## RICE UNIVERSITY

# Exploring aspects of nonequilibrium physics with quantum impurity problems

by

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#### ABSTRACT

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Traditionally the study of quantum mechanical ensembles was focused on the exploration of their equilibrium properties: the program has consisted of the classification of the quantum mechanical states of matter, and the identification of the striking phase transitions between them. On the other hand, questions about the out of equilibrium properties of quantum ensembles have largely remained academic until fairly recently. Particularly, the rapid technological progress in the field of atomic physics has enabled experimental demonstrations of nontrivial out of equilibrium phenomena which moreover are describable in terms of relatively simple theoretical models with a few parameters. Thus the time is ripe for a theoretical exploration of nonequilibrium physics. To this end, quantum impurity models offer a natural and simple starting point for studying nonequilibrium phenomena in the context of ultracold atoms, and pave the way toward the study of more complicated systems. I will discuss how the impurity-bath model offers a clean, simple realization of rich phenomenology including the dynamics of polaron formation as well as the orthogonality catastrophe, and can be engineered using dilute mixutres of cold atomic gases. Moreover I will demonstrate how impurity models are also embedded in the more complicated physics of the response of a one-dimensional system to an external perturbation, or a sudden local parameter change. Lastly, I will describe the approach to equilbrium of a more complicated system, the one dimensional Bose gas, following a sudden parameter change, and discuss some of the important questions which arise in this connection: does a quantum mechanical system thermalize? What is the appropriate asymptotic description of a nonequilibrium state? Does such a system retain a memory of its initial state?

# Dedication

A healthy balance of both a scientific and human element, which is not to say that the two are easily separable, was *essential* to the completion of this work.

I would like to explicitly acknowledge several special scientists and humans who left an especially strong mark.

Firstly my parents, Shashi and Rajeswari, whose support, encouragement, motivation, and affection have always been constant and unconditional. Although the bulk of our interaction during the period of my graduate career have largely been *virtual* – enabled variously by low quality phone connections, video-conferencing, emails and instant messages – its impact has been assuredly *real*.

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I mention Adilet last, but only because he has all but robbed me of words; I still cannot talk of him without deep sadness. It was my great privilege to have been his first student. It was awesome to encounter such a *singular* human being as him, at once immeasurably gifted, able and approachable. Although his time with us was cut absurdly short, the mark he has left is quite permanent: I still reguarly find myself asking "what would Adilet do", when approaching a new problem, and hopefully will always try to abide by his almost impossibly high standard.

# Contents

	Abs	tract	ii	
1	Preface			
	1.1	Introduction	1	
	1.2	Outline	3	
<b>2</b>	A١	broad overview	7	
	2.1	The arrow of time	7	
	2.2	The "quantum" arrow of time	9	
		2.2.1 Relaxation in integrable systems: GGE	13	
	2.3	The microscopic origins of friction	16	
		2.3.1 Impurity physics in ultracold gases	18	
	2.4	Hidden 1D physics in impurity models and vice versa $\ldots$	23	
3	As	single impurity in a quantum mechanical bath	<b>27</b>	
	3.1	Introduction	27	
	3.2	Model of impurity in a quantum bath	27	
	3.3	Exchange statistics of the bath	28	
		3.3.1 Bosons	28	
		3.3.2 Fermions	30	
	3.4	Interactions between impurity and bath	31	
	3.5	Lee-Low-Pines transformation	32	
	3.6	General phenomenology of impurity in a bath	33	
		3.6.1 Single particle states: Problem of local scatterer	34	

		3.6.2	Many-body spectrum	35
	3.7	RF sp	ectroscopy as dynamical problem	37
		3.7.1	Direct and inverse RF: momentum resolved spectra $\ldots$ .	38
		3.7.2	Calculating many-body overlaps	40
4	Im	purity	y in a bath of bosons	42
	4.1	Introd	luction	42
	4.2	Impur	rities in a BEC	42
	4.3	Polare	on ground state in BEC	44
		4.3.1	Lee-Low-Pines transformation	45
		4.3.2	Mean-field polaron solution	47
		4.3.3	Binding energy of the polaron	48
		4.3.4	Effective mass of the polaron	50
		4.3.5	Quasiparticle residue	52
	4.4	Analy	sis of RF spectra	55
		4.4.1	Generic features of the RF response	55
		4.4.2	Direct RF: Transition from interacting to non-interacting state	61
		4.4.3	Inverse RF: Transition from noninteracting to interacting state	63
	4.5	Concl	usions and Outlook	70
		4.5.1	Relation to experimental systems	71
		4.5.2	Related problems	72
<b>5</b>	Im	purity	y in a Fermionic bath	76
	5.1 Introduction		luction	76
	5.2	Physic	cs of OC in cold atoms	76
	5.3	Expor	nents of response at threshold singularities	80
		5.3.1	X-ray edge exponent	81
		5.3.2	Exponents in the the presence of bound state	83
		5.3.3	Exponents due to the bottom of band effect	84

vii

	5.4	Prefactors of response at threshold singularities			
		5.4.1	Prefactor of conventional edge singularity	88	
		5.4.2	Prefactor of response in the presence of bound state	89	
		5.4.3	Prefactor of response at higher threshold	90	
6	Co	rrelat	ion prefactors of 1D quantum liquids	92	
	6.1	Introd	luction	92	
	6.2	2 Effective field theory in 1D			
	6.3	.3 Results from effective field theory		94	
		6.3.1	Distribution of spectral weight among states	97	
		6.3.2	Prefactors of dynamic response functions	102	
	6.4	Pertu	bative calculation of form factors	105	
		6.4.1	Calculation of $A_{0,+}(k)$	107	
		6.4.2	Calculation of $A_{1,-}(k)$	111	
		6.4.3	Calculation of $A_{1,+}(k)$	114	
		6.4.4	Calculation of prefactor $C_1$	117	
		6.4.5	Calculation of prefactor $A_2$	119	
		6.4.6	Calculation of prefactor $A_{0,-}(k)$	123	
	6.5	Summ	ary	136	
7	Co	rrelat	ion prefactors: exactly solvable models	139	
	7.1	Introd	luction	139	
	7.2	Overv	iew	139	
	7.3	Result	s from effective field theory	141	
		7.3.1	Prefactors of equal-time correlators	142	
		7.3.2	Prefactors of singularities in dynamic response	145	
	7.4	Dynar	nic structure factor of CSM	149	
	7.5	Prefa	ctors of the Lieb-Liniger Bose Gas	156	
		7.5.1	Form Factors	157	

		7.5.2	Thermodynamic Limits and Finte Size corrections 159		
		7.5.3	Evaluation of $M_1$		
		7.5.4	Obtaining term $M_2$		
		7.5.5	Fredholm Determinants		
		7.5.6	Thermodynamic Limit of Form Factors		
		7.5.7	Numerical Results		
	7.6	Concl	usions and Summary of Results		
		7.6.1	Prefactors of equal-time correlators		
		7.6.2	Prefactors of the singularities of the dynamic structure factor . 224		
		7.6.3	Prefactors of the singularities of the spectral function 226		
8	Q Quantum much of interacting 1D Dags mag				
0	Qu		In quench of interacting 1D bose gas 250		
	8.1	Introd	luction		
	8.2	The model			
	8.3	Divergence of the local conserved charges			
	8.4	q-boson regularization			
	8.5	The density $\rho_{\rm LL}(\lambda)$			
	8.6	Correlation functions in the final state			
	8.7	Strongly interacting final state			
	8.8	Summ	nary		
Appendices 242					
$\mathbf{A}$	Ap	pend	ix to impurity in BEC 243		
	A.1	UV regularization of polaron binding energy			
	A.2	Path i	integral formulation of time dependent overlap		
B Appendix to correlation prefactors I 251					
	B 1 Multiplet Summation Bule				
	D.1 multiplet summation fulle $\ldots \ldots 201$				

		B.1.1 $n_+ = 1$	252
		B.1.2 $n_+ = 2$	252
		B.1.3 $n_+ = 3$	253
	B.2	Identities involving Poly-Gamma functions	253
	B.3	Principal Value Integrals: Interior and Edge Singularities	254
С	Ap	pendix to correlation prefactors II 2	255
	C.1	$\Gamma$ products and Barnes G function	255
	C.2	Principal Value Integrals: Interior and Edge Singularities	256
	C.3	Special Property of Barnes Function	256
	C.4	The Fredholm Determinant	257
D	Ap	pendix to Interaction quench of 1D Bose gas	260
	D.1	Local conserved charges in the $q$ -boson hopping model $\ldots \ldots \ldots$	260
	D.2	Expectation values of the charges in the initial state	262
	D.3	Pattern for expectation values in the BEC state	266
	D.4	Padé–Fourier approximation	268
	Bib	bliography	269

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# Chapter 1

# Preface

#### **1.1** Introduction

The study of the equilibrium properties of interacting quantum mechanical ensembles has a mature history. The central theme of this study has been understanding and characterizing the diverse zoo of quantum mechanical states of matter, and the striking phase transitions between them. In this enterprise, although there remain interesting unresolved questions, particularly on the nature and properties of strongly correlated matter, from a conceptual standpoint, the "big picture" is clear.

The situation is entirely different with regard to the properties of quantum ensembles out of equilibrium. Historically, questions about nonequilibrium properties have largely been academic curiosities. Indeed, even the central question: "how does a system obeying unitary, i.e. time reversal invariant, quantum mechanical evolution, relax?", is only just starting to be satisfactorily resolved.

Such apparent neglect is very understandable: realizing quantum evolution of a system taken far out of equilibrium is enormously challenging in generic systems – environmental influences which constantly measure the quantum system and provide a dephasing mechanism, are extremely hard to eliminate. Moreover, in dense condensed matter, collisions provide a relaxation mechanism which rapidly brings the system into thermal equilibrium. Thus coherent nonequilibrium dynamics typically occurs over an extremely short time scale, and is therefore hard to observe.

Theoretically, it has been difficult to model realistic nonequilibrium systems. Moreover, even the more modest goal of taking known theoretical models out of equilibrium "on paper" has been met with resistance: the standard tools applicable to equilibrium problems seldom directly apply in the non equilibrium situation, and each instance of a problem seems to require specialized approaches leading some to comment: "every nonequilibrium system is out of equilibrium in its own way".

Yet, far from being hopelessly doomed, nonequilibrium physics has seen a recent surge of interest and activity. What has brought about this change? To a large extent, the rapid advances of the past decades in the field of atomic physics have been a major motivating factor. The unprecedented control over interatomic interactions, external trapping potentials, and internal states of ultracold atoms, allows the realization of systems and associated phenomena previously unattainable in condensed matter. In particular two key advances were i) the ability to dynamically tune interactions via Feshbach resonances, ii) the ability to manipulate system geometries using optical lattices. It is now very realistic, and almost routine, to engineer clean realizations of simple models and to dynamically tune their couplings, moreover models can even be realized in lower spatial dimensions where exotic out of equilibrium physics is expected to occur, by optically confining the system. Such dynamic and precise control of these isolated system puts the study of nonequilibrium quantum dynamics within reach of experimentalists.

Furthermore, while relaxation in solid state systems occurs on the picosecond timescale, and is accessibly only using cutting edge ultrafast pulsed lasers, the low temperatures and dilute conditions of atomic systems stretches that time scale to milliseconds, within which standard experimental measurements can be made. Additionally, the mechanisms of relaxation in cold atoms is intrinsically different from solid state systems; in the latter, electrons are the system of study, and phonons, which can be thought of as an unwanted environmental influence, provide the relaxation mechanism. In well isolated atomic gases, there are no phonons, and relaxation if any is mediated by interactions in the system of interest. Such a system lends itself to a "barebones" theoretical model that is nonetheless a complete and accurate description of the experimental system, and admits a rich phenomenology. Thus, in addition to being experimentally feasible, the study of nonequilibrium phenomena has now also become appealing to theorists and bears the promise of making fundamental conceptual progress.

The time is thus ripe to explore theoretical aspects of nonequilibrium physics which are especially applicable to systems of ultracold atoms. Moreover it is illuminating to proceed from the domain of simple models, towards more complex ones.

## 1.2 Outline

The following body of work will examine theoretical models of interacting quantum systems with the goal of describing some of their out of equilibrium properties. In this regard, two central questions which will be addressed are:

- What is the role played by impurities embedded in a quantum mechanical environment?
- How should the out of equilibrium quantum state of a system be described, and how does it differ from the ground state?

While a priori these questions seem unrelated, the central theme of this thesis is the essential role played by quantum impurities in understanding the out of equilibrium physics of quantum many-body systems. On the one hand, the impurity-bath model is of intrinsic interest: it represents a clean, simplified, experimentally accessible system in which to study nonequilibrium dynamics in a controlled setting. Indeed, there has been a flurry of activity centered around realizing quantum impurity physics using cold atomic gases. The low temperatures, diluteness and precise control over interatomic interactions and internal states of atoms has naturally lent itself to the study of quantum impurity models; additionally a toolbox of experimental techniques such as Feshbach resonances, and spectroscopic probes using the absorption of radiofrequency (RF) light has allowed the study of the out of equilibrium behavior of these systems.

On the other hand, quantum impurity problems are often embedded in a more complicated problem, and pave the way to understanding the essential underlying phenomenology of the model. In the present context, it will be seen that the response of a 1D system to an influx of energy, from an external probe, or from an abrupt parameter change, can be understood in terms of a quantum impurity model. When such systems are analyzed by separating their high and low energy parts, it turns out that the essential physics can be understood by considering an effective model of an impurity, representing the high energy parts of the system, propagating through a bath of low-energy excitations.

The following chapters comprise a body of work exploring these notions in more detail:

Chapter 1 will provide a broad overview of the material covered here, and will put the work in context of prior research, emphasizing the specific questions taken up in this thesis.

Chapter 2 will set the stage for a detailed exploration of quantum impurity physics. A simplified impurity model will be presented, which will display the basic phenomenology of such systems: a single, structureless impurity immersed in a quantum mechanical bath. The bath of particles, which interact with the impurity via pairwise contact interactions can be either bosonic or fermionic, leading to dramatically different behavior. Additionally, some recent developments of atomic physics which lend themselves to the realization of impurity physics will be mentioned.

Chapter 3 will examine the impurity model in great detail focusing on a bosonic bath, where the manifestation of the essential polaronic physics of the impurity will be discussed in the context of recently developed experimental techniques. Details of the calculation of radiofrequency absorption spectra will be provided, showing how the signature of polaronic physics might be inferred. It will be seen that the calculation of spectra involves solving the more general out of equilibrium problem of the dynamics of an impurity which is suddenly introduced into a bath.

Chapter 4 will explore the physics of an impurity in a fermionic environment. The phenomenon of the "Orthogonality catastrophe" will be discussed, along with a description of the recent realization of this phenomenon using cold atomic gases. In this context, the characterization of this phenomenon using radiofrequency spectroscopy, and the details of the corresponding theoretical calculation will be presented, and will highlight the "hidden" one-dimensional structure of the problem.

Chapter 5 will consider the response of one-dimensional (1D) systems to external probes. It will be seen that again the physics of the orthogonality catastrophe emerges in this problem, which maps onto an impurity propagating through a bath of excitations. As an application of this interesting connection, a calculation of the asymptotic form of correlation functions of 1D quantum systems will be presented, which involves relating the prefactors in correlation functions to the finite size scaling of certain matrix elements (form factors). Chapter 6 will apply the general technique presented in the previous Chapter to a few exactly solvable models. With the aim of obtaining exact analytic expressions for the asymptotic forms of correlation functions, a technical procedure for carefully treating finite size effects in integrable models will be developed. Finally exact analytic forms for the prefactors of the long-distance behavior of equal time correlation functions as well as prefactors of singularities of dynamic response functions of the Calogero-Sutherland, and Lieb-Liniger models will be presented.

Chapter 7 will examine the effect of a global parameter change on a quantum mechanical system, and will emphasize the special role played by integrability, i.e. the existence of local quantities which remain conserved in the course of quantum evolution, which gives rise to a form of quantum memory. Specifically, The effect of abruptly switching on pair-wise short-range interactions in an initially non-interacting 1D Bose gas is studied within the framework of the "Generalized Gibbs Ensemble", a method of properly construction a statistical description of a system with a proliferation of conserved quantities. The calculation will clearly demonstrate the deviation in the predictions made using such an ensemble, from those of the canonical ensemble, and will thus highlight the amount of memory retained by such a system of its initial state.

## Chapter 2

# A broad overview

The aim of this chapter is to put the work presented in the following chapters into perspective. Starting with a more philosophical discussion of the origins of the study of out of equilibrium physics, recent conceptualizations of relaxation in closed quantum systems will be discussed. The close interplay between theory and experiments with ultracold atoms will be highlighted, and some of the important recent work in this area will be reviewed.

In parallel, microscopic irreversibility in quantum systems will be discussed in the context of impurity models, where the question of the quantum origins of friction was first posed. Recent realizations of impurity models using systems of ultracold atoms will be discussed, emphasizing opportunities for the systematic study of nonequilibrium phenomena.

### 2.1 The arrow of time

We receive almost daily demonstrations that a system that is taken out of equilibrium eventually relaxes - a steaming cup of tea left unattended will cool to room temperature, a cloud of smoke will dissipate and rarefy until it disappears, and one never sees a broken egg spontaneously reassemble. However, this apparent "fact of life" was surprisingly difficult to establish rigorously. The difficulty stems from the fact that for relaxation to occur in a system governed by the laws of mechanics, irreversibility must emerge from a mathematical framework that is manifestly reversible; indeed, the explicit mathematical forms of the microscopic laws of physics are symmetric with respect to the direction of time. Yet, this clearly flies in the face of common experience, which suggests that the passage of time has a well defined direction.

It was Boltzmann's famous work [1] that provided the necessary microscopic proof that enabled conceptual progress to be made in this regard. Boltzmann considered a gas of colliding molecules which obey Newtonian mechanics. His key insight was in attributing an inherently stochastic character to the behavior of the system – the velocity of a molecule after a collision arises from a distribution, and it is this randomness that allows irreversibility to emerge. The resulting behavior of such an ensemble can be captured by a nonlinear kinetic equation that leads to entropy increasing behavior, thus *orienting* the arrow of time.

This notion can be formalized as the property of "ergodicity", and explains thermalization in classical systems. A classical system may be prepared in a very special initial configuration, however, in the course of time evolution almost all particle trajectories quickly begin to look alike, *independently of their initial conditions*, because nonlinear equations drive them to explore a constant-energy manifold of phase space, ergodically. As a consequence, the trajectories of the constituent particles cover a fixed energy manifold uniformly with respect to a statistical measure, the microcanonical measure of Gibbs, a characteristic which we succinctly describe as "thermal". \*

<sup>\*</sup>There is a notable exception: namely systems which are "integrable", i.e. have quantities independent of their energy and each other, that are also conserved during time evolution. Such systems are constrained further and do not ergodically explore a constant-energy manifold of phase space, but rather only sub manifolds which are consistent with their conserved quantities. Such systems *do not* thermalize.

## 2.2 The "quantum" arrow of time

It is quite reasonable to ask the same question about a quantum mechanical system: how can a closed quantum mechanical system, that is prepared in a pure initial state, that is however *not* the ground state, ever relax? Indeed, in the most trivial case, if the system is prepared as an eigenstate of its quantum Hamiltonian, it will *never* relax, but rather undergo endless stationary evolution, accumulating a time dependent phase, but otherwise remaining unchanged:

$$|\psi(t)\rangle = e^{iHt}|\psi_0\rangle = e^{iE_{\psi_0}t}|\psi_0\rangle; \quad H|\psi_0\rangle = E_{\psi_0}|\psi_0\rangle. \tag{2.1}$$

However, consider a more interesting scenario: suppose the system were prepared in a pure quantum state, but nonetheless such a state were not the eigenstate of the Hamiltonian governing the time evolution of such a system, what then? More generally, under what circumstances will a quantum mechanical ensemble admit a statistical description analogous to the classical system described earlier, and how does thermalization occur, if at all?

A version of these questions was addressed as early as 1929 by von Neumann [2] who outlined necessary criteria to recover the analog of the Boltzmann H theorem in the quantum mechanical context. Although his proof was microscopic, and he considered closed quantum systems, his criteria for "quantum ergodicity" were too general to be of practical use.<sup>†</sup>

<sup>&</sup>lt;sup>†</sup>von Neumann obtained bounds on the deviations of entropy, and generic bulk observables from their time averages. Intuitively one would expect that if such deviations were to always remain small then the system shows self averaging, and by extension admits an ensemble description. A guarantee of the smallness of von Neumann's bounds amount to very technical conditions on the spectrum of eigenvalues. They suffice to distinguish interacting and non-interacting systems, but not e.g. integrable and nonintegrable interacting systems.

The question was revived in the early 90s, and was addressed much more concretely [3, 4]. In particular, the idea of "eigenstate thermalization" was introduced independently by the authors of Refs. [3, 4]. Under this hypothesis, thermal behavior emerges at the level of quantum eigenstates themselves; more precisely, the expectation value of an observable  $\hat{A}$  calculated with any eigenstate  $|\alpha\rangle$  of the Hamiltonian in a window of energies  $E_{\alpha} \pm \Delta E$ , reproduces the average of  $\hat{A}$  calculated in a microcanonical shell with average energy  $E_{\alpha}$ . While this statement could be shown rigorously in the semi-classical limit of a quantum systems whose classical counterparts admit chaotic dynamics, a completely general proof is as yet absent. Nonetheless, thermalization of closed quantum systems can be explained by assuming eigenstate thermalization as a hypothesis.

While these early works were leisurely explorations of abstract concepts, and had a strongly academic flavor, the discussion took on a more urgent tone when the Weiss group unveiled the results of its "Quantum Newton's Cradle" in 2006. In this experiment, a cold atomic gas of interacting bosons was confined to one spatial dimension (1D), split into two spatially separated parts, and allowed to recombine (see Fig. 2.1). The experimental result, which has since attained iconic status, was that the two separated pieces underwent many collisions while oscillating back and forth in the trap, but failed to recombine. The upshot was that the system failed to reach a thermal equilibrium, and this fact was manifested even in traditional observables like the momentum distribution. Moreover it was also shown that the same experiment performed using a three dimensional gas, relaxed to a thermal distribution after a few collisions.

It turns out that the 1D Bose gas realized using cold atomic gases, is quite accurately described by a theoretical model first considered by Lieb and Liniger. This

Figure 2.1 : The Quantum Newton's cradle: shown schematic representation on the left. Momentum distribution along the longitudinal direction clearly demonstrates "memory"; consistent oscillations with no recombination of atomic clouds.

model has a special mathematical property; it is a "quantum integrable" model (see [5, 6] for a more "philosophical" discussion of integrability) – it contains an infinite number of local charges<sup>‡</sup>, including energy density, which remain conserved in the

<sup>&</sup>lt;sup>‡</sup> A more "physical" understanding of integrability can be developed by considering scattering properties of particles (see e.g. Sutherland's very readable book [5]); in an integrable system any n-particle scattering event can be factorized into a sequence of two-particle scattering events. One way to account for the lack of thermalization within a quasi-classical picture is by noting that in Boltzmann's kinetic equation, thermalization occurs only when there is a finite amplitude for (at least) three particle scattering processes, since energy-momentum conservation ensures that for

course of quantum evolution. Within the framework of classical mechanics, an analogous system is said to be in involution – it is constrained to explore only a special region of phase space, a multidimensional torus, in stark contrast to a generic system which explores phase space ergodically; since ergodic exploration of phase space is the key mechanism responsible for thermalization in classical systems, an integrable system does not thermalize. One can imagine that a quantum integrable model taken out of equilibrium, is similarly constrained to explore a smaller state space than its nonintegrable counterparts. Thus one can reasonably expect, and indeed finds, different relaxation behavior for integrable and nonintegrable systems.

The results of the quantum Newton's cradle experiment galvanized the field. The discussion of relaxation of closed quantum systems was attacked with renewed vigor, and the idea of eigenstate thermalization [3, 4] was revisited, with particular attention paid to the difference between integrable and non-integrable systems [7, 8, 9] and was aided at least in part by independent numerical studies of relaxation [10, 11]. Essential questions included: when does eigenstate thermalization occur, and how can it be violated? What is the nature of the transition between ergodic and non-ergodic behavior as a function of some integrability breaking parameter? (see Ref. [12] for a comprehensive review).

A careful study of the asymptotics of density-density correlators and momentum distribution function for hard-core bosons in 1D showed that the transition from nonthermal to thermal behavior in finite size systems takes the form of a crossover controlled by the strength of the integrability breaking perturbation and the system size [8]. Thus, if integrability is broken by a sufficiently strong perturbation ergodic

two-particle scattering events momenta of particles are either preserved or simply exchanged thus disallowing relaxation.

behavior emerges, related to the validity of the eigenstate thermalization hypothesis [7], and the non-ergodic behavior of integrable models can be seen to originate from wide state-to-state fluctuations of the expectation value of natural observables around the microcanonical average [9].

These studies greatly advanced the understanding of relaxation in closed quantum systems, and firmly established the major distinction between integrable and nonintegrable systems. However, a prescriptive technique for describing steady-states of integrable systems was sorely missing, leading to the question, if integrable systems do not thermalize, then is it possible to apply methods of quantum statistical mechanics to such systems? If so, then what is the appropriate ensemble description of an integrable system?

#### 2.2.1 Relaxation in integrable systems: GGE

A major breakthrough occurred when Rigol et al. [13] formalized the quantum statistical description of a closed integrable system by introducing the idea of a "Generalized Gibbs Ensemble" (GGE). The idea behind the GGE dates back to Jaynes [14, 15] who first made the connection between information theory and statistical mechanics. Jaynes showed that the canonical ensembles of statistical mechanics emerged naturally when one posed the central problem of statistical mechanics as the construction of an ensemble description of a system in the *least biased way*, while simultaneously using all known information about the system. Seen in this light, Jayne's prescription was to maximize entropy, thus minimizing "bias", but at the same time constraining the energy of the system to be a fixed constant E, with an associated Lagrange multiplier,  $\beta$ , the inverse temperature. The number of particles N can be similarly constrained by assigning a chemical potential  $\mu$ . The solution of this variational problem yields the grand canonical ensemble, as promised.

Rigol et al., generalized this idea for integrable models[13], where in addition to the energy, one also knows that additional charges are conserved. For the particularly simple case of a noninteracting model, the explicit form of such charges is known: they are simply the mode occupations of the system. Assigning Lagrange multipliers, generalized chemical potentials, associated with each of the conserved charges beyond energy, one obtains the appropriate ensemble description for quantum integrable systems.

At this stage, the reader might realize a conceptual difficulty - one typically thinks of an ensemble description of a system as a mixed state. However, it is patently impossible for a system initially starting in a pure state, time evolved by a unitary Hamiltonian, to end up in a mixed state. It turns out, however, that subsystems of the time evolved system are consistent with a reduced density matrix description, obtained by tracing out degrees of freedom, which characterizes a mixed state. Conceptually, one can imagine that the parts of the system which were traced out, act as a "bath" for the rest of the system to equilibrate. Indeed, by now there is substantial evidence [16] that such a reduced density matrix constructed for a time evolved closed quantum system is thermal for generic systems, and given by the GGE for integrable systems.

The GGE, which started out as a conjecture, was shown to hold rigorously for quadratic models in Ref. [17]. Initially it was studied mostly in models which could be mapped to quadratic bosonic or fermionic systems where the conserved charges are given by the mode occupation numbers. While some of these models are paradigmatic, like the Ising or Luttinger models, a prominent class of nontrivial integrable systems was not sufficiently explored, namely those solvable by the Bethe ansatz (BA).

The difficulty in constructing the GGE for BA solvable models lies in the highly nontrivial form of the conserved charges for these models. In Chapter 8, the GGE solution of the 1D Bose gas quenched from a noninteracting initial state to an arbitrary final state will be presented, and will highlight the technical challenges in constructing such a solution: it will be seen that the interplay of contact interactions, which are zero-range in space, and the instantaneous quench, which is zero-range in time, will lead to pathological ultraviolet divergences for the natural choice of conserved charges entering the GGE. Although the divergences can be regularized, the required procedure is highly nontrivial. In short, since the divergences stem from zero-range interactions in the model, an artificial lattice spacing could serve as a natural UV regulator for the purposes of calculations. Such a procedure should reproduce cutoff independent results for physical observables which are expected to be finite, e.g., temperature of the system after quench, values of local correlators, etc. However a naive implementation of a lattice cutoff is doomed to fail because it breaks the integrability of the original model of the 1D Bose gas, and after all integrability is central to the agenda. In fact, the correct procedure involves mapping the original model to an *integrable* lattice model, where the interaction quench must be simulated, the GGE solved, and the results mapped back onto the original model. This procedure was carried out in Ref. [18], but could only take a finite number of conserved charges into account. For many practical purposes, such a "truncated GGE" suffices to make physical predictions. In particular this question was extensively studied in Ref. [19, 20], where it was shown that the conserved charges typically grow in complexity by including correlations between a monotonically increasing number of sites for a lattice model. Thus to correctly predict local correlators which extend only over a small number of sites, a small number of conserved charges suffices to construct a valid GGE [18, 19, 20].

## 2.3 The microscopic origins of friction

In parallel to the previous discussion of relaxation in a closed quantum system, an independent question concerning irreversibility can be posed about the emergence of friction in a quantum mechanical system. Once again we are confronted by the apparent paradox of irreversibility emerging out of reversible dynamical laws. Consider for example Ohm's law which relates current to an applied electric field:

$$j = \sigma E. \tag{2.2}$$

It is hard to imagine that Ohm's law could arise in a time-reversal invariant system, since under time reversal the current j changes sign, but the electric field E does not, leading to a contradiction. However, if one were to introduce a phenomenological damping term of the form:

$$m\ddot{q} = -\kappa\dot{q} + eE,\tag{2.3}$$

which breaks time reversal symmetry, then the equilibrium solution of such an equation readily yields the required law:

$$\dot{q} = \frac{eE}{\kappa}.\tag{2.4}$$

In classical systems, such a friction term naturally appears in the equation of motion of a particle, due to random collisions with a background gas. The resulting motion is called Brownian and represents a field of study on its own (see, e.g. Zwanzig's book [21] for an excellent discussion).

One way to account for such a damping term within a quantum mechanical framework is to consider a coupling between a particle and a quantum mechanical environment, with the resulting system described by the Lagrangian [22, 23]

$$\mathcal{L} = M\dot{q}^2 + q(t)\sum_{\mathbf{k}} c_{\mathbf{k}} x_{\mathbf{k}}(t) + \sum_{\mathbf{k}} (m\dot{x}(t)^2 + \omega_{\mathbf{k}} x(t)^2).$$
(2.5)

Here the particle has coordinate q(t), and the quantum environment is modeled as a collection of harmonic oscillators that are linearly coupled to the particle's coordinate. By considering a path integral for the propagator of the particle, we can integrate out the quantum environment, leading to an effective action for the particle given by:

$$S = \int_0^t dt' \left[ M \dot{q}(t')^2 - i \int_0^{t'} dt'' \sum_{\mathbf{k}} c_{\mathbf{k}} \frac{e^{i\omega_{\mathbf{k}}(t'-t'')}}{m\omega_{\mathbf{k}}} q(t')q(t'') \right].$$
 (2.6)

It is straightforward to verify<sup>§</sup> that the saddle point of this equation indeed leads to an equation of motion of the particle with a friction term proportional to its velocity

$$M\ddot{q} + \int_0^t \sum_{\mathbf{k}} dt' \frac{c_{\mathbf{k}}}{m\omega_{\mathbf{k}}^2} \cos\left[\omega_{\mathbf{k}}(t-t')\right] \dot{q}(t') = 0$$
(2.7)

Eq. (??) above describes "quantum Brownian motion". Note that in contrast to the classical analog, e.g. Eq. (2.3), the friction term takes involves integration over a time-dependent kernel. In general, such a term signals the presence of "non-Markovian" dynamics.

One way to see this is to observe how the fluctuation dissipation theorem is modified for the time-dependent friction above; whereas the memory-less Markovian case corresponds to the force on the particle at different times being uncorrelated[21, 22, 23]:

$$\langle F(t)F(0)\rangle = 2\kappa T\delta(t),$$
(2.8)

<sup>&</sup>lt;sup>§</sup>An alternate derivation based on solving the coupled equations of motion for particle and environment is presented in Ref. [23]

it can be shown [22, 23] that for the model above,

$$\langle F(t)F(0)\rangle = T\sum_{\mathbf{k}} \frac{c_{\mathbf{k}}}{m\omega_{\mathbf{k}}^2} \cos(\omega_{\mathbf{k}}t),$$
(2.9)

which clearly allows temporal correlations to build up.

More generally, let us observe that the time-dependent kernel in Eq. (??) arose when the bath was integrated out in the simple model above. In fact, this is a generic phenomenon although the explicit form of the kernel may vary: integrating out a Gaussian bath coupled linearly to a function of impurity coordinates will *always* generate a corresponding quadratic term in impurity coordinates which will depend on two times. Moreover, the kernel generated will always depend on the correlation function of the bath. As a consequence, in general, if the dynamics of the bath alone has a typical "correlation time"  $\tau$ , then dynamics of the impurity occurring on timescales  $t \lesssim \tau$  will experience the effect of bath correlations, i.e. the bath "remembers" the history of interactions with the impurity, while over long times  $t \gg \tau$  the memory of the bath is lost, and the friction on the particle starts to resemble white noise.

In light of the theoretical richness of even simple impurity models, and the opportunities they present for the careful study of non trivial, uniquely quantum mechanical effects, it is interesting to consider the recent developments within the field of ultracold atoms.

#### 2.3.1 Impurity physics in ultracold gases

Not long after the realization of Bose Einstein Condensation (BEC) in 1995[24, 25, 26] and the subsequent creation of a quantum degenerate gas of fermions in 1999 [27], these systems are now routinely engineered in laboratory settings. While early work emphasized the phenomenology stemming from the observable macroscopic coherent wave properties of these systems, with recent technological advances, the systems considered and the phenomena probed have become more sophisticated[28]. In this regard, two advances cannot be understated: (i) the ability to dynamically tune interatomic interactions using Feshbach resonances [29], and (ii) the ability to change the confining geometry of the systems using optical lattices. It is this latter development that even allows for the dimensionality of the systems to be changed.

More relevant to our present discussion, it has now become possible to engineer dilute mixtures of quantum degenerate bosonic and fermionic gases [30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41]. Moreover the concentrations of the constituents can be varied, setting the stage for quantum impurity models. Although the model of quantum Brownian motion described by Eq. (2.5) is appealing for its theoretical simplicity, a more natural model in systems of cold atoms is the related polaron model [42, 43, 44].

A common measure of interactions in a quantum mechanical system involves introducing a hypothetical extra particle into the system, and quantifying the ease with which the extra particle propagates in the system, i.e. its Green's function – for a noninteracting system the extra particle simply ignores the rest of the system (beyond obeying exchange statistics) and behaves like a free particle, while for a strongly interacting system its identity is completely lost as it becomes entangled with every other particle in the system. In the case of a quantum impurity model, the situation described earlier is no longer hypothetical, but rather directly determines the fate of the impurity; the "polaron" is the name given to the stable quasiparticle (if any) formed by the impurity, when it is allowed to interact with a quantum mechanical system.

The polaron model again involves a quantum impurity and a bath, but the cou-

pling between the two is significantly more complicated. In the physical cold atom systems, interactions occur dominantly via two-particle scattering events, i.e. a pairwise density-density contact interaction. Such an interaction can be modeled as

$$H_{\rm int} = g_{\rm IB} \int d\mathbf{x} \rho_{\rm I}(\mathbf{x}) \rho_{\rm B}(\mathbf{x}). \qquad (2.10)$$

In the first quantized notation used earlier, the density of the impurity  $\rho_I$  can be expressed as:

$$\rho_{\mathrm{I}}(\mathbf{x}) = \delta(x - \hat{q}) = \sum_{\mathbf{k}} e^{ik(x - \hat{q}).}$$
(2.11)

from which it is clear that the coupling of the impurity to the bath is no longer linear in the impurity coordinate  $\hat{q}$ .

Historically the polaron model was studied as a model of electron-phonon interactions [45, 42, 46, 47] where the role of the impurity was played by electrons propagating through a bath of phonon excitations. Subsequently the problem was invoked in numerous settings electron-phonon interactions [42], the propagation of muons in a solid [48], transport in organic transistors [49], the physics of giant magnetoresistance materials [50], and high  $T_C$  cuprates [51].

Most recently, the polaron problem was considered in the context of quantum impurities in ultracold atomic gases [44, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76].

Although one traditionally thinks of transport measurements in order to study out of equilibrium problems with polarons, the cold atom system presents a different set of tools and associated problems. One particularly interesting probe of impurity physics is radio frequency (RF) spectroscopy. An RF pulse changes the internal state of the impurity atom without modifying its momentum. Thus for a  $\downarrow$ -impurity-bath initial state with momentum p, energy  $E_{i\downarrow}$ , denoted  $|i_{\downarrow p}\rangle$ , the RF absorption cross section can be computed within Fermi's Golden Rule from

$$I(p,\omega) = \sum_{n} |\langle n_{\uparrow p} | \hat{V}_{\rm RF} | i_{\downarrow p} \rangle|^2 \delta(\omega - (E_{n\uparrow} - E_{i\downarrow})), \qquad (2.12)$$

where all states  $|n_{\uparrow p}\rangle$  of  $\uparrow$ -impurity-bath system with total momentum p are summed over. The RF transition operator  $\hat{V}_{\rm RF} \sim |\uparrow\rangle\langle\downarrow|$  instantaneously changes the internal state of the impurity, but the quantum mechanical state of the impurity-BEC system is otherwise unmodified by it, i.e. the initial state of the system  $|i_{\downarrow p}\rangle$  is quenched. Using standard manipulations (see e.g. [77, 78]) the last expression can be rewritten as

$$I(p,\omega) = \operatorname{Re}\frac{1}{\pi} \int_0^\infty dt e^{i\omega t} A_p(t)$$
(2.13)

$$A_p(t) = e^{iE_{i\downarrow}t} \langle i_{\uparrow p} | e^{-i(\mathcal{H}_b + \mathcal{H}_I + H_{\text{int}\uparrow})t} | i_{\uparrow p} \rangle, \qquad (2.14)$$

where frequency  $\omega$  is measured relative to the atomic transition frequency between states  $|\downarrow\rangle$  and  $|\uparrow\rangle$  of the bare impurity, and where we denoted  $|i_{\uparrow p}\rangle = \hat{V}_{\text{RF}}|i_{\downarrow p}\rangle$ .

Due to the instantaneous nature of the RF spin-flip, the state  $|i_{\uparrow p}\rangle$  is identical to the initial state of the  $\downarrow$ -impurity bath system in all respects, *except the internal state of the impurity*. Consequently,  $|i_{\uparrow p}\rangle$  state is different from, and therefore higher in energy than, the  $\uparrow$ -impurity-bath ground state at momentum  $p, |0_{\uparrow p}\rangle$ . Thus it is more convenient to formulate the physical problem underlying the RF response as a dynamical one, rather than a traditional calculation of a ground state observable. Indeed, expression (3.26) has the form of the quantum propagation amplitude, related to the Loschmidt echo[79]), where an eigenstate of the Hamiltonian  $\mathcal{H}_b + \mathcal{H}_I + \mathcal{H}_{int\downarrow}$ needs to be time evolved with  $\mathcal{H}_b + \mathcal{H}_I + \mathcal{H}_{int\uparrow}$ .

Thus such a measurement is geared toward measuring the effect of a "quantum quench" of the impurity-bath system. Moreover the correlator  $A_p(t)$ , above can also

be measured directly in the time domain using the Ramsey sequence discussed in Ref. [78], and can provide insight into the dynamics of polaron formation.

Chapter 4 will discuss the polaron model, focusing on the case of an impurity in a bosonic bath. While many earlier works either failed to distinguish between or else avoided the study of equilibrium and nonequilibrium measurements of RF spectra, in Ref. [80] which forms the basis of the discussion of Chapter 4, we take care to treat the relevant out of equilibrium correlator  $A_p(t)$  correctly. Moreover we study the time-evolution of the velocity profile of an injected impurity, and study its relaxation into a nonequilibrium steady state.

Although the polaron model was originally studied as a model of fermionic impurities in a bosonic bath, the diversity of cold atom systems makes it equally feasible to study the effects of an impurity in a fermionic bath. Indeed, the polaron is a viable quasiparticle in higher dimensional fermionic systems [44, 52, 53, 54, 55, 56, 57, 58, 59, 76]. It bears emphasis however, that while the observed physics is well described by polaronic physics in the case of a generic impurity-Fermi gas system, the case of a heavy impurity is significantly different.

It was shown by Anderson [81] that the ground state of a Fermi gas with an infinitely massive impurity is orthogonal to the ground state in the absence of the impurity. This property has a dramatic consequence for the polaron discussed earlier – in particular the "weight" of the polaronic state is characterized by precisely the overlap between the ground states with and without the impurity, and in the case of the Fermi gas with a static impurity this weight is seen to disappear, leading to the destruction o the polaron. Moreover, the decay of the overlap manifests in the time-dependent correlator discussed earlier, and shows a characteristic power law behavior.

This unique behavior emerges from rich underlying physics: the orthogonality of the ground states results from a catastrophic divergence in the density of states of low-energy excitations generated in the Fermi gas due to its interactions with the impurity. Although divergences can often be cut off or carefully regularized, such an infrared (IR) divergence is quite physical, and is in fact the signature of 1D physics.

## 2.4 Hidden 1D physics in impurity models and vice versa

The 1D physics underlying the orthogonality catastrophe (OC) arises in the following way: a structureless localized impurity is sufficient for the OC to manifest. Following in Anderson's footsteps, if we imagine such an impurity was embedded at the center of a large sphere containing a Fermi gas, then it is only those fermions that occupy the *s*-wave channel which respond to the presence of the impurity (the wavefunctions of fermions in higher angular momentum states have nodes at the origin, where the impurity sits). The Schrödinger equation obeyed by the only relevant fermions is purely radial and therefore one dimensional. It takes a small leap to further realize that the significance of this hidden 1D nature manifests when counting the density of states for excitations that are generated near the Fermi surface due to the introduction of the impurity. Since the impurity solely, or more generally, primarily, affects the s-wave Fermions, which moreover have such a 1D geometry, there is divergence in the density of states for low-energy excitations. This divergence is just the van Hove singularity characteristic to 1D systems [77, 82, 206].

It will be shown in Chapter 5 how an effective 1D field theory, namely the Luttinger liquid (with modified boundary conditions) can be used to characterize the OC, and to extend the analysis for OC in cold atoms. In fact, the OC physics controlled by the excitations in the vicinity of the Fermi surfaces is ubiquitous in solid state systems, and is controlled by Fermi liquid theory. On the other hand, away from the Fermi surface fermionic quasiparticles are not well defined in 3D interacting systems, and thus one cannot usually probe contributions to OC from the bottom of the dispersion band. For spinless fermions in cold atoms, however, the bottom of the band contributions are well defined, since interactions between atoms in the s-wave channel are absent, allowing us to identify well defined fermionic excitations at all energies. In particular, we will show how the bottom of the Fermi band leads to a cusp in the absorption spectrum at energy  $E_F$  (corresponding to the energy difference between the Fermi surface, and the band bottom) above the absorption threshold (which occurs exactly at the Fermi surface, where gapless excitations originate).

While the discussion above makes it clear that the framework used to study 1D systems serves as a valuable tool to analyze the physics of OC, interestingly, the study of 1D systems also benefits from this connection. Indeed, it had long been observed that 1D quantum systems universally show "threshold singularities" reminiscent to OC, in their structure factors or spectral functions [270],  $S(k, \omega)$ . The latter characterize the response of the system to a perturbation with energy  $k, \omega$  (the perturbation might be due to tunneling a particle into the system, or else creating a density or spin fluctuation). The threshold singularities arise for the following reason: there is a well defined kinematic threshold for generating an excitation in the system, which corresponds to the smallest excitation  $\omega_k$  that the system admits at momentum k. Moreover, there is a continuum of gapless excitations that can also be generated in the system at arbitrarily low energy and momentum, which give rise to a power-law tail in the response, starting exactly at the kinematic threshold. These two facts combine to give threshold singularities in responses. The question then is whether this behavior can be correctly described by the Luttinger liquid, the effective field

theory of 1D systems.

Although the Luttinger liquid, is a powerful tool, it is severely lacking in a crucial way. The theory requires an essential simplification – one has to replace the "true" dispersion of the system one wishes to describe, with a linearized dispersion for the theory to work [205, 82]. Naturally such a description correctly predicts asymptotic properties of these systems – but it clearly will not correctly predict, e.g., the aforementioned threshold singularities, which require at the very least, the full dispersion relation of the system beyond a linearized caricature.

It is at this point that the connection between OC physics and 1D systems becomes a useful computational tool. A series of works [219, 220, 221, 224, 136, 231, 232, 234, 227, 83] exploited this connection to characterize the response of generic 1D systems to external probes. The basic idea was to identify the dominant excitations of the system involved in producing threshold singularities in responses. These excitations naturally separate into high and low energy parts – the high energy part corresponds to creating an excitation at energy near  $\omega_k$  and momentum k, while the low-energy excitations occur at  $k \approx 0$  (0 corresponds to the Fermi level  $k_F$ ). It turns out that an effective model which treats the high energy excitation as a mobile impurity, and the the low energy excitations as a bath, correctly predicts all universal features of the response of 1D systems to probes, and goes well beyond the crude predictions made using a linearly dispersing Luttinger liquid.

Chapters 6 and 7, explore one aspect of this connection and discuss a technique for calculating asymptotic properties of the correlation functions of 1D quantum liquids. In particular, one defect of the effective theory described above is that it can only predict correlation functions up to an overall prefactor. One typically considers such prefactors "non-universal" which is synonymous with "hopeless to calculate". However, it turns out that there is additional structure hidden in the effective description. One can show that analyzing the finite size corrections to correlation functions within the field theoretical framework strongly constrains the so called "non-universal" prefactors. Although the prefactors will depend on microscopic aspects of the model described, there is an explicit relation which will allow them to expressed in terms of a single matrix element which will need to be calculated for the underlying model. Chapters 6 spells out the details of the general framework, and demonstrates how the relation arises within a perturbative treatment. Chapter 7 discusses the actual calculation of matrix elements for exactly solvable models, which allow analytic progress to be made.

Thus it is seen that impurity models, while simple in and of themselves, not only admit phenomenological richness, but are quite central to the understanding of more complicated systems.
# Chapter 3

# A single impurity in a quantum mechanical bath

## 3.1 Introduction

In this chapter a simple model of the impurity-bath system is presented, with an eye toward dilute mixtures of cold atoms, and its general phenomenology analyzed. In Chapters 3, 4 we will discuss the phenomenology of a single impurity, interacting with a quantum mechanical bath in great detail. Here a rudimentary description of such systems is presented by focusing on a simplified version of the model of a single impurity in a bath. The goal is to provide a guide to the more in depth analysis of the following chapters by reviewing the general landscape of the impurity model, as well as the essential theoretical and experimental tools that are available.

## 3.2 Model of impurity in a quantum bath

In the Chapters 4 and 5 we will discuss the phenomenology of a single impurity, interacting with a quantum mechanical bath in great detail. This chapter is devoted to the essential phenomenology of such systems, and focuses on a simplified version of the model of a single impurity in a bath. This simple model, which proves surprisingly rich, can be described by the Hamiltonian

$$H = H_{\rm imp} + H_{\rm bath} + H_{\rm int.}$$
(3.1)

We will consider a single impurity of mass M with canonically conjugate momentum  $\hat{\mathbf{p}}$  and position  $\hat{\mathbf{x}}$ . Thus we may express the dynamics of the impurity using

$$H_{\rm imp} = \frac{\hat{\mathbf{p}}^2}{2M}.\tag{3.2}$$

Next, we will consider the surrounding bath, which may be comprised of fermions or bosons. Its exchange statistics are encoded in the commutation relations of the bath operators:

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}]_{\pm} = \delta_{\mathbf{k}, \mathbf{k}'}. \tag{3.3}$$

## 3.3 Exchange statistics of the bath

Using dilute systems of cold atomic gases quantum degenerate states of bosons as well as fermions are now routinely realized. Moreover the viability of preparing mixtures of such gases has also been repeatedly demonstrated (see e.g., Refs. [30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41]); thus we consider below both cases, a bath of bosons as well as fermions.

### 3.3.1 Bosons

A bosonic bath under similar circumstances typically will contain weak interactions and can be described by the Hamiltonian

$$H_{\text{bath,b}} = \sum_{\mathbf{k}} \frac{k^2}{2m} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + g_{bb} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} b_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}'-\mathbf{q}} b_{\mathbf{k}'} b_{\mathbf{k}}.$$
(3.4)

Typically, such a bosonic system is treated within the Bogoliubov prescription [84]: the vast majority of bosons are assumed to have formed a Bose-Einstein condensate (BEC), with a small number of uncondensed bosonic excitations. To account for this phenomenon, one uses the fact the lowest momentum mode  $\mathbf{k} = 0$  is macroscopically occupied and consequently the  $|BEC\rangle$  ground state of the system has the property:

$$b_{\mathbf{k}=\mathbf{0}}^{\dagger}|\text{BEC}\rangle \approx b_{\mathbf{k}=\mathbf{0}}|\text{BEC}\rangle \approx \sqrt{\rho_0}|\text{BEC}\rangle,$$
(3.5)

where  $\approx$  symbol expresses the fact that in writing the relations we have neglected a term of O(1) in comparison to  $\sqrt{\rho_0}$ , and assumed that the state with one more or less condensed particle is the same as  $|\text{BEC}\rangle$ . This is equivalent to assuming a coherent state like property for the BEC [85, 86].

The relations (3.5) suggest the replacement of the operators  $b_{\mathbf{k}=0}^{\dagger}$ ,  $b_{\mathbf{k}=0}$  by the cnumber  $\rho_0$ , effectively separating out the condensed fraction with density  $\rho_0$ . The Hamiltonian is then expanded to quadratic order in operators around the condensed state, using the smallness of  $1/\rho_0$  to justify neglecting the remainder, for weak interactions.

Such a procedure will however lead to the anamolous terms of the form:

$$g_{\rm bb}\rho_0 b_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger}, \quad g_{\rm bb}\rho_0 b_{\mathbf{k}} b_{-\mathbf{k}},$$

which can be treated by performing a canonical transformation:

$$\beta_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} + v_{\mathbf{k}} b_{\mathbf{k}}, \qquad (3.6)$$

choosing.

Thus one obtains the resulting quadratic Hamiltonian

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}}, \qquad (3.7)$$

in which the effects of interactions enter through a renormalization of the dispersion of quasiparticles

$$\omega_{\mathbf{k}} = ck\sqrt{1 + \frac{(k\xi)^2}{2}}.$$
(3.8)

In the bargain we have introduced two new constants which capture the effect of interactions on the quasiparticles.  $c = \sqrt{\frac{gn}{m}}$  is the speed of sound of the superfluid bosons, while  $\xi = \frac{1}{\sqrt{2mc}}$  is the "healing length" of the BEC. One defining property of the BEC is the presence of "off-diagonal long range order" [87]. The healing length is the correlation length for such order in the presence of interactions. It may also be interpreted more qualitatively as the "quasi-particle" separation length.

## 3.3.2 Fermions

The description of a quantum degenerate gas of fermions realized with cold atoms is much simpler by contrast [88]. Exchange statistics lead to a key difference between gases of bosons and fermions. In particular, in a single-component Fermi gas, s-wave scattering, the dominant mode of interatomic interactions in cold atoms, is inhibited due to the Pauli exclusion principle. This effect has dramatic consequences on e.g., the cooling mechanisms based on evaporation, where thermalization plays a crucial role, which explains in part the late realization of degenerate Fermi gases in contrast to Bose gases []. The achievement of low temperatures in Fermi gases was realized with the use of sympathetic cooling techniques either employing two different spin components of the same Fermi gas or adding a Bose gas component as a refrigerant. Though the relevant temperature scale providing the onset of quantum degeneracy is the same in both cases, on the order of  $T \approx \rho^{2/3}/m$ , unlike in the Bose case, where quantum statistical effects are associated with the occurrence of a phase transition to the Bose-Einstein condensed phase, in a noninteracting Fermi gas the quantum degeneracy temperature corresponds only to a smooth crossover between a classical and a quantum behavior.

Thus the bath Hamiltonian in the case of fermions is simply the free fermionic

Hamiltonian

$$H_{\text{bath,f}} = \sum_{\mathbf{k}} \frac{k^2}{2m} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}, \qquad (3.9)$$

where we made explicit the fact that a dilute system of single component fermions is essentially non-interacting.

## 3.4 Interactions between impurity and bath

As a simple model of impuprity-bath interactions, we consider pairwise "contact", i.e. zero-range interactions. Moreover in the context of ultracold atoms, such a model is indeed reasonable. Thus if the density of the bath at position  $\mathbf{x}$  is given by

$$\rho(\hat{x}) = \sum_{q} e^{i\mathbf{q}\cdot\hat{\mathbf{x}}} \rho_q,$$

then the impurity-bath interactions can be expressed as

$$H_{\rm int.} = g_{\rm IB} \sum_{\mathbf{q}} e^{i\mathbf{q}.\hat{\mathbf{x}}} \rho_{\mathbf{q}}.$$
 (3.10)

Here,  $g_{\rm IB}$  models the microscopic short-range interaction between the atoms. In systems of ultracold atoms the effective range of interactions between atoms (on the order of the van der Waals length) is the smallest length scale. Consequently, interatomic interactions can be modeled as having zero range[89, 28], and the microscopic host-impurity interaction  $g_{\rm IB}$  can further be expressed using the impurity-bath s-wave scattering length  $a_{\rm IB}$  (see Appendix A).

While the mixture of first and second quantization in Hamiltonian (3.1) appears unusual, it is a convenient when dealing with a single impurity. Moreover, expressed in this form, it is possible to perform a canonical rotation of the Hamiltonian (3.1) which effectively suppresses impurity degrees of freedom, at the cost of an induced interaction of the bath which gets generated.

# 3.5 Lee-Low-Pines transformation

There exists a canonical transformation introduced by Lee, Low, and Pines[90] (LLP), that singles out the conserved total momentum of the system:

$$\tilde{\mathcal{H}} = e^{iS} \mathcal{H} e^{-iS}$$
, with  $S = \hat{\mathbf{x}} \cdot \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}$ , (3.11)

$$e^{iS}\hat{b}_{\mathbf{k}}e^{-iS} = \hat{b}_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}, e^{iS}\hat{\mathbf{p}}e^{-iS} = \hat{\mathbf{p}} - \sum_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}.$$
(3.12)

We may write the transformed Hamiltonian as

$$\tilde{\mathcal{H}} = \frac{1}{2M} \left( \mathbf{p} - \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} \right)^2 + g_{\text{IB}} \sum_{\mathbf{k},\mathbf{k}'} \hat{b}_{\mathbf{k}'}^{\dagger} \hat{b}_{\mathbf{k}} + \tilde{\mathcal{H}}_{\text{bath}}, \qquad (3.13)$$

The canonical transformation leads to an effective Hamiltonian of the bath in which the explicit impurity degrees of freedom were absent. However, the presence of the impurity manifests in two ways:

1. There is a *local* scattering potential for the bath particles

$$g_{\rm IB} \sum_{\mathbf{k},\mathbf{k}'} \hat{b}^{\dagger}_{\mathbf{k}'} \hat{b}_{\mathbf{k}}, \qquad (3.14)$$

2. There is an induced interaction between the bath particles

$$\frac{1}{M} \sum_{\mathbf{k},\mathbf{k}'} \mathbf{k}.\mathbf{k}' (\hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}) (\hat{b}_{\mathbf{k}'}^{\dagger} \hat{b}_{\mathbf{k}'}).$$
(3.15)

Thus the effect of impurity-bath interaction is entirely encoded in a local scattering potential, while the quantum dynamics of the impurity is encoded in the induced interaction of the bath. This can be explicitly verified by taking the limit  $M \to \infty$ under which the impurity is rendered static, and the induced interaction term (3.15) disappears.

## 3.6 General phenomenology of impurity in a bath

The analysis above suggests considering in detail the model of a local scatterer in a non-interacting bath of bosons or fermions, to understand the essential physics of this system.

The Hamiltonian in this case has to the quadratic form

$$H = \int d\mathbf{r}\psi^{\dagger}(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + g_{\rm IB}\right)\psi(\mathbf{r}) = \sum_{\mathbf{k},\mathbf{k}'} \left(\delta_{\mathbf{k},\mathbf{k}'}\frac{k^2}{2m} + g_{IB}\right)b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}'},\qquad(3.16)$$

and describes the effect of a local scatterer on a system of non-interacting particles. In fact, this simple system comprising decoupled single particle states can be completely solved by first solving the single particle problem of a particle in a  $\delta$ -potential. The many-body states of the system can then be constructed out of the single particle states.

Such a seemingly trivial solution still admits richness; the problem of an impurity in a free Fermi gas was first studied by Anderson [81], by constructing the many-body states as Slater determinants of scattered single particle states. The solution consists the essential ingredients of the Orthogonality catastrophe, which demonstrates the impossibility of an infinite mass impurity in a Fermi gas to form a stable quasiparticle. In contrast, for the case of an impurity in a bosonic bath, one recovers the polaron, the stable quasiparticle formed by the impurity.

Although ground state properties can be trivially obtained from such a solution, its real power lies in its application to the full dynamical problem of the response of the quantum system to the sudden introduction of an impurity, pertinent to inverse impurity RF spectroscopy [78, 91], as will be demonstrated in the following sections.

#### 3.6.1 Single particle states: Problem of local scatterer

Here we solve the single particle problem of free particles (fermions or bosons) confined to a sphere of radius R scattered by a local potential which, without loss of generality, we insert at the origin of coordinates. This leads to the Hamiltonian

$$H_{1p} = -\frac{\nabla^2}{2m} + g_{IB}\delta(x), \qquad (3.17)$$

which for a finite spherically symmetric system simply yields a spectrum of states given by

$$\phi_{1p,k}(r) = \frac{\mathcal{N}}{\sqrt{4\pi}} \frac{\sin(\tilde{k}x + \delta(\tilde{k}))}{x}, \quad \tilde{k} + \delta(\tilde{k})/R = k, \quad k = \frac{\pi m}{R}, \quad m = 1, 2, 3... \quad (3.18)$$

with

$$\delta(k) = \tan^{-1} \left( k a_{\rm IB} \right), \qquad (3.19)$$

the s-wave phase shift due to scattering, expressed in terms of the measurable impuritybath scattering length  $a_{\rm IB}$ , and  $\mathcal{N}$  a normalization factor given by:

$$\mathcal{N} = \sqrt{\frac{2}{R} \left( 1 + \frac{\sin(2\delta(\tilde{k}))}{\tilde{k}R} \right)}$$
(3.20)

Additionally for positive scattering length  $a_{\rm IB} > 0$ , the system admits a bound molecular state:

$$\phi_{\rm b}(r) = \frac{1}{\sqrt{2\pi a (1 - e^{-2R/a})}} \frac{e^{-r/a}}{r}.$$
(3.21)

Thus the single particle problem has been exactly solved: for  $a_{\rm IB} < 0$ , we find propagating states with additional phase shifts due to impurity scattering; for  $a_{\rm IB} > 0$ , we find in addition to the propagating states, a bound state with energy  $E_b = \frac{1}{2ma_{\rm IB}^2}$ . The GS energy for the single particle problem is given by:

$$E_{a_{\rm IB}<0} = \frac{\tilde{k}_{\rm min}^2}{2m} = \frac{1}{2m} \left(\frac{\pi^2}{R^2} - 2\frac{\pi^2 a_{\rm IB}}{R^3}\right), \qquad (3.22)$$

$$E_{a_{\rm IB}>0} = -\frac{1}{2ma_{\rm IB}^2}.$$
(3.23)

It is clear that the single particle ground state energy has a non-analyticity as a function of  $\frac{1}{a_{\text{IB}}}$ : the second derivative of the ground state energy changes discontinuously as we sweep from small negative scattering length to small positive scattering length. We expect this simple physics to also persist in the many-body situation described in the next subsection, where we should rightly call this phenomenon a quantum phase transition.

### 3.6.2 Many-body spectrum

The solution of the single particle problem for a local scatterer renders the construction of the full many-body spectrum of the impurity-bath system trivial for non-interacting baths. The many-body states are simply Fock states formed from the exact single particle states, and directly encode the exchange statistics of the bath.

It is straightforward to verify that such states recover the expected physical properties of the impurity-bath ground states. In particular, the ground state phase diagram of the Bose polaron, shown in Fig. can be obtained by forming condensates of the appropriate single particle states. The phase diagram proves surprisingly rich – the ability to tune interactions between the impurity and background Bose gas to be both positive and negative scattering lengths, allows for the formation of different species of quasiparticles. For small negative scattering lengths, one obtains the stable attractive Bose polaron shown in blue. As the unitarity limit is approached, it becomes increasingly favorable for the impurity to bind to the bosons and form a molecule, leading to a transition to a molecular state. The state with a single boson bound to the impurity corresponds to the molecular state identified in [75], and is the analog of the molecular quasiparticle identified also in Fermi systems with mobile impurities [53, 52]. Additionally at high energies it becomes possible to form another quasiparticle, the so called repulsive polaron [57] shown in red, a metastable state which becomes destabilized due to decay into the molecular state.

Figure 3.1 : Ground states and physically relevant stationary states of the impurityboson system. The energy of three different types of states is plotted as a function of inverse impurity-boson scattering length; the attractive polaron (blue), repulsive polaron (red), and the molecular state (black). The attractive polaron becomes degenerate with the molecular state at unitarity, but their second derivatives are discontinuous indicating a second order phase transition.

For fermions one does not expect to recover a polaronic quasiparticle, but rather

one expects to find a signature of the Orthogonality catastrophe [?, ?, 206, ?]. Indeed, this phenomenon too is recovered, but as will be shown in the next section, its signature manifests in a dynamical observable.

## 3.7 RF spectroscopy as dynamical problem

An RF pulse changes the internal state of the impurity atom without modifying its momentum. Thus for a  $\downarrow$ -impurity-BEC initial state with momentum p, energy  $E_{i\downarrow}$ , denoted  $|i_{\downarrow p}\rangle$ , the RF absorption cross section can be computed within Fermi's Golden Rule from

$$I(p,\omega) = \sum_{n} |\langle n_{\uparrow p} | \hat{V}_{\rm RF} | i_{\downarrow p} \rangle|^2 \delta(\omega - (E_{n\uparrow} - E_{i\downarrow})), \qquad (3.24)$$

where all states  $|n_{\uparrow p}\rangle$  of  $\uparrow$ -impurity-BEC system with total momentum p are summed over. The RF transition operator  $\hat{V}_{\rm RF} \sim |\uparrow\rangle\langle\downarrow|$  instantaneously changes the internal state of the impurity, but the quantum mechanical state of the impurity-BEC system is otherwise unmodified by it, i.e. the initial state of the system  $|i_{\downarrow p}\rangle$  is quenched. Using standard manipulations (see e.g. [77, 78]) the last expression can be rewritten as

$$I(p,\omega) = \operatorname{Re}\frac{1}{\pi} \int_0^\infty dt e^{i\omega t} A_p(t)$$
(3.25)

$$A_p(t) = e^{iE_{i\downarrow}t} \langle i_{\uparrow p} | e^{-i(\mathcal{H}_b + \mathcal{H}_I + H_{\text{int}\uparrow})t} | i_{\uparrow p} \rangle, \qquad (3.26)$$

where frequency  $\omega$  is measured relative to the atomic transition frequency between states  $|\downarrow\rangle$  and  $|\uparrow\rangle$  of the bare impurity, and where we denoted  $|i_{\uparrow p}\rangle = \hat{V}_{\text{RF}}|i_{\downarrow p}\rangle$ .

Let us emphasize again: due to the instantaneous nature of the RF spin-flip, the state  $|i_{\uparrow p}\rangle$  is identical to the initial state of the  $\downarrow$ -impurity bath system in all respects, except the internal state of the impurity. Consequently,  $|i_{\uparrow p}\rangle$  is different from, and therefore higher in energy than, the  $\uparrow$ -impurity-bath ground state at momentum  $p, |0_{\uparrow p}\rangle$ . Thus it is more convenient to formulate the physical problem underlying the RF response as a dynamical one, rather than a traditional calculation of a ground state observable. Indeed, expression (3.26) has the form of the quantum propagation amplitude, related to the Loschmidt echo[79]), where an eigenstate of the Hamiltonian  $\mathcal{H}_b + \mathcal{H}_I + \mathcal{H}_{int\downarrow}$  needs to be time evolved with  $\mathcal{H}_b + \mathcal{H}_I + \mathcal{H}_{int\uparrow}$ .  $A_p(t)$  can also be measured directly in the time domain using the Ramsey sequence discussed in Ref. [78]. Analysis of (3.26) serves the central goal of this paper: the calculation of impurity RF spectra.

#### 3.7.1 Direct and inverse RF: momentum resolved spectra

Two varieties of RF spectroscopy are commonly used to probe impurity physics in cold atoms: direct and inverse RF. In the present context, direct RF involves preparing the system with the impurity initially in an interacting state, i.e. in Eq.(3.24), the state  $|i_{\downarrow p}\rangle = |0_{\downarrow p}\rangle$  will correspond to the interacting impurity-bath state, e.g., a polaron with momentum p. The RF pulse then flips the impurities to a final state in which they are non-interacting, i.e.,  $a_{\text{IB},\uparrow} \approx 0$ . For the inverse RF measurement, the scenario above is reversed, and the impurity is initially in a non-interacting state, i.e.  $|i_{\downarrow p}\rangle = |\mathbf{p}\rangle_{\downarrow} \otimes |0\rangle$  will correspond to the decoupled momentum  $\mathbf{p}$  bare impurity-bath ground state, with  $|0\rangle$  the the ground state of the bath, and the RF pulse flips the impurities to an interacting final state, i.e.  $a_{\text{IB},\uparrow} \neq 0$ .

Typically one is interested in performing a momentum resolved RF measurement. In the case of direct RF, a time-of-flight measurement following the RF pulse will directly yield the polaron momentum distribution since, after the impurity atoms are transferred to the  $\uparrow$  state, they propagate ballistically without being scattered by the host atoms. The combined time-of-flight and RF absorption measurements can be interpreted as momentum resolved RF spectroscopy [92, 93, 56]. Offsetting this advantage, the finite lifetime of the polaron [75] \* may pose a challenge to the initial adiabatic preparation of the system required for this measurement. On the other hand, for the inverse RF measurement, in which interactions are absent for the initial state of the impurity, the problem of finite polaron lifetime can be circumvented [57] but momentum resolution is more challenging to obtain.

We proposed [80] the following momentum-resolved *inverse* RF measurement. An external force that acts selectively on impurity atoms (e.g. through a magnetic field gradient) can be used to impart a finite initial momentum

$$p_0 = -\nabla V_{\text{ext},\downarrow} \Delta T, \qquad (3.27)$$

where  $p_0$ , the center of the momentum distribution of  $\downarrow$ -impurities is the momentum transferred by applying a state-selective external potential gradient  $\nabla V_{\text{ext},\downarrow}$  for a time  $\Delta T$  to the impurities. An RF pulse would then transfer the initially weakly interacting impurities to an interacting final state. The known transferred momentum  $p_0$ , combined with the absorption of RF, would yield a momentum resolved RF spectrum. Since the experiment is done at a finite concentration of impurity atoms to obtain the total absorption cross section  $I(p, \omega)$  would need to be averaged over the impurity momentum distrubtion (see e.g., the Supplementary materials of Ref. [53]), with width given by the thermal de Broglie wavelength, or by the inverse of the distance

<sup>\*</sup>For positive scattering length, the pair-wise impurity-boson interaction potential admits a bound state, leading to an impurity-bath ground state formed out of bound particles, that is much lower in energy than the repulsive polaron which is formed out of scattered bosons. Consequently the repulsive polaron is a metastable state with a finite lifetime after which it will decay into the molecular state.

between impurity atoms (if they are fermionic and obey the Pauli exclusion principle). Typically the width is expected to be small due to the low temperature and diluteness of the impurities. The advantage of such a measurement is its insensitivity to the polaron lifetime as it requires no adiabatic preparation [57], while also allowing a momentum resolved measurement, but at the cost of repeated measurements to resolve a finite momentum range.

## 3.7.2 Calculating many-body overlaps

We will use a technique originally due to Levitov and Klich for calculating timedependent observables of a free many-body system. They showed that for such systems, the relevant observables can be cast as a determinant over matrices expressed in the basis of single particle states.

We are interested in the many-body overlap of the form

$$A(t) = \langle \psi_i | e^{i \hat{\mathcal{H}}_{\downarrow} t} e^{-i \hat{\mathcal{H}}_{\uparrow} t} | \psi_i \rangle, \qquad (3.28)$$

which we can more generally formulate as

$$A(t) = \operatorname{Tr} \left[ \hat{N}_{0} e^{i\hat{\mathcal{H}}_{\downarrow} t} e^{-i\hat{\mathcal{H}}_{\uparrow} t} \right]$$
  
$$= \frac{\operatorname{Tr} \left[ e^{-\beta\hat{\mathcal{H}}_{\downarrow}} e^{i\hat{\mathcal{H}}_{\downarrow} t} e^{-i\hat{\mathcal{H}}_{\uparrow} t} \right]}{\operatorname{Tr} \left[ e^{-\beta\hat{\mathcal{H}}_{\downarrow}} \right]},$$
  
(3.29)

where  $\hat{N}_0$  is the many-body density matrix describing the initial configuration of the system. In the second line, to prove the formula with ease, we have described such an initial state as the equilbrium state of the initial Hamiltonian at temperature  $1/\beta$ ; in general all that is required is a density-matrix characterization of the initial state of the system.

To make progress we require the following Lemma []: consider an arbitrary manybody operator  $\hat{\mathcal{A}}$  constructed out of single particle operators  $\hat{a}$  as:

$$\hat{\mathcal{A}} = \sum_{i,j} \hat{a}_{ij} \hat{b}_i^{\dagger} \hat{b}_j, \qquad (3.30)$$

where  $\hat{b}_i$  are the annihilation operators which express the particles in the second quantized form. The following lemma allows us to express traces over many-body states of the system in terms of the single particle operators:

$$\operatorname{Tr}\left[e^{\hat{\mathcal{A}}}e^{\hat{\mathcal{B}}}\right] = \det(1 - \xi e^{\hat{a}}e^{\hat{b}})^{\xi},\tag{3.31}$$

with

$$\xi = \begin{cases} +1, & \text{for fermions,} \\ -1, & \text{for bosons.} \end{cases}$$
(3.32)

The lemma above allows us to express the time-dependent overlap as

$$A(t) = \left[\frac{\det\left(1 - \xi e^{-\beta\hat{h}_{\downarrow}} e^{i\hat{h}_{\downarrow}t} e^{-i\hat{h}_{\uparrow}t}\right)}{\det\left(1 - \xi e^{-\beta\hat{h}}\right)}\right]^{-\xi}.$$
(3.33)

Identifying  $\hat{n}_0 = \frac{1}{1 - e^{-\beta \hat{h}}}$ 

The relevant quantity for overlap calculation is

$$A(t) = \det\left(1 \pm \hat{n}_0 e^{i\hat{h}_{\downarrow}t} e^{-i\hat{h}_{\uparrow}t} \mp \hat{n}_0\right)^{\pm 1},$$
(3.34)

for fermions (upper), bosons (lower) respectively.

Thus knowledge of the single particle spectrum as obtained in Sec. 3.6.1 suffices to calculate the dynamic correlator Eq. (3.26) and its associated Fourier transform, the impurity RF absorption spectral function, both of which are observable. These quantities will be explored in more depth in the following chapters.

# Chapter 4

# Impurity in a bath of bosons

## 4.1 Introduction

Following the general discussion in Chapter 3 of impurity physics in the context of ultracold atoms, this chapter contains a detailed analysis of heavy mobile impurities in a Bose gas. The impurity is known to form a quasiparticle called a polaron, but the dynamical properties of this system are less well explored. Here we discuss how to probe the polaronic physics using RF spectroscopy in cold atoms. Moreover, while treating the problem of calculating the "inverse" RF spectra, we will come across the problem of characterizing an impurity which is suddenly introduced into a BEC, and explore the resulting nonequilibrium dynamics.

## 4.2 Impurities in a BEC

We assume that the concentration of impurity atoms is low, so we can neglect interactions between them, and discuss individual impurity atoms. Thus we consider a single impurity of mass M, which has two internal (e.g. hyperfine) states  $|\uparrow\rangle, |\downarrow\rangle$ , immersed in a BEC of a different type of atom of mass m. The Hamiltonian of the system is given by

$$\mathcal{H} = \mathcal{H}_b + \mathcal{H}_I + |\uparrow\rangle \otimes \langle\uparrow |\mathcal{H}_{\text{int}\uparrow} + |\downarrow\rangle \otimes \langle\downarrow |\mathcal{H}_{\text{int}\downarrow}, \tag{4.1}$$

where  $\mathcal{H}_b$  is the BEC Hamiltonian,  $\mathcal{H}_I = \frac{\hat{p}^2}{2M}$  is the Hamiltonian of the impurity atom with momentum  $\hat{p}$ , and  $\mathcal{H}_{int\sigma}$  describes a density-density interaction of the bosons with impurity in state  $\sigma$  at position  $\hat{\mathbf{x}}$ :

$$\mathcal{H}_{\text{int}\sigma} = g_{\text{IB},\sigma} \rho_{\text{BEC}}(\hat{\mathbf{x}}), \qquad (4.2)$$

where  $g_{\text{IB},\sigma}$  models the microscopic short-range interaction between the atoms. Since we treat systems of ultracold atoms for which the effective range of interactions between atoms (on the order of the van der Waals length) is the smallest length scale, inter-atomic interactions can be modeled as having zero range[89, 28], and the microscopic host-impurity interaction can be described using the s-wave scattering length  $a_{\text{IB},\sigma}$  of the impurity in state  $\sigma$  with the surrounding BEC (see also Appendix A).

We will restrict our discussion to weakly-interacting Bose gases, well described by the Bogoliubov approximation [84], in which the condensed ground state of the Bose gas is treated as a static "mean field", and excitations are modeled as a bath of free phonons.

$$\mathcal{H}_b = \sum_{\mathbf{k}\neq\mathbf{0}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}, \quad \omega_{\mathbf{k}} = ck \sqrt{1 + \frac{(k\xi)^2}{2}}, \quad (4.3)$$

where  $\xi = 1/(\sqrt{2}mc)$  is the healing length, c the speed of sound in the BEC,  $k = |\mathbf{k}|$ , and where we took  $\hbar = 1$ . In this framework the interaction (4.2) between impurity and bosons can be rewritten as a sum of two terms. The first captures the "mean-field" interaction of the BEC ground state with the impurity, and the second encodes the impurity interactions with the Bogoliubov excitations. The density of the excitations can be expressed as a linear combination of phonon creation and annihilation operators, and leads to the following explicit form of the interaction Hamiltonian:

$$\mathcal{H}_{\text{int}\sigma} = \frac{2\pi a_{\text{IB},\sigma}}{\mu} n_0 + \sum_{\mathbf{k}} V_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\hat{\mathbf{x}}} (\hat{b}_{\mathbf{k}} + \hat{b}_{-\mathbf{k}}^{\dagger}), \qquad (4.4)$$

with [73]

$$V_{k\sigma} = \frac{2\pi a_{IB\sigma} \sqrt{N_0}}{\mu} \left(\frac{\xi k}{\sqrt{2 + (\xi k)^2}}\right)^{1/2}.$$
 (4.5)

Here  $N_0$  is the number of atoms in the condensate, with the corresponding density  $n_0$ , and  $\mu = (m^{-1} + M^{-1})^{-1}$  is the reduced mass of the impurity.

The above approximations hold so long as the impurity-boson interaction does not significantly deplete the condensate, leading to the condition [61, 65]

$$|a_{\mathrm{IB},\sigma}|\xi^{-1} \ll 1.$$
 (4.6)

Our treatment of the impurity-BEC system ignores the phenomenology of strongcoupling physics e.g., near a Feshbach resonance [75], which lies beyond the parameter range (4.6). The model (4.3), (4.4), with parameters (4.5), in its regime of validity, constitutes a generalized Fröhlich model of polarons in ultracold BECs [70, 71, 72, 73].

## 4.3 Polaron ground state in BEC

In order to characterize polaronic phenomena manifested in RF spectra, it is useful to review the ground state properties of polarons in BECs.

It is possible to tune interactions between ultracold atoms to be effectively attractive or repulsive using Feshbach resonances [94]. Correspondingly, the Bose polaron comes in two varieties associated with effective attraction ( $a_{\text{IB},\sigma} < 0$ ) and repulsion ( $a_{\text{IB},\sigma} > 0$ ) between the impurity and the BEC. Moreover at strong coupling there is an additional transition of the attractive polaron into a bound molecular state [75]. We will only discuss the regime of weak impurity-Bose interactions which satisfy the condition (4.6) and are captured by our Fröhlich model (4.3), (4.4), with parameters (4.5).

We note that the authors of Ref. [75] also considered the spectral properties of impurities in a BEC, but considered the regime of strong impurity-bose coupling which occurs in the vicinity of the Feshbach resonance. Their approach, inspired in part by Chevy's variational wavefunction description of fermionic polarons [95, 96], separates the spectral contributions of the bound molecules and the repulsive polarons on the repulsive side of the Feshbach resonance ( $a_{\text{IB},\sigma} > 0$ ). However their selective resummation scheme does not reduce to the exact solution in the case of a heavy impurity, and consequently misses the physics of the orthogonality catastrophe [97] in low dimensions. Thus it does not accurately describe the precise lineshape of the incoherent part of RF spectra.

Although the analysis of the ground state of the polaron model has been carried out previously in Refs. [43, 98], we present it here to motivate our later study of dynamics as a generalization of the approach to the ground state.

#### 4.3.1 Lee-Low-Pines transformation

There exists a canonical transformation introduced by Lee, Low, and Pines[90] (LLP), that singles out the conserved total momentum of the system:

$$\widetilde{\mathcal{H}} = e^{iS} \mathcal{H} e^{-iS}, \text{ with } S = \widehat{\mathbf{x}}. \sum_{\mathbf{k}} \mathbf{k} \widehat{b}_{\mathbf{k}}^{\dagger} \widehat{b}_{\mathbf{k}},$$
(4.7)

$$e^{iS}\hat{b}_{\mathbf{k}}e^{-iS} = \hat{b}_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}, e^{iS}\hat{\mathbf{p}}e^{-iS} = \hat{\mathbf{p}} - \sum_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}.$$
(4.8)

We may write the transformed Hamiltonian as

$$\tilde{\mathcal{H}} = \frac{1}{2M} \left( \mathbf{p} - \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} \right)^{2} + \sum_{\mathbf{k}} V_{\mathbf{k}} (\hat{b}_{\mathbf{k}}^{\dagger} + \hat{b}_{-\mathbf{k}}) \\
+ \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}},$$
(4.9)

where without loss of generality we projected the full Hamiltonian onto the sector  $\sigma = \uparrow$ ; the same can be done in the other sector.

The LLP transformation eliminates the impurity degree of freedom by isolating the conserved total momentum  $\mathbf{p}$  of the system which becomes a parameter of the effective Hamiltonian (4.9). The simplification comes at the cost of an induced interaction between the Bogoliubov excitations, which enocodes the quantum dynamics of the impurity, and vanishes in the  $M \to \infty$  limit of a static localized impurity.

It was argued in Refs. [99, 100] that the existence of a finite momentum ground state implies symmetry breaking, and consequently, a phase transition corresponding to the "self-localization" transition of Landau and Pekar [46]. Although we will discuss states of the Hamiltonian (4.9) with arbitrary total momentum p, it was established rigorously in Ref. [101] that a large class of Fröhlich type models with gapless phonons, including the present one, can only admit a ground state with p = 0.

We will consider eigenstates of Hamiltonian (4.9) with finite total momentum p, which are not "true" global ground states in the above sense, but are nonetheless required to calculate momentum resolved RF spectra using the time dependent overlap (3.26). The symmetry breaking in the present context is not spontaneous, but rather due to the injection of an impurity with finite momentum into the BEC. We will use the term "polaron ground state" to refer to the lowest-energy eigenstate of Hamiltonian (4.9) with a given total momentum p. We approximate such states using a mean-field treatment.

### 4.3.2 Mean-field polaron solution

For a localized impurity  $M \to \infty$ , Hamiltonian (4.9) decouples into a sum of independent harmonic oscillators, each of which has a coherent state as its ground state [102]. Consequently the many-body ground state in this limit is a decoupled product of coherent states:

$$|0_{M\to\infty}\rangle = \prod_{\mathbf{k}} e^{\beta_{\mathbf{k}}\hat{b}^{\dagger}_{\mathbf{k}} - \beta^{*}_{\mathbf{k}}\hat{b}_{\mathbf{k}}}|0\rangle, \quad \beta_{\mathbf{k}} = -\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}.$$
(4.10)

Moreover we expect by continuity \* that for an impurity with a large, finite mass M, we can approximate the true ground state by an optimally chosen product of coherent states:

$$|0_{\downarrow p}\rangle = \prod_{\mathbf{k}} e^{\alpha_{\mathbf{k}}^{\mathrm{MF}} \hat{b}_{\mathbf{k}}^{\dagger} - (\alpha_{\mathbf{k}}^{\mathrm{MF}})^{*} \hat{b}_{\mathbf{k}}} |0\rangle, \qquad (4.11)$$

with  $\alpha_{\mathbf{k}}^{\text{MF}}$  determined by minimizing the total energy of the system  $E(\{\alpha_{\mathbf{k}}\}) = \langle 0_{\downarrow p} | \tilde{\mathcal{H}} | 0_{\downarrow p} \rangle$ , which can be cast as a mean field self-consistency condition

$$\alpha_{\mathbf{k}}^{\mathrm{MF}} = -\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}} + \frac{k^{2}}{2M} - \frac{k_{\parallel}}{M} \left(p - \Xi[\alpha_{\mathbf{k}}^{\mathrm{MF}}]\right)}, \qquad (4.12)$$
$$\Xi[\alpha_{\mathbf{k}}] \equiv \sum_{\mathbf{k}} k_{\parallel} |\alpha_{\mathbf{k}}|^{2}.$$

where we denote the total phonon momentum projected in the direction  $k_{\parallel} \equiv \frac{\mathbf{p}}{|\mathbf{p}|}$  by the parameter  $\Xi$ . The set of self-consistency conditions (4.13) can then be reformulated as a *single scalar equation* for  $\Xi$ :

$$\Xi = \sum_{\mathbf{k}} \frac{k_{\parallel} V_{\mathbf{k}}^2}{\left(\omega_{\mathbf{k}} + \frac{k^2}{2M} - \frac{k_{\parallel}}{M} \left(p - \Xi\right)\right)^2}.$$
(4.13)

<sup>\*</sup>Note that unlike for a fermionic bath, for which the infinitely massive impurity is a singular limit displaying the orthogonality catastrophe, for bosons the infinite mass limit is smoothly connected to a system with a heavy impurity; this can be verified by examining the effect of recoil on the density of states [103].

Having approximated the polaron ground state wavefunction using Eq. (4.13), we can calculate the polaron binding energy, effective mass, and the overlap with the bare impurity.

### 4.3.3 Binding energy of the polaron

The binding energy is defined as the difference between the ground state energy of the polaron at zero momentum and the energy of a BEC with a non-interacting impurity atom:

$$E_{B} = \langle 0_{\uparrow p=0} | \mathcal{H} | 0_{\uparrow p=0} \rangle - \langle 0 | \otimes \langle p = 0 | \mathcal{H}_{b} + \mathcal{H}_{I} | 0 \rangle \otimes | p = 0 \rangle$$

$$= \langle 0_{\uparrow p=0} | \mathcal{H} | 0_{\uparrow p=0} \rangle - 0$$

$$= \sum_{\mathbf{k}} \frac{\left[ \left( 1 + \frac{k_{\parallel}}{M} \Xi \left( \omega_{k} + \frac{k^{2}}{2M} \right)^{-1} \right)^{-1} - 2 \right]}{\left( \omega_{k} + \frac{k^{2}}{2M} + \frac{k_{\parallel}}{M} \Xi \right)} V_{k}^{2} + \frac{\Xi^{2}}{2M},$$

$$(4.14)$$

where we took an expectation value using the state (4.11) optimized according to Eq. (4.13). Note that we did not include the mean field energy of the interactions between condensend bosons and the impurity  $E_{\rm MF} = \frac{2\pi a_{\rm IB,\sigma} n_0}{\mu}$ , in the binding energy.

The binding energy is a well defined physical observable, which must moreover be expressible in terms of the *s*-wave scattering length, by virtue of the universality of interactions in cold atoms (see Appendix A). However, a naive evaluation of the sum in Eq. (4.14) leads to an ultraviolet (UV) divergence. The appearance of UV divergences in physical observables is a direct consequence of poorly approximating the fundamentally different physics at atomic length scales. Indeed, our zero-range model Eq. (4.2) pathologically couples microscopic degrees of freedom to the physically relevant long distance degrees of freedom. However, in order to describe universal properties which are insensitive to microscopic physics, we require a means of safely and justifiably decoupling microscopic and macroscopic scales.

To this end we found it most convenient to evalute Eq. (4.14) using dimensional regularization [104], which is equivalent to the regularization scheme based on a momentum cutoff used in Refs. [61, 73, 75]. The regularization amounts to the subtraction of the leading divergence in the binding energy which takes the form

$$E_{\rm B}^{\rm div} \to -\left(\frac{2\pi a_{{\rm IB},\sigma}}{\mu}\right)^2 n_0 \sum_{\mathbf{k}} \frac{2\mu}{k^2}.$$
 (4.15)

Physically such a subtraction can be justified by considering the total interaction energy of the BEC and impurity:

$$E_{\rm int} = E_{\rm B} + E_{\rm MF}.\tag{4.16}$$

and expressing the mean field interaction energy of the condensate in terms of the "bare" coupling to the impurity  $g_{\text{IB},\sigma}$  from Eq. (4.2):

$$E_{\rm MF} = g_{\rm IB,\sigma} n_0. \tag{4.17}$$

The bare coupling can be related to the physical impurity-boson s-wave scattering length using the Lippman-Schwinger equation

$$\frac{1}{g_{\text{IB},\sigma}} = \frac{\mu}{2\pi a_{\text{IB},\sigma}} - \sum_{\mathbf{k}} \frac{2\mu}{k^2},$$
(4.18)

which yields the following expression for the mean-field energy, accurate to second order in  $a_{\text{IB},\sigma}$ :

$$E_{\rm MF} = \frac{2\pi a_{\rm IB,\sigma} n_0}{\mu} + \left(\frac{2\pi a_{\rm IB,\sigma}}{\mu}\right)^2 n_0 \sum_{\bf k} \frac{2\mu}{k^2}.$$
 (4.19)

Indeed, the second term on the right hand side is precisely the "subtracted infinity" required to eliminate the divergence (4.15). Thus we obtain a well-behaved binding

energy which can be expressed in closed form for a localized impurity with  $M \to \infty$ 

$$E_{B,\text{reg.}}^{M\to\infty} = -\frac{2\sqrt{2\pi a_{\text{IB},\sigma}^2 n_0}}{\mu\xi} < 0, \qquad (4.20)$$

and must be evaluated numerically for finite mass impurities. The details of the regularization procedure used to obtain Eq. (4.20) are presented in Appendix A.

We will later need the generalized binding energy for a finite momentum polaron, i.e. Eq. (4.14) with  $p \neq 0$ . As shown in Sec. 4.4.2, the latter quantity will contribute a shift of the RF signal relative to the atomic transition rate between  $\uparrow$  and  $\downarrow$  of the bare impurity.

### 4.3.4 Effective mass of the polaron

In the absence of interactions, the bare impurity propagates as a free particle with a quadratic dispersion  $\varepsilon_{\rm I} = \frac{p^2}{2M}$ . It is useful to conceptualize the polaron also as a propagating object – a wave packet – composed of an impurity dragging a cloud of bosonic excitations. Such a dressing of the impurity will naturally imply propagation with an effectively heavier mass. We can identify the effective mass of the polaron from its group velocity by requiring the polaron dispersion to take the form  $\varepsilon_{\rm polaron} = \frac{p^2}{2M^*}$ . Then from the definition of the polaron group velocity we find

$$v_{\text{polaron}} \equiv \frac{\partial}{\partial p} \varepsilon_{\text{polaron}} = \frac{p}{M^*}$$
$$= \partial_p \left( \langle 0_{\uparrow p} | \tilde{\mathcal{H}} | 0_{\uparrow p} \rangle - \langle 0_{\uparrow p=0} | \tilde{\mathcal{H}} | 0_{\uparrow p=0} \rangle \right)$$
$$\frac{p}{M^*} = \frac{p}{M} - \langle 0_{\uparrow p} | \sum_{\mathbf{k}} k \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} | 0_{\uparrow p} \rangle, \qquad (4.21)$$

where in the second line we expressed the polaron dispersion as the energy difference between the system at finite momentum p and zero momentum. We can express Eq. (4.21) in terms of the mean field solution to find

$$\frac{M}{M^*} = 1 - \frac{\Xi}{p},$$
 (4.22)

with the parameter  $\Xi$ , the total momentum of the bosons, obtained by solving Eq. (4.13).

Here we note an interesting feature of the mean-field treatment above. One finds that for a certain parameter regime, no mean-field solution can be found due to a singularity in the self-consistency Eq. (4.13). The singularity arises when the denominator of the right hand side of Eq. (4.13) admits a zero for small k:

$$0 = \omega_{\mathbf{k}} + \frac{k^2}{2M} - \frac{k_{\parallel}}{M} \left( p - \Xi[\alpha_{\mathbf{k}}^{\mathrm{MF}}] \right) \xrightarrow{k \ll 1/\xi} ck - \frac{pk_{\parallel}}{M^*},$$

where we used Eq. (4.22) to obtain the right hand side.

Thus we find that the mean-field treatment breaks down when

$$v^* = \frac{p}{M^*} > c. (4.23)$$

The criterion (4.23) is reminiscent of Landau's criterion for dissipationless transport through a superfluid [61], with one important difference. The usual criterion is a purely kinematic bound obtained by weighing the relative advantage for an impurity to emit excitations, and does not include the effects of interactions. The remarkable feature of Eq. (4.23) is the role of interactions: it is not the *bare impurity* velocity that is compared to the sound speed, but rather the *effective polaron* velocity. Due to the strong dependence of the effective mass on interactions, one finds that for a large enough interaction the *polaron* is subsonic, although the corresponding bare impurity in the absence of interactions would be supersonic.

In Fig. 4.1 we plot the critical strength of interactions for which we find polaronic solutions. We interpret the lack of solutions in the unshaded region of the figure as a break down of our ansatz. Our ansatz implicitly assumes a well defined polaronic quasiparticle, which fails to describe the impurity at supersonic velocities; indeed, the authors of Ref. [75] reported a decay of the Bose polaron into the continuum, above the critical velocity given by Landau's criterion.

Figure 4.1: Mean-field solutions are obtained in the shaded region, while in the upper unshaded region no solutions can be found within our ansatz. The line separating the regions corresponds to the condition (4.23) reminiscent of the Landau criterion. In the absence of interactions the separation occurs at the usual subsonic to supersonic transition point p/M = c.

## 4.3.5 Quasiparticle residue

The quasiparticle residue directly quantifies the component of the bare impurity that remains in the interacting ground state. Although it is usually extracted from the residue of the pole of the impurity Green's function [105], it may also be obtained as the overlap between the free and dressed impurity wavefunction. Since the impurity degrees of freedom drop out of the problem due to the Lee-Low-Pines transformation, we obtain the quasiparticle weight from the overlap of the phonon vacuum  $|0\rangle$  and the interacting phonon ground state  $|0_{\downarrow,p}\rangle$ :

$$Z = |\langle 0|0_{\uparrow p} \rangle|^{2}$$

$$= \exp\left[-\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2}}{\left(\omega_{\mathbf{k}} + \frac{k^{2}}{2M} - \frac{k_{\parallel}}{M} \left(p - \Xi[\alpha_{\mathbf{k}}^{\mathrm{MF}}]\right)\right)^{2}}\right]$$

$$= \exp\left[-\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2}}{\left(\omega_{\mathbf{k}} + \frac{k^{2}}{2M} - \frac{pk_{\parallel}}{M^{*}}\right)^{2}}\right], \qquad (4.24)$$

where we used Eq. (4.22) in the last line to relate the quasiparticle weight and the effective mass.

In Fig. 4.2, we plotted the quasiparticle residue on a logarithmic scale, in the 3-D case as a function of the impurity-BEC mass ratio, and interaction strength; strong interactions as well as small mass ratio quickly suppresses Z. One finds that in spatial dimensions D = 2, 3, a quantum impurity in a weakly-interacting BEC always forms a quasiparticle, although with exponentially suppressed weight for growing interaction strength. Moreover, at a given impurity-BEC interaction strength, quasiparticle residue is *larger* for *heavier* impurities, and retains a finite value even in the  $M \to \infty$  limit. This should be contrasted to impurities in a Fermi gas with quasiparticle residue that has the opposite dependence on mass. In particular due to Anderson's Orthogonality Catastrophe (OC) [97] the quasiparticle residue Z = 0 for localized impurities with  $M \to \infty$  in a Fermi sea in 1-,2-,and 3-D. Interestingly, for D = 1, the expression (4.24) contains an infrared divergence which again leads to Z = 0, and signals OC even for localized impurities in 1-D Bose gases. The mechanism of the OC, namely the catastrophic emission of excitations in response to an impurity.

Figure 4.2: (a)Log plot of the quasiparticle weight (which is exponentially small) as a function of interaction strength, represented by the dimensionless quantity  $a_{\text{IB},\sigma}\sqrt{n_0\xi}$ , i.e. ratio between the mean free path of the impurity and the length scale over which bosons are localized), and mass ratio between impurity and bosons  $m_r = M/m$ . For any moderate interaction strength, the quasiparticle weight is almost negligible, corresponding to an extremely strong renormalization of the impurity. (b) Quasiparticle weight Z plotted as a function of interaction strength  $a_{\text{IB},\sigma}\sqrt{n_0\xi}$  for a fixed mass ratio of  $m_r = 2.5$ 

occurs independently of the exchange statistics of the many-body environment and is mainly due to the kinematic confinement of 1-D systems [106].

We will in Sec. 4.4 show that the quasiparticle residue Z is directly measurable via RF spectroscopy, and manifests as the weight of the coherent part of the signal.

## 4.4 Analysis of RF spectra

In Sec. 3.7 we showed that in order to obtain RF spectra, the relevant quantity is the time-dependent overlap (3.26), i.e. the propagation amplitude of the initial  $\downarrow$ -impurity-BEC state by the Hamiltonian associated with the  $\uparrow$ -impurity-BEC system:

$$A_p(t) = e^{iE_{i\downarrow}t} \langle i_{\uparrow p} | e^{-i\mathcal{H}t} | i_{\uparrow p} \rangle, \qquad (4.25)$$

where we used  $|i_{\uparrow p}\rangle = \hat{V}_{\rm RF}|i_{\downarrow p}\rangle$ , with  $|i_{\downarrow p}\rangle$  the initial state of the  $\downarrow$ -impurity-BEC system at momentum p energy  $E_{i\downarrow}$ , and  $\hat{V}_{\rm RF} = |\uparrow\rangle\langle\downarrow|$ . Note that in order to use the LLP transformed  $\uparrow$ -impurity-BEC Hamiltonian we must consider the effect of the transformation on  $|i_{\uparrow p}\rangle$ , however in the cases of interest to us  $|i_{\uparrow p}\rangle$  involves the phonon vacuum, which is invariant under LLP.

The RF spectral response of the impurity is simply obtained as the Fourier transform of Eq. (4.25). First, in Sec. 4.4 A we discuss general features of the time dependent overlap (4.25). In Sec 4.4 B,C, we explicitly calculate the overlap and corresponding RF spectra for direct and inverse RF protocols.

### 4.4.1 Generic features of the RF response

Starting from a straightforward Lehmann expansion [105] of the RF response, and resolving the identity in terms of eigenstates  $|m_{\uparrow p}\rangle$  of the time-evolving Hamiltonian,

with energy  $E_{m\uparrow}$ , we obtain:

$$I(p,\omega) = \operatorname{Re} \frac{1}{\pi} \int_{0}^{\infty} dt e^{i(\omega+E_{i\downarrow})t} \langle i_{\uparrow p} | e^{-i\tilde{\mathcal{H}}_{\uparrow}t} | i_{\uparrow p} \rangle$$
  
$$= \sum_{m} \operatorname{Re} \frac{1}{\pi} \int_{0}^{\infty} dt e^{i(\omega+E_{i\downarrow}-E_{m\uparrow})t} |\langle m_{\uparrow p} | i_{\uparrow p} \rangle|^{2}$$
  
$$= \operatorname{Re} \frac{1}{\pi} \int_{0}^{\infty} dt e^{i(\omega-\Delta_{0})t} Z_{\uparrow\downarrow} \times$$
  
$$\left(1 + \sum_{m\neq 0} e^{i\Delta_{m}t} \frac{|\langle m_{\uparrow p} | i_{\uparrow p} \rangle|^{2}}{Z_{\uparrow\downarrow}}\right), \qquad (4.26)$$

with

$$Z_{\uparrow\downarrow} = |\langle 0_{\uparrow p} | i_{\uparrow p} \rangle|^2, \Delta_m = E_{m\uparrow} - E_{i\downarrow}, \qquad (4.27)$$

where  $|0_{\uparrow p}\rangle$  is the ground state of the  $\uparrow$ -impurity-BEC Hamiltonian (4.9).

We expect the low energy contribution to  $I(p, \omega)$  to be dominated by the long time limit of the integrand for which, due to dephasing, we find:

$$I\left(p,\omega\ll\frac{c}{\xi}\right) = \lim_{t\to\infty} Z_{\uparrow\downarrow}\left(1+\sum_{m\neq0}e^{i\Delta_m t}\frac{|\langle m_{\uparrow p}|i_{\uparrow p}\rangle|^2}{Z_{\uparrow\downarrow}}\right)$$
  

$$\to Z_{\uparrow\downarrow}.$$
(4.28)

This dephasing mechanism separates a coherent and incoherent contribution which constitute the total RF signal:

$$I(p,\omega) = I_{\rm coh}(p,\omega) + I_{\rm incoh}(p,\omega), \qquad (4.29)$$

with the coherent part given by

$$I_{\rm coh}(p,\omega-\Delta_0) = Z_{\uparrow\downarrow}\delta(\omega-\Delta_0). \tag{4.30}$$

From Eq. (4.27) we find that the weight of the coherent peak of the impurity RF response is determined by the overlap between the initial state of the  $\downarrow$ -impurity-BEC

system, and the ground state of the final  $\uparrow$ -impurity-BEC system (the RF operator  $\hat{V}_{\text{RF}}$  abruptly changes the impurity internal state, but otherwise leaves the impurity-BEC state unmodified, i.e.  $|i_{p\downarrow}\rangle \rightarrow |i_{p\uparrow}\rangle$  must be thought of as a sudden quench). The center of the peak occurs at the energy difference between the initial and final states  $E_{0,\uparrow} - E_{i\downarrow}$  measured with respect to the bare atomic transition rate of the impurity between its internal states.

In the case of the direct and inverse RF protocols considered here, the weight of the coherent peak is in fact the quasiparticle weight Z defined in Eq. (4.24). Indeed, for the direct RF protocol the impurity is initially in the polaronic ground state  $|i_{\downarrow p}\rangle = |0_{\downarrow p}\rangle$ , while the ground state of the non-interacting  $\uparrow$  –impurity-BEC system is decoupled, i.e. in this case  $|0_{\uparrow p}\rangle = |\mathbf{p}\rangle_{\uparrow} \otimes |0\rangle$ , thus

$$Z_{\uparrow\downarrow}^{\text{directRF}} = |\langle 0|0_{\uparrow p}\rangle|^2. \tag{4.31}$$

For the inverse RF protocol the  $\downarrow$  –impurity is initially non-interacting with the bosons, and after the RF spin-flip,  $|i_{\uparrow p}\rangle = |\mathbf{p}\rangle_{\uparrow} \otimes |0\rangle$ , while the ground state of the interacting  $\uparrow$  –impurity-BEC system is the polaronic ground state  $|0_{\uparrow p}\rangle$ , leading to

$$Z_{\uparrow\downarrow}^{\text{inverseRF}} = |\langle 0_{\uparrow p} | 0 \rangle|^2.$$
(4.32)

Since the impurity degrees of freedom drop out of the problem due to the LLP transformation, in both Eqs. (4.31) and (4.32), the overlap between initial state and final ground state defined in Eq. (4.27) reduces to the overlap of the *phonon vacuum*  $|0\rangle$ and the interacting *phonon* ground state  $|0_{\uparrow p}\rangle$  (see also Sec. 4.3.5).

Although the Lehmann analysis (4.26) demonstrates the existence of an incoherent contribution to the RF signal, it does not specify its structure without additional knowledge about the many body eigenstates of the system. Interestingly, again for the particular case where one of the two internal states of the impurity is non-interacting with the BEC, the asymptotic behavior of the incoherent part of the RF is also constrained by exact relations.

This fact was demonstrated e.g. by the authors of Refs. [107, 108], by relating the high-frequency impurity RF response to the momentum distribution of the many-body system n(k). Fermi's golden rule for the RF transition rate of impurity atoms between non-interacting and interacting internal states can be expressed as the convolution[108] of the free propagator of the impurity in the non-interacting state, and its spectral function  $A(k, \omega) = -2 \text{Im}G(k, \omega)$  in the interacting state, where G is the interacting Green's function:

$$I(\omega) = \sum_{\mathbf{k}} \int d\Omega A(k,\Omega) n(\Omega) \delta(\Omega - \omega - \varepsilon_k).$$
(4.33)

Here  $n(\Omega)$  is the distribution function of the many-body environment at energy  $\Omega$ . To isolate the high frequency contribution, one can integrate the expression Eq. (4.33) by parts, and use the sum rule  $\int d\Omega A(\mathbf{k}, \Omega) n(\Omega) = n(\mathbf{k})$  [105] to obtain

$$I(\omega \to \infty) \approx \sum_{\mathbf{k}} n(\mathbf{k} \to \infty) \delta(\omega - \varepsilon_{\mathbf{k}}), \qquad (4.34)$$

where n(k) is the momentum distribution of the many-body environment of the impurity. The authors of Refs. [107, 108] considered RF spectroscopy of fermions, but in the expression above, exchange statistics only enter through n(k). Interestingly the large momenta structure of n(k), which determines the high frequency RF response, is *insensitive* to exchange statistics [109, 110] and allows us to directly generalize the argument for bosons. In particular, for large momenta n(k) displays a universal power-law tail [111, 112, 113, 110]:

$$n(\mathbf{k} \to \infty) \to C/k^4.$$
 (4.35)

This form was discovered by Tan [111, 112] who identified the "contact" C as the density of pairs of atoms, whose binary collisions are responsible for the emergence of

this universal feature. The asymptotic behavior (4.35) of the momentum distribution in turn constrains the asymptotic behavior of the RF response:

$$I(\omega \to \infty) \propto \begin{cases} C\omega^{-3/2} & \text{in } 3\text{-}D, \\ C\omega^{-2} & \text{in } 2\text{-}D, \end{cases}$$
(4.36)

leading to universal high-frequency RF tails that have been noted in various contexts for systems of interacting bosons and fermions[114, 115, 107, 110, 108].

Dimensionality of the system plays a crucial role in determining the precise form of the RF singal. For the high frequency incoherent part of the RF discussed above, different power law tails emerged in 2-*D* and 3-*D*, due to the dimensional dependence of the many-body density of states. Moreover, as discussed in Sec. 4.3.5 the quasiparticle weight, *Z*, which controls the coherent part of the RF signal, attains a finite albeit exponentially small value in 2-*D*, and 3-*D*, while it displays a characteristic infrared divergence in 1-*D*. The latter phenomenon signals the orthogonality catastrophe intrinsic to the kinematically constrained phase space of 1-*D* systems. Here, the spectrum is dominated by a power-law decay (the 1*D* generalization of the incoherent part adds a subleading  $1/\omega$  correction to the leading log-divergence):

$$I(\omega - \Delta) \approx C |\omega - \Delta|^{-\alpha}, \qquad (4.37)$$

where the exponent  $\alpha(a_{IB})$  depends on the phase shift induced by scattering of the impurity [78] and within our formalism is given by the first order Born result  $\alpha \sim n_0^2 a_{\text{IB},\uparrow}^2$ .

With this general phenomenology of the RF response in mind, we performed a detailed microscopic calculation of the time dependent overlap (3.26) by generalizing the mean-field approach to polaron ground states of Sec. 4.3 to the problem of impurity dynamics.

Figure 4.3 : RF spectra for different initial impurity interaction strengths. The quantity  $a_{\text{IB},\sigma}\sqrt{n_0\xi}$  is a dimensionless ratio between the mean free path of the impurity and the length scale over which bosons are localized (a non-interacting BEC has completely delocalized bosons). We observe that the spectral weight starts almost entirely in the coherent part of the spectrum, corresponding to a nearly free impurity, and gradually shifts to higher energies as more excitations of the BEC are generated by increasing impurity-bose interactions. The spectra presented above were obtained for an experimentally relevant mass ratio M/m of 2.5; there is a weak dependence of the spectra on mass ratio, and is not observable on the scale shown here.

#### 4.4.2 Direct RF: Transition from interacting to non-interacting state

In the direct RF measurement, the system is first adiabatically prepared in the polaronic ground state, i.e.  $|i_{\downarrow p}\rangle = |0_{\downarrow p}\rangle$ . Since the system is non-interacting in its final state, the time evolving Hamiltonian in this case is simply that of free Bogoliubov bosons,  $\mathcal{H}_b = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}$ .

We showed in Sec.4.3 that the ground state can be approximated as a product of coherent states, see Eq. (4.11), which moreover becomes exact in the case of an infinitely heavy impurity. Thus the problem of calculating the time-dependent overlap reduces to free evolution of product coherent states:

$$A_{p}(t) = \langle 0_{\uparrow p} | e^{-i\mathcal{H}_{b}t} | 0_{\uparrow p} \rangle$$
  
$$= \prod_{\mathbf{k}} \langle 0 | e^{\alpha_{\mathbf{k}}^{\mathrm{MF}} \hat{b}_{\mathbf{k}}^{\dagger} e^{-i\omega_{\mathbf{k}}t} - (\alpha_{\mathbf{k}}^{\mathrm{MF}})^{*} \hat{b}_{\mathbf{k}} e^{i\omega_{\mathbf{k}}t}} | 0 \rangle, \qquad (4.38)$$

with  $\alpha_{\mathbf{k}}^{\text{MF}}$  obtained from solving Eq. (4.13); in the limit of a localized impurity with  $M \to \infty, \, \alpha_{\mathbf{k}} \to -\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}$ , and there one obtains the exact solution to the time dependent overlap.

We find that the overlap amplitude decays quickly from unity to an exponentially small limiting value with an oscillatory envelope:

$$A_{p}(t \to \infty) \to Ze^{-i\Delta t}, \quad \Delta = \Delta_{1} + \Delta_{2},$$

$$Z = \exp\left[-\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2}}{\left(\omega_{\mathbf{k}} + \frac{k^{2}}{2M} - \frac{\mathbf{p}\cdot\mathbf{k}}{M^{*}}\right)^{2}}\right],$$

$$\Delta_{1} = \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2}}{\left(\omega_{\mathbf{k}} + \frac{k^{2}}{2M} - \frac{\mathbf{p}\cdot\mathbf{k}}{M^{*}}\right)^{2}} + \frac{2\pi}{\mu}n_{0}a_{\mathrm{IB},\sigma},$$

$$\Delta_{2} = \frac{p^{2}}{2M}\left(1 - \frac{M}{M^{*}}\right) \qquad (4.39)$$

Here Z is the quasiparticle residue defined in Eq. (4.24), and is in agreement with the general analysis of Sec. 4.4.1.  $\Delta$  denotes the energy difference between interacting

and non-interacting ground states, and consists of two contributions:  $\Delta_1$  includes the "mean-field" shift due to the interaction of impurity with the static BEC ground state, and the finite momentum generalization of the binding energy defined in Eq. (4.14), and  $\Delta_2$  which accounts for the change in effective mass of the impurity. As in the ground state case, the (generalized) binding energy was regularized as described in Appendix A.

The RF absorption spectrum can be simply obtained by Fourier transforming Eq. (4.38). We present a few sample spectra in Fig. 4.3. The RF absorption spectrum of the impurity contains a coherent and incoherent contribution as expected from the general analysis presented in Sec. 4.4.1

$$I(p,\omega) = I_{\rm coh}(p,\omega) + I_{\rm incoh}(p,\omega).$$

The coherent peak is determined entirely by the long time limit of Eq. (4.38) which is the quasiparticle residue defined in Eq. (4.24).

$$I_{\rm coh}(p,\omega-\Delta) = Z\delta(\omega-\Delta), \qquad (4.40)$$

with  $\Delta$  defined in Eq. (4.39)

The spectrum contains additionally a broad incoherent part corresponding to the short time dynamics of polaron destruction due to excitations generated when the impurity-BEC interactions are removed in the course of the direct RF:

$$I_{\rm incoh}(p,\omega-\Delta) = \frac{{\rm Re}}{\pi} \int_{0}^{\infty} dt' e^{i(\omega-\Delta)t} \left(A_p(t)e^{i\Delta t} - Z\right).$$
(4.41)

For concreteness, we present the leading high and low frequency behavior of the RF spectrum in the exactly solvable case of a localized impurity; it is straighforward but tedious to obtain identical results for mobile impurities. By expanding the exponential
in Eq. (4.41) to leading order, we can approximate Eq. (4.41) using

$$I_{\rm incoh}(\omega - \Delta) \approx \operatorname{Re} \frac{Z}{\pi} \int_{0}^{\infty} dt e^{i(\omega - \Delta)t} \sum_{\mathbf{k}} \left| \frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right|^{2} e^{-i\omega_{\mathbf{k}}t}$$
$$= Z \sum_{\mathbf{k}} \left| \frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right|^{2} \delta(\omega - \Delta - \omega_{\mathbf{k}})$$
$$= Z \int \frac{d\Omega}{2\pi^{2}} \frac{(\sqrt{2\Omega^{2} + 1} - 1)^{d/2}}{\Omega^{2}\sqrt{2\Omega^{2} + 1}} \delta(\omega - \Delta - \Omega)$$
$$= \frac{Z}{2\pi^{2}} \frac{(\sqrt{2(\omega - \Delta)^{2} + 1} - 1)^{d/2}}{(\omega - \Delta)^{2}\sqrt{2(\omega - \Delta)^{2} + 1}}.$$
(4.42)

Thus we find the following limiting behaviors of the incoherent RF response:

$$I_{\rm incoh}\left(\omega - \Delta \gg \frac{c}{\xi}\right) \propto \begin{cases} (\omega - \Delta)^{-3/2}, & \text{in } 3\text{-}D.\\ (\omega - \Delta)^{-2} & \text{in } 2\text{-}D, \end{cases}$$

$$I_{\rm incoh}\left(\omega - \Delta \ll \frac{c}{\xi}\right) \propto \begin{cases} (\omega - \Delta), & \text{in } 3\text{-}D. \end{cases}$$

$$(4.43)$$

$$I_{\rm incoh}\left(\omega - \Delta \ll \frac{c}{\xi}\right) \propto \begin{cases} (\alpha - \Delta)^2 & \text{in } 2-D. \end{cases}$$

$$(4.44)$$

We see that the high frequency tails of the RF spectra in Eqs. (4.41)-(4.43) are in agreement with the general functional form required by Eq. (4.36). This provides a non-trivial consistency check to our microscopic approach. We now generalize our approach to consider the more complicated dynamics involved in the inverse RF measurement.

#### 4.4.3 Inverse RF: Transition from noninteracting to interacting state

In the inverse RF measurement impurities are transferred from an initially noninteracting state to an interacting state, with  $a_{\text{IB},\uparrow}$  finite and  $a_{\text{IB},\downarrow} \approx 0$ . We again consider the time dependent overlap (3.26), but the associated dynamics cannot be reduced to free evolution as in the direct RF in Sec. 4.4.2. However, the case of the localized impurity is once again amenable to an exact solution, and inspires an approximate treatment of the mobile impurity.

#### Dynamics of a localized impurity

Like the ground state of the localized impurity-BEC system, the time evolving wavefunction of the system is also a product of coherent states, but with *time dependent* parameters.

The initial free Hamiltonian  $\mathcal{H}_b$  is modified after the switch on of interactions to  $\mathcal{H}_b + \mathcal{H}_{int}$ . Crucially, the two Hamiltonians are related by a canonical transformation. We introduce the displacement operators  $D(\alpha) = e^{\sum_{\mathbf{k}} (\alpha_{\mathbf{k}} \hat{b}^{\dagger}_{\mathbf{k}} - \alpha^{*}_{\mathbf{k}} \hat{b}_{\mathbf{k}})}$  which shift the mode operators

$$D^{-1}(\alpha)\hat{b}_{\mathbf{k}}D(\alpha) = \hat{b}_{\mathbf{k}} + \alpha_{\mathbf{k}}.$$

Then, for the appropriate choice of shift  $\alpha_{\mathbf{k}} = \frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}$ , we find  $D^{-1}(\mathcal{H}_b + \mathcal{H}_{\text{int}})D = \mathcal{H}_b + \Delta$ , with  $\Delta$  a constant number. Thus we can directly solve the time-evolution of the initial state using the displacement operators as follows:

$$\begin{aligned} |\phi_{M\to\infty}(t)\rangle &= e^{i(\mathcal{H}_b + \mathcal{H}_{\rm int})t}|0\rangle \\ &= e^{-i\Delta t}D^{-1}\left(\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right)e^{iH_b t}D\left(\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right)|0\rangle \\ &= e^{-i\Delta t}\prod_{\mathbf{k}}e^{\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}(\hat{b}_{\mathbf{k}} - \hat{b}_{\mathbf{k}}^{\dagger})}e^{\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}(\hat{b}_{\mathbf{k}}^{\dagger} e^{-i\omega_{\mathbf{k}}t} - \hat{b}_{\mathbf{k}}e^{i\omega_{\mathbf{k}}t})}|0\rangle, \end{aligned}$$

leading to an expression for the wavefunction of the form:

$$|\phi_{M\to\infty}(t)\rangle = e^{-\Psi(t)-i\Delta t} \prod_{\mathbf{k}} e^{\frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}}(e^{-i\omega_{\mathbf{k}}t}-1)b_{\mathbf{k}}^{\dagger}}|0\rangle, \qquad (4.45)$$

with

$$\Psi(t) \equiv \sum_{\mathbf{k}} \left| \frac{V_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right|^2 (1 - e^{-i\omega_{\mathbf{k}}t}), \ \Delta \equiv \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} + \frac{2\pi}{\mu} a_{\mathrm{IB},\downarrow} n_0.$$

#### Dynamics of a finite mass impurity

Inspired by the exact time evolving wavefunction of the localized impurity-BEC system, a product of time dependent coherent states, we make an analogous ansatz for finite mass impurity-BEC system:

$$|\phi(t)\rangle = e^{-i\chi(t)} e^{\sum_{\mathbf{k}} \alpha_{\mathbf{k}}(t)\hat{b}_{\mathbf{k}}^{\dagger} - \frac{1}{2}|\alpha_{\mathbf{k}}(t)|^{2}}|0\rangle.$$
(4.46)

The variational wavefunction (4.46) represents a mean-field approach to dynamics: the wavefunction factorizes for individual phonons, so each phonon indexed by momentum  $\mathbf{k}$  evolves in an effective time-dependent oscillator Hamiltonian, whose frequency  $\omega_{\mathbf{k}}(t)$  is renormalized by the other phonon modes.

Projecting the Schrödinger equation onto the variational state (4.11) (see e.g. [116, 117]) we obtain equations of motion for the variational coherent state parameters:

$$\dot{\chi}(t) = \frac{p^2}{2M} - \sum_{\mathbf{k},\mathbf{k}'} \frac{\mathbf{k}.\mathbf{k}'}{2M} |\alpha_{\mathbf{k}}|^2 |\alpha_{\mathbf{k}'}|^2 + \frac{1}{2} \sum_{\mathbf{k}} V_{\mathbf{k}}(\alpha_{\mathbf{k}} + \alpha_{\mathbf{k}}^*),$$

$$i\dot{\alpha}_{\mathbf{k}}(t) = \left(\Omega_{\mathbf{k}} - \frac{\mathbf{p}.\mathbf{k}}{M} + \frac{\mathbf{k}}{M} \cdot \sum_{\mathbf{k}'} \mathbf{k}' |\alpha_{\mathbf{k}'}(t)|^2\right) \alpha_{\mathbf{k}}(t) + V_{\mathbf{k}},$$

$$(4.47)$$

with  $\Omega_{\mathbf{k}} = \omega_{\mathbf{k}} + \frac{k^2}{2M}$ .

We solved the differential Eq. (4.47) numerically using a standard computational package <sup>†</sup>. We found that the inverse RF spectrum is qualitatively quite similar to the direct RF spectrum calculated in the previous subsection. In light of the general phenomenology of RF responses presented in Sec. 4.4.1, the similarity between the two

<sup>&</sup>lt;sup>†</sup>Solutions of Eqs. (4.47) are naively UV divergent. Imposing a sharp cut-off gives rise to unphysical oscillations at the cut-of frequency. To avoid this problem we introduced a soft cut-off  $V_k \rightarrow V_k e^{-k^2/2\Lambda^2}$ , choosing  $\Lambda$  large enough to obtain converged results for relevant observables.

RF spectra is not surprising, since both involve transitions between interacting and non-interacting impurity-BEC states, which constrains the high and low frequency parts of the RF response.

#### Dynamical ansatz as optimal estimate of time-dependent overlap

Here we demonstrate that the time-dependent mean-field approach, which is tailored to solve the *general* dynamics of the interacting Hamiltonian, gives a good semiclassical approximation to the specific propagation amplitude in Eq. (3.26). Using the LLP transformation, this amplitude can be written as

$$A_{p}(t) = \langle i_{\uparrow p} | e^{-i\mathcal{H}t} | i_{\uparrow p} \rangle = \langle 0 | e^{-i\mathcal{H}t} | 0 \rangle$$

$$= \langle 0 | e^{-i\left[\frac{1}{2M}\left(p - \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}\right)^{2} + \sum_{\mathbf{k}} (\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + V_{\mathbf{k}} (\hat{b}_{\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}}))\right]^{t} | 0 \rangle,$$

$$(4.48)$$

where the phonon vacuum  $|0\rangle$ , is time evolved by the Hamiltonian (4.9) for a given time t, and the overlap of the resulting state is measured with respect to the initial vacuum.

As an alternative approach to calcuating such a propagation amplitude, we may formulate Eq. (4.48) as a path integral, i.e. a sum over configurations of the semiclassical velocity profile of the impurity, and compare the mean-field ansatz with the saddle point of such a path integral (see Appendix B for more details).

We obtain the path integral formulation by introducing into the time-dependent overlap (4.48) a classical field  $\varphi(t)$ , corresponding to the fluctuating impurity velocity. This is justified by the Hubbard-Stratonovich (HS) identity, which is typically used in equilbrium quantum field theory to decouple interacting systems by using a random variable to mimic fluctuations of the system. In a similar spirit, we use  $\varphi(t)$  to decouple the interaction between bosons in Eq. (4.48) and introduce a corresponding path integral to sum over all configurations of  $\varphi(t)$ :

$$A_{p}(t) = \int \mathcal{D}[\varphi(t)] e^{i \int_{0}^{t} dt' \frac{M}{2} \varphi(t')^{2}}$$

$$\times \quad \langle 0| e^{-i \int_{0}^{t} dt' \left[\varphi(t') \cdot \left(p - \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}\right) - \sum_{\mathbf{k}} (\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + V_{\mathbf{k}} (\hat{b}_{\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}})) \right]} |0\rangle.$$

$$(4.49)$$

As seen above, the HS decoupling reduces the originally interacting bosonic Hamiltonian to a quadratic form, allowing us to integrate out the bosons exactly. We may then approximate the resulting path integral, now over  $\varphi(t)$  alone, by a saddle point treatment:

$$\varphi_{s}(t') = \frac{\mathbf{p}}{M} + \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2} \mathbf{k}}{M} \int_{t'}^{t} dt_{1} \int_{0}^{t'} dt_{2} \times e^{-i \int_{t_{2}}^{t_{1}} dt'' (\omega_{\mathbf{k}} - \mathbf{k}.\varphi_{s}(t''))}.$$
(4.50)

The details of our derivation of Eq. (4.49) and its saddle point Eq. (4.50) are provided in Appendix B. Our saddle point approximation yields an optimal  $\varphi_s(t)$ , shown in Fig. 4.4, which we can then use to evaluate the time-dependent overlap Eq. (4.48). We checked that this approach is in agreement with the results of the time-dependent mean-field analysis, but at significantly greater numerical effort.

Thus we conclude that the mean-field ansatz for the dynamics of the impurity, optimally estimates the RF response. In the remainder we present the main features of the dynamical mean-field solution.

#### Inverse RF and non-equilbrium dynamics

Although the prominent features of the RF spectrum appear identical for the direct and inverse RF there are differences in the details: both measurements involve Hamiltonian evolution of a non-eigenstate (see Eq. (3.26)), however the inverse measurement involves more complicated dynamics compared to the direct RF; the dynamics of the latter are trivially determined by a non-interacting Hamiltonian (see Sec. 4.4.2). However, due to the strong impurity renormalization by BEC interactions, the complicated non-equilibrium dynamics of the impurity do not manifest in spectra, which are enveloped by the exponentially small spectral weight Z (see Eq. (4.41)).

Fortunately our dynamical mean field solution Eq. (4.47) approximates the full time dependence of the system and can be used to study observables beyond the RF spectrum.

We studied the time-evolution of the momentum of the impurity, following the abrupt switch on of interactions. The results plotted in Fig. 4.5 show how the impurity relaxes to a steady state at long times. For weak interactions, the impurity loses a small portion of its momentum to the bosonic bath, corresponding to a minimally dressed polaron with large quasiparticle weight. The steady state momentum of the impurity decreases rapidly with interactions which we interpret as the onset of strong dressing and a reduction in quasi-particle weight. We also point out a surprising feature emerging at strong interactions – decaying oscillations in the impurity momentum. We conjecture that quenching the impurity interaction to large values excites a long lived internal excitation of the emergent polaron; unfortunately no signature of this phenomenon manifests in the RF spectrum due to exponential suppression of weight for strong interactions, but it would be interesting to study this behavior in an experiment directly probing the non-equilibrium dynamics of the impurity, e.g. exciting the internal structure of the polaron by resonantly driving it in a trap. Note that such transient oscillations in the relaxation dynamics of impuritybath systems appears to be a generic phenomenon and have been observed previously, e.g. Ref. [118, 119]

We emphasize that although the coherent peak of the RF spectrum is characterized

by the ground state of the interacting impurity-BEC system (see Sec. 4.4.1), the steady-state reached by the impurity following a sudden switch on is *different* from the interacting ground state. This can be seen formally by taking the long-time limit of the expectation value of an arbitrary observable  $\hat{O}$ . Performing a spectral decomposition of this quantity highlights the appropriate ensemble description of the steady state of the system:

$$\lim_{t \to \infty} \langle i_{\uparrow p} | \hat{O}(t) | i_{\uparrow p} \rangle \to \sum_{n} | \langle i_{\uparrow p} | n_{\uparrow p} \rangle |^2 \langle n_{\uparrow p} | \hat{O} | n_{\uparrow p} \rangle, \qquad (4.51)$$

The right hand side expressed in terms of  $|n_{\uparrow p}\rangle$ , the time-independent eigenstates of the final Hamiltonian, represents the Diagonal Ensemble which characterizes the long time behavior of a generic closed quantum system [7]. Clearly the steady state of the system is different from its ground state and is in fact an ensemble which includes the ground state, but also contains additional excitations.

Within our formalism we approximate the dynamics of the system using a time dependent product of coherent states. We expect that such an approximation can also capture the long-time steady state expectation value of operators, i.e. the long time limit of the coherent state product approaches Eq. (4.51). We found strong evidence of this fact; we plotted in Fig. 4.6 the steady state (SS) and ground state (GS) group velocity of the impurity defined as:

$$v_{\rm SS,GS} = \frac{p_{\rm SS,GS}}{M},\tag{4.52}$$

where the steady-state value of the impurity velocity was calculated using the long time limit of our coherent state product Eq. (4.46), while the ground state value was calculated using Eq. (4.11). We observe a quantitative difference between the two quantities. The quasiparticle residue Z (see Eq. (4.24)) on the other hand is approximately equal (difference typically less than 1 part in  $10^6$  for many different parameters) when calculated using the two states. This supports the picture of the impurity steady-state we put forward in Eq. (4.51), and is also consistent with the general argument about the coherent peak of the RF response presented in Sec. 4.4.1

### 4.5 Conclusions and Outlook

We studied the fate of quantum impurities in BECs, and discussed the manifestation of polaron physics in RF spectroscopy. Population imbalanced dilute mixtures of degenerate ultracold atoms, either Bose-Fermi[30, 31, 32, 33, 34, 35] or Bose-Bose[36, 37, 38, 39, 40, 41] mixtures, in which the role of the majority many-body environment is played by bosons, are the ideal settings in which to explore this rich physics. We require sufficiently low temperatures for which the bosonic environment will condense and can be modelled as a weakly interacting BEC. Crucially the atoms playing the role of quantum impurities should have hyperfine structure which can typically be addressed by RF pulses, and we require control over the interactions between impurity in different hyperfine levels and BEC. Ideally one of the hyperfine levels should be weakly interacting with the BEC, which will allow the faithful realization of the predictions in our article.

Experiments are always done at low, but finite temperature, while our approach models the system at zero temperature. We expect the zero-temperature approximation to be quite reasonable for a Bose gas well below the transition temperature  $(T \ll T_c)$ , since in this regime the number of thermal excitations scales as  $\propto T^4$ [84], and corrections to equilbrium properties of the impurity-Bose system will be vanishingly small. Additionally we expect impurity dynamics to only be modified at long times on the order  $t \gtrsim \hbar/T$ , as was seen in e.g. Ref. [78]. Thus for  $T \ll T_c$  all the relevant phenomena reported in the present chapter will be observable at shorter, experimentally accessible time scales. The inverse of the time scale also sets a resolution limit on the spectral properties of the impurity, which can be interpreted as the characteristic scale of thermal broadening of sharp features such as the polaronic peak.

The modest requirements discussed above are attainable using currently available experimental systems and techniques, thus we expect that our predictions can be tested in the near future. We consider a few particularly relevant experiments below.

#### 4.5.1 Relation to experimental systems

Bose-Bose mixtures of Rb<sup>87</sup>-K<sup>41</sup> [37, 39] and Rb<sup>87</sup>-Cs<sup>133</sup> [38, 41], as well as the Bose-Fermi mixture of Na<sup>23</sup>-K<sup>40</sup>[35], are promising candidates in which to realize the polaronic physics of heavy impurities in BECs. In the three systems considered the heavy impurities, respectively Rb<sup>87</sup>, Cs<sup>133</sup>, K<sup>40</sup>, have intrinsic mass ratio  $M/m \approx 2$  with respect to the BEC atoms, which can be further enhanced by a state-selective optical lattice. Moreover all of the experimental systems satisfy the criteria outlined previously: low temperatures sufficient to achieve BEC are routinely attained, atoms can be reliably trapped, inter-atom interactions can be tuned via carefully mapped out Feshbach resonances, and impurity atoms have hyperfine levels which can be addressed using RF. To quantify the impurity-BEC interactions which can be attained in these systems, we define a dimensionless ratio,  $g_{\text{eff}} = \xi n_0 a_{IB}^2$ , between the average correlation length of the BEC ~  $\xi$  to the mean-free path of the impurity ~  $1/(n_0 a_{IB}^2)$ . We find that for the systems considered, intermediate interactions up to  $g_{\text{eff}} \approx 2 - 3$ can be attained using resonant tuning of scattering lengths, while ensuring the condition Eq. (4.6) for the validity of our theoretical approach is satisfied.

#### 4.5.2 Related problems

Our treatment in the present chapter missed aspects of strong coupling physics near a Feshbach resonance which are experimentally accessible, and theoretically rich. Given the possibility to form bound molecules for large positive impurity-boson interactions, it is quite possible that the system admits a polaron to molecule phase transition – this is especially pertinent, given the impossibility of quantum phase transitions in Fröhlich type models, and thus will clearly involve physics beyond such a model. Moreover, as a more non-trivial probe of the rich phase diagram afforded by the impurity-BEC system, it would be interesting to study the decay of the attractive polaron into the "true" molecular ground state of the system.

The dynamics of polaron formation, and internal excitation structure of polarons are relatively unexplored areas of research. Indeed, within our current framework we observed coherent oscillations in the course of the relaxation of the impurity into a polaronic state (see Fig. 4.5), which we interpreted as signatures of the internal structure of the polaron. It would be worthwhile devising a more elaborate theoretical description of the internal structure of the polaron, which may be probed in an experiment by resonantly driving the impurity-BEC system, and could shed light on the dynamics of polaron formation. One can also consider other non-trivial probes of polaron dynamics, such as the effect of driving Bloch oscillations of lattice impurities [120]. Such a scenario is particularly exciting as it is experimentally feasible using optical lattices.

Figure 4.4 : (a) Real part of the (rescaled) solution of saddle point Eq. (4.50) plotted for  $m_r = 75.0, \sqrt{n_0\xi}a_{\mathrm{IB},\sigma} = .25, p/Mc = .6$ ; we obtained a family of trajectories parameterized by  $t_{\mathrm{f}}$ , the total propagation time for which the amplitude Eq. (4.48) was required. Each individual trajectory is a time-evolving function of  $t < t_{\mathrm{f}}$ , and can be interpreted (after rescaling) as the time-dependent momentum of the impurity. Note the symmetry of the saddle point trajectories around  $t = t_{\mathrm{f}}/2$ , which arises because they optimize Eq. (4.48), the amplitude for a time-evolving state to return to its initial value. This is in contrast to the time-dependent mean-field solution which simply propagates forward to the steady state at time  $t_{\mathrm{f}}$  (c.f. Fig. 4.5). (b) Imaginary part of the saddle point trajectories are shown for the same parameters. The imaginary part shares the symmetry property of the real part, but is typically smaller in magnitude. While it does not lend itself to direct interpretation as the physical momentum of the impurity, it is necessary to properly optimize the propagation amplitude when expressed as a path integral Eq. (4.49).

Figure 4.5: Impurity momentum as a function of t after switching on interactions. Strong interactions lead to small asymptotic impurity momentum (corresponding to heavy effective mass). Additionally the momentum develops decaying oscillations associated with internal mode of the polaron.

Figure 4.6 : (Color online) The asymptotic velocity attained by the impurity as a function of impurity-BEC interaction  $a_{\rm IB}$ , for a given initial momentum in the non-equilibrium steady-state (NESS, solid red) and the ground state (GS, dashed black).

# Chapter 5

# Impurity in a Fermionic bath

### 5.1 Introduction

In this final chapter treating impurity models in the context of cold atoms, localized impurities in a Fermi gas are considered. It is shown how the techniques of atomic physics can be used to explore new regimes and manifestations of Anderson's orthogonality catastrophe (OC), which could not be accessed in solid-state systems. To supplement the exact technique described in Chapter 3, here an alternate "phenomenological" calculation is presented, which relies on exploiting the "hidden" one-dimensional structure of the problem.

## 5.2 Physics of OC in cold atoms

How can we use currently available experimental tools of ultracold atoms to study several key aspects of the problem of the orthogonality catastrophe (OC) in manybody fermionic systems? The core of this problem is understanding the response of a Fermi gas to a suddenly introduced impurity. This question was originally considered in the context of the X-ray absorption spectra in metals [77].

As discussed in Chapter 4, we consider a quantum degenerate mixture of two types of atoms, e.g. a Bose-Fermi mixture or a Fermi-Fermi mixture. We assume that one type of atom has a much lower density than the other and we will refer to it as an impurity atom. We always take the majority atoms, which we call host atoms, as fermionic. Two types of atoms can have very different polarizability hence it is possible to apply an optical lattice that provides a strong trapping potential for impurity atoms while it has very little effect on the host fermions. The hyperfine spin states of impurity atoms can be manipulated using RF fields, which allows to switch between weakly and strongly interacting states with respect to host fermions and thus introduce time dependent impurities in the Fermi gas [57, 56].

In ultracold atoms one can perform measurements of OC in frequency domain by doing RF spectroscopy on impurity atoms. However, as we discuss below, it is also illuminating to measure S(t) in time domain using Ramsey type interference. The idea of the proposed experiment is as follows: initially, the impurity is in the down-state  $|\downarrow\rangle$ , and the fermions are in the ground state  $|\psi_0\rangle$ . Then, the Ramsey interferometry is performed: at time t = 0, a  $\pi/2$  pulse is applied, such that the system is driven into the superposition state  $\frac{|\downarrow\rangle+|\uparrow\rangle}{\sqrt{2}} \otimes |\psi_0\rangle$ . The two states evolve differently since they have different evolution with the Fermi sea:

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}|\downarrow\rangle \otimes e^{-i\hat{H}_i t}|\psi_0\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle \otimes e^{-i\hat{H}_f t}|\psi_0\rangle.$$
(5.1)

The fermions stay undisturbed in the first state, while the impurity scattering excites multiple electron-hole pairs in the state entangled with the  $|\uparrow\rangle$  spin state. Performing a second  $\pi/2$  pulse after time t, and measuring  $\langle \Psi(t)|\hat{S}_x|\Psi(t)\rangle$  gives:

$$\langle \hat{S}_x(t) \rangle = \operatorname{Re} \langle \psi_0 | e^{i\hat{H}_i t} e^{-i\hat{H}_f t} | \psi_0 \rangle = \operatorname{Re} S(t)$$

In the equation above we neglected the trivial phase factor arising from the energy difference of states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . Thus, the Ramsey interferometry provides a direct measurement of the OC overlap. One can also use the Hahn spin echo, as well as more complicated spin-echo-type sequences, to create processes in which the impurity switches between different states multiple times. As we show below the response of

the Fermi gas to such processes is characterized by a power-law decay of the overlap, with an exponent *enhanced* compared to the case of usual OC.

The predicted faster decay of the spin-echo response goes against the atomic physics intuition; it stems from the fact that the spin-echo sequence does not "undo" the evolution of the Fermi gas under impurity scattering, but instead, creates a state in which the impurity pseudospin and Fermi gas are strongly entangled. From the experimental point of view spin echo experiments should have an additional advantage that they allow to cancel slow fluctuations of the magnetic field.

What are the new universal characteristics that one can find in S(t) (or in the corresponding absorption spectra  $S(\omega)$  at intermediate time scales? One feature is oscillations of S(t) on the timescale  $\hbar E_F^{-1}$  on the attractive side of the Feshbach resonance. These oscillations give rise to a cusp in the absorption spectrum at energy  $E_F$  above the absorption threshold. The origin of this feature is a singularity in the density of states at the band bottom in one dimension (OC is essentially a 1D problem since only s-wave scattering is important). This provides an interesting connection to the problem of "beyond Luttinger liquid" physics in 1D (see Ref. [83] for a review). As the Feshbach resonance is approached from the attractive side  $(k_F a \rightarrow -\infty)$ , the cusp develops into a true singularity with universal exponent 1/4, but the peak is finite for any finite value of  $k_F a$  with a characteristic shape described by a universal function, see Eq. (5.18). We note that the many-body response considered here, namely  $S(\omega)$ , is somewhat unique for ultracold atoms in the vicinity of a Feshbach resonance, since it shows a singular response only exactly at the resonance. In conventional BCS-BEC studies ?, most of the measured quantities change only smoothly across the crossover region  $(-1 \le k_F a \le 1)$  and do not show any singularity exactly at the resonance.

We emphasize, that the universal response coming from the bottom of the band

is a unique feature of ultracold spinless fermions, and makes it possible to investigate universal phenomena which generically take place in 1D systems [83] using 3D atomic clouds. Indeed, the universal behavior coming from the excitations in the vicinity of the Fermi surfaces is ubiquitous in solid state systems, and is controlled by Fermi liquid theory. On the other hand, away from the Fermi surface fermionic quasiparticles are not well defined in 3D interacting systems, and thus bottom of the band contributions to the orthogonality catastrophe cannot be probed in solid state systems. For spinless fermions, bottom of the band contributions are well defined, since interactions between atoms in the s-wave channel are absent, thus fermionic excitations are well defined for all energies. Experiments with ultracold atoms also provide an opportunity to quantitatively test the breakdown of the notion of the Fermi liquid quasiparticle away from Fermi surface when weak interactions between fermions are introduced (e.g. via p-wave channel or by studying a spin-1/2 mixture).

On the repulsive (a > 0) side, a bound state of energy

$$E_b = -\frac{\hbar^2}{2ma^2} \tag{5.2}$$

separates from the bottom of the band and a true edge of support corresponds to this bound state being occupied [?]. Another singularity at energy larger by  $E_F - E_b$ corresponds to this bound state being empty. Since the system at this energy is adiabatically connected to a true threshold on the attractive side, we will continue to call it a threshold on the repulsive side as well. The bottom of the band cusp also survives on the attractive side close to the resonance, leading to a characteristic three peak structure.

Furthermore, OC experiments with ultracold atoms should make it possible to study quantum variables that are not accessible in electron systems. For example, full energy of an interacting many-body system can be measured [282, 253]. Several experiments with ultracold atoms demonstrated that it is possible to measure not only the average values but also fluctuations of quantum observables [196, 290]. In some cases even full distribution functions have been obtained [291]. In the quantum impurity system, following the impurity potential quench the system will not be in an energy eigenstate and the full distribution function of the total energy should also exhibit power-law type singularities. Full counting statistics of scattering processes should also provide an intriguing connection to an extensive theoretical research in mesoscopic physics, which however was notoriously difficult to study in experiments in solid state systems. The intriguing new feature of experiments with ultracold atoms is that full counting statistics can be measured for fermions in specific energy windows rather than in the whole energy range.

These interesting features can be captured by the approach described in Chapter. 3, where first the single particle problem interacting with a local scatterer is solved, and the solution used to evaluate many-particle states and correlators. However such a calculation represents a brute force approach, and in order to gain further insight into the results, as well as to predict asymptotics beyond numerical accuracy, a more phenomenological approach is described below.

## 5.3 Exponents of response at threshold singularities

In the previous section, we saw that the response of the Fermi gas to an impurity displays characteristic threshold singularities. Here we provide a more microscopic account of the origin of these singularities: the first threshold corresponds to the energy difference between the ground states in the presence and absence of the impurity. There are additional thresholds, shadow bands, corresponding to final states with excitations of particles from the bottom of the Fermi sea to just above the Fermi level followed by the usual shake-up for the Fermi sea manifested by the creation of many low energy particle-hole pairs. The energy associated with the  $n + 1^{th}$  threshold, with  $n \ge 0$ , is given by

$$\omega_n = \Delta E + nE_F,$$
  
$$\Delta E = -\int_0^{E_F} \frac{d\xi}{\pi} \delta(\xi),$$
 (5.3)

where  $\Delta E$ , the shift in ground state energy due to the presence of the impurity is given in terms of the phase shift  $\delta(\xi)$  of the state with energy  $\xi$ , due to the impurity, and  $E_F$  is the Fermi energy corresponding to the energy cost of promoting a particle from the bottom of the band E = 0 to the Fermi level.

In order to characterize these singularities carefully, our strategy will be to exploit the hidden one-dimensionality of the localized impurity in the Fermi gas. Our model essentially treats the impurity as a structureless local scatterer. Thus all the scattering physics occurs solely in the *s*-wave channel of the Fermi gas. Since the radial wave functions of states in this channel obey a 1D Schrödinger equation (albeit with modified boundary conditions), in the spirit of Ref. [82, 206] we will map the fermions in this channel onto the Luttinger liquid, the 1D Fermi gas, with appropriate boundary conditions (see e.g. Ref. [206] for details).

With this mapping in place, we will freely use the well developed field theoretical toolset available in 1D, namely bosonization [206, 82]

#### 5.3.1 X-ray edge exponent

First we show how we obtain the conventional X-ray edge exponent, i.e. the power law of the response at the first threshold  $\omega_0 = \Delta E$ . Let us notate annihilation operators for the electrons near the Fermi level  $\psi(x)$ , and the impurity d(x). We can write the following Hamiltonian describing their dynamics:

$$H_0 = -\int dx i v_F \psi^{\dagger}(x) \partial_x \psi(x),$$
  
$$H_{\rm int} = \int dx V_0 \delta(x) d^{\dagger}(x) d(x) \psi^{\dagger}(x) \psi(x),$$
 (5.4)

where the scattering potential  $V_0$  due to the impurity is characterized by the scattering length *a*. We proceed by bosonizing [206] the conduction electrons near the Fermi level using

$$\psi(x) \propto e^{i\phi(x)},\tag{5.5}$$

with

$$[\phi(x'), \phi(x)] = i\pi \operatorname{Sign}(x - x'). \tag{5.6}$$

We may remove the term representing the interaction between  $\psi$ , d entirely by applying the rotation

$$U = e^{i \int dx \frac{\delta_F}{\pi} \phi(x) d^{\dagger}(x) d(x)}.$$
(5.7)

We can convince ourselves by comparing the effect of the transformation on the electron operator that  $\delta_F$  is indeed the phase picked up by the electrons near the Fermi level due to scattering off the impurity, which we know from the solution of the one-body problem is  $\delta_F$ =-tan<sup>-1</sup>( $k_F a$ ).

Thus the propagator we need can be obtained using

$$S(t) = e^{-i\Delta Et} \langle d^{\dagger}(0,t)d(0,0) \rangle_{H_0+H_{\text{int}}}$$

$$= \langle U^{\dagger}d^{\dagger}(0,t)UU^{\dagger}d(0,0)U \rangle_{H_0}$$

$$= e^{-i\Delta Et} \langle d^{\dagger}de^{-i\frac{\delta_F}{\pi}\phi(0,t)}e^{i\frac{\delta_F}{\pi}\phi(0,0)} \rangle_{H_0}$$

$$= Ce^{-i\Delta Et}e^{-\frac{\delta_F^2}{2\pi^2}\langle(\phi(0,t)-\phi(0,0))^2\rangle}$$

$$= Ce^{-i\Delta Et}(iE_Ft+0)^{-\frac{\delta_F^2}{\pi^2}}, \qquad (5.8)$$

where we have used the conservation of impurity number  $\langle d^{\dagger}d \rangle = 1$  since the impurity does not have dynamics. The prefactor *C* is beyond the scope of field theory alone and will be discussed below. The RF response e.g. can be obtained via the Fourier transform of the correlator above

$$S(\omega - \omega_0) = C \int dt e^{i(\omega - \omega_0)t} (iE_F t + 0)^{-\frac{\delta_F^2}{\pi^2}} = \frac{2\pi C\theta(\omega - \omega_0)}{\Gamma\left(\frac{\delta_F^2}{\pi^2}\right)} |\omega - \omega_0|^{\frac{\delta_F^2}{\pi^2} - 1}$$
(5.9)

#### 5.3.2 Exponents in the the presence of bound state

The delta potential for attractive scattering length a > 0 admits a bound state of energy  $-\frac{1}{a^2}$ . In this case there will be two thresholds one at the usual edge, and the other corresponding to the bound state energy i.e.

$$\omega_0 = \Delta E, \quad \omega_b = \Delta E + E_F - E_b, \quad E_b = -1/a^2.$$
(5.10)

#### Threshold singularities

The exponent of the singularity in the response at  $\omega_0$  will be the usual one i.e.

$$S(\omega - \omega_0) = \frac{2\pi C\theta(\omega - \omega_0)}{\Gamma\left(\frac{\delta_F^2}{\pi^2}\right)} |\omega - \omega_0|^{\delta_F^2/\pi^2 - 1},$$
(5.11)

but when the bound state is present, the scattering phase shift at the Fermi level is modified. We may simply replace the phase shift at the Fermi level in the absence of a bound state  $\frac{\delta_F}{\pi}$ , with  $\frac{\delta_F}{\pi} + 1$ . This is consistent with the fact that the bound state induces an additional  $\pi$  scattering phase shift (see e.g. *Quantum Mechanics Sec. 133, pg. 557*). Since we put the phase shift into the bosonization calculation by hand, we can correctly predict threshold exponents in vicinity of  $\omega_b$  as

$$S(\omega - \omega_b) = \frac{2\pi C_b \theta(\omega - \omega_b)}{\Gamma\left(\left(1 + \frac{\delta_F}{\pi}\right)^2\right)} |\omega - \omega_b|^{\left(1 + \frac{\delta_F}{\pi}\right)^2 - 1}.$$
(5.12)

#### 5.3.3 Exponents due to the bottom of band effect

Numerical results in [78] indicate that a strong peak develops at the energy corresponding to the bottom of the band as unitarity is approached. This phenomenon and the full structure of  $S(\omega)$  at  $k_F|a| \gg 1$  can be understood as a simple interplay between few-body physics happening near the bottom of the band, and physics of multiple particle-hole excitations being created at the Fermi surface. Such an interplay between many-body and few-body physics is a characteristic feature of ultracold atom physics.

We can extend the calculation above to analyze the response  $S(\omega)$  in the vicinity of

$$\omega_1 = \Delta E + E_F,\tag{5.13}$$

where the impurity excites a particle from the bottom of the band to just above the Fermi level, leaving behind a holes at the band bottom, denoted by b(x). To perform this calculation, we need to include the dynamics associated with the non-linear bottom of the band, where electrons cannot be naively bosonized. We may write the following Hamiltonian describing the dynamics of the hole and its interaction with the impurity:

$$H_b = \int dx \left[ b^{\dagger}(x) \partial_x^2 b(x) + a\delta(x) b^{\dagger}(x) d^{\dagger}(x) b(x) d(x) \right], \qquad (5.14)$$

with mass of the holes m = 1/2.

One is now interested in propagators of the form

$$S_n(t) = e^{-i(\Delta E + nE_F)t} \langle [(\psi b^{\dagger})^n d^{\dagger}](0, t) [(\psi^{\dagger} b)^n d](0, 0) \rangle$$
(5.15)

In the case where n = 1, i.e. the threshold  $\omega_1 = \Delta E + E_F$ , the Hamiltonian for the bottom of the band becomes that of one particle interacting with a local scatterer.

In the time domain, the contributions from the Fermi surface excitations and the dynamics of the hole at the bottom of the band factorize. The former contributions manifest as the usual power laws with unitary phase shift, while the latter can be simply evaluated within two-body theory.

We are interested in the response

$$S(t) = e^{-i(\Delta E + E_F)t} \langle \psi(t)b^{\dagger}(t)U^{\dagger}d^{\dagger}(t)U\psi^{\dagger}(0)b(0)U^{\dagger}d(0)U \rangle_{H_0+H_b}$$
  

$$= C_1 e^{-i(\Delta E + E_F)t} \langle \psi(t)\psi^{\dagger}(t)e^{-i\frac{\delta_F}{\pi}\phi(0,t)}e^{i\frac{\delta_F}{\pi}\phi(0,0)} \rangle_{H_0} \langle b^{\dagger}(t)d^{\dagger}(t)b(0)d(0) \rangle_{H_b}$$
  

$$= C_1 e^{-i(\Delta E + E_F)t} \langle e^{i(1-\frac{\delta_F}{\pi})\phi(0,t)}e^{-i(1-\frac{\delta_F}{\pi})\phi(0,0)} \rangle_{H_0} \langle b^{\dagger}(t)d^{\dagger}(t)b(0)d(0) \rangle_{H_b}$$
  

$$= C_1 e^{-i(\Delta E + E_F)t} (iE_F t + 0)^{-(1-\frac{\delta_F}{\pi})^2} \langle b^{\dagger}(t)d^{\dagger}(t)b(0)d(0) \rangle_{H_b} + reg., \quad (5.16)$$

where reg. denotes the terms whose Fourier transform is regular at  $\omega_1$ , and the prefactor  $C_1$  is beyond the scope of the field theory alone. Note that the very important consequence of Eq. (5.16) is that the contribution from the vicinity of the Fermi surface and contribution from the bottom of the band factorize in the time representation.

The two-body problem of the core-hole interacting with the impurity can be solved by expanding the bottom of the band fermion creation and annihilation operators in Fourier modes with coefficients  $\chi_k(x) = \sqrt{\frac{2}{R}} \sin(kx + \delta_k)$ :

$$\langle [b^{\dagger}d^{\dagger}](0,t)[bd](0,0)\rangle = \sum_{kk'} \langle e^{iE_{k}t}\chi_{k}(0)\chi_{k'}(0)b_{k}^{\dagger}d^{\dagger}b_{k'}d\rangle$$

$$= \frac{2}{R}\sum_{k}e^{ik^{2}t}\sin(\delta_{k})\sin(\delta_{k'})\sum_{k'} \langle b_{k}^{\dagger}b_{k'}\rangle$$

$$= \int_{0}^{\infty} \frac{d\varepsilon}{\pi}\frac{\sqrt{\varepsilon}a^{2}}{1+\varepsilon a^{2}}e^{i\varepsilon t}$$

$$= \frac{e^{i\frac{3\pi}{4}}}{\sqrt{\pi E_{F}t}} + \frac{e^{-i\frac{t}{a^{2}}}}{a}\left(\operatorname{Erf}\left(\frac{\sqrt{-it}}{a}\right) - 1\right)$$

$$\xrightarrow{t \to \infty} \frac{a^{2}}{2\sqrt{\pi}}\frac{1}{(iE_{F}t-0)^{3/2}} + O(t^{-5/2}).$$

$$(5.17)$$

The full crossover of the lineshape as a function of  $|\omega - \omega_1|$  can be obtained from the careful convolution of the terms in Eq. (5.16):

$$S_{a<0}(\omega - \omega_1) = C_1 \operatorname{Re} \int \frac{dt}{\pi} e^{i(\omega - \omega_1)t} \times \left(\frac{1}{(iE_F t + 0)^{1/4}} \int \frac{d\varepsilon}{\pi} \frac{\sqrt{2m\varepsilon}}{\varepsilon - E_b} e^{i\varepsilon t}\right)$$
  

$$\approx \frac{2\pi C_1}{\Gamma(1/4)(E_F)^{1/4}} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \theta \left(\omega - \omega_1 + \varepsilon\right) \left(\omega - \omega_1 + \varepsilon\right)^{-3/4} F(\varepsilon),$$
  

$$F(\varepsilon) = \frac{2\sqrt{\varepsilon/E_F}}{\varepsilon - E_b}$$
(5.18)

Thus we encounter a peculiar situation, when the full many-body response is represented as a convolution of the two-body probability to excite a hole  $F(\varepsilon)$  and the Fermi surface contribution.

The amplitude to excite a hole  $F(\varepsilon)$  with energy within interval  $d\varepsilon/(2\pi)$  is given by

$$F(\varepsilon) = \theta(\varepsilon) \frac{2\sqrt{\varepsilon/E_F}}{E_b + \varepsilon} + \theta(k_F a) \frac{4\pi\delta(\varepsilon - E_b)}{k_F a}.$$
(5.19)

To obtain this result, we have combined the result of Eq. (5.17) with the additional contribution from the bound state for a > 0.

Thus, the total  $S(\omega)$  is expressed in terms of  $F(\varepsilon)$  as

$$S(\omega) \approx \frac{1.74\pi}{\Gamma(1/4)(E_F)^{1/4}} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \theta(\omega - \omega_1 + \varepsilon) \times (\omega - \omega_1 + \varepsilon)^{-3/4} F(\varepsilon),$$
(5.20)

where we have already substituted the value of the phase shift at unitarity. Instead of evaluating  $C_1$  at unitarity, it is more convenient to fix the prefactor in Eq. (5.20) via threshold prefactor C (evaluated in the next subsection) as

$$\lim_{k_F a \to \infty} (k_F a) C(k_F a) = 0.868, \tag{5.21}$$

and  $\omega_1 \approx \frac{E_F}{2\hbar}$  at unitarity. The prefactor in Eq. (5.20) is fixed by the condition that one should get C at the threshold.

Although for  $0 < \varepsilon \ll |E_b|$  function  $F(\varepsilon)$  behaves as  $\propto \sqrt{\varepsilon}$ , for  $|E_b| < \varepsilon$ , it behaves as  $\propto 1/\sqrt{\varepsilon}$ . Right at unitarity the scale  $E_b$  disappears, and one obtains in  $S(\omega)$  the divergence with the universal exponent 1/4 and a universal shoulder ratio:

$$S(\omega) \approx \frac{1.74|\omega - \omega_1|^{-1/4}}{(E_F)^{3/4}} \times \left[\theta(\omega - \omega_1)\frac{\Gamma(1/2)}{\Gamma(3/4)} + \theta(\omega_1 - \omega)\frac{\Gamma(1/4)}{\Gamma(1/2)}\right].$$
(5.22)

for  $k_F a = \infty$  and  $|\omega - \omega_1| \ll E_F$ . For large but finite negative  $k_F a$ , this peak gets smeared out at energies of the order of  $|E_b|$  from its maximal value. On the repulsive side, the true bound state with energy  $E_b$  "pinches off" from the bottom of the band with an exponent 3/4 and a prefactor which vanishes as  $\propto 1/(k_F a)$ . Thus for large but finite  $k_F a > 0$  the universal form of  $S(\omega)$  has a characteristic double peak structure.

## 5.4 Prefactors of response at threshold singularities

The field theory prediction of the response of the fermions to an impurity gives the correct power laws of the threshold singularities but the prefactors,  $C, C_b, C_1$ in Eqs. (5.8),(5.12), (5.18) are undetermined. However, by using the conformal invariance of the field theory describing the fermions close to the Fermi level, we can obtain these prefactors. The procedure for evaluation of the prefactor here is very similar in spirit to a recently proposed method to evaluate prefactors in dynamic response functions of 1D quantum liquids [121, 122], which will be taken up in more detail in the following chapter.

Here we will give a broad overview, and specifically discuss the applicability of the more general technique to the particular case of pre factors of the response of the free Fermi gas to an impurity.

#### 5.4.1 Prefactor of conventional edge singularity

Let us consider how Eq. (5.8) is modified in a finite size system for times of the order of  $t \sim R/v_F$ , where finite size quantization becomes important. On the one hand from expansion in terms of intermediate states, one expects (we will not explicitly write the energy  $\Delta E$  here)

$$C\left(\frac{1}{iE_Ft+0}\right)^{\left(\frac{\delta_F}{\pi}\right)^2} \approx \sum_{\tilde{m}} |\langle \tilde{m}|FS \rangle|^2 e^{-iE_{\tilde{m}}t},\tag{5.23}$$

where the sum needs to be performed over low-energy states with energies approximately quantized in units of  $\omega_{min} = v_F \pi / R$ ,

$$E_{\tilde{m}} = \tilde{m}\omega_{min}, \quad \tilde{m} \ge 0, \tag{5.24}$$

and  $\tilde{m} = 0$  corresponds to the ground state of the final Hamiltonian,  $|\tilde{\text{FS}}\rangle$ , i.e. a phase shifted Fermi sea. To evaluate the distribution of the spectral weights between various states for small  $\tilde{m}$ , one can first periodically continue Eq. (5.8) using conformal invariance, and then evaluate explicitly a spectral weight for  $\tilde{m} = 0$  (ground state overlaps).

In the spirit of Refs. [121, 122], we may write then Fourier series expansion

$$C\left(\frac{1}{iE_Ft+0}\right)^{\left(\frac{\delta_F}{\pi}\right)^2} \to C\left(\frac{-i\omega_{min}e^{i\omega_{min}t}}{2E_F\sin\frac{\omega_{min}t}{2}-i0}\right)^{\left(\frac{\delta_F}{\pi}\right)^2}$$
$$= C\sum_n B(n,\alpha) \left(\frac{\omega_{min}}{E_F}\right)^{\alpha} e^{-in\omega_{min}t},$$
(5.25)

where

$$\alpha = \left(\frac{\delta_F}{\pi}\right)^2,\tag{5.26}$$

$$B(n,\alpha) = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)\Gamma(n+1)}.$$
(5.27)

Comparing the right hand sides of Eqs. (5.23), (5.25) implies  $n = \tilde{m}$ , giving

$$C = \lim_{R \to \infty} \left(\frac{k_F R}{\pi}\right)^{\left(\frac{\delta_F}{\pi}\right)^2} |\langle \tilde{FS} | FS \rangle|^2$$
(5.28)

Thus the problem of evaluating the prefactor is reduced to determining the finite size matrix element specified above. This can be straightforwardly eavaluated by performing a finite size scaling analysis on the overlap between the ground states of the initial and final Hamiltonians for a finite size system. Fortunately as they are both Fock states, such an overlap can be calculated from the single particle wavefunctions, and the many-body overlap is expressed as a Slater determinant of single particle overlaps, i.e.

$$\langle \tilde{FS}|FS \rangle = \det(\langle \psi_i | \tilde{\psi}_j \rangle), \quad i, j = 1, ..., N.$$
 (5.29)

The determinant is numerically evaluated for various system sizes and the prefactor is obtained from a power-law fit, see Fig. 5.1.

#### 5.4.2 Prefactor of response in the presence of bound state

To obtain the prefactor  $C_b$  in Eq. (5.12), we follow the same procedure as for the conventional threshold prefactor, except with the trivial modification of the exponent due to the enhancement of the phase shift at the Fermi level by  $\pi$  due to the bound state. This leads to:

$$C_b = \lim_{R \to \infty} \left(\frac{k_F R}{2\pi}\right)^{\left(1 + \frac{\delta_F}{\pi}\right)^2} |\langle FS|\tilde{FS} + \text{boundstate} \rangle|^2.$$
(5.30)

The state  $|FS + boundstate\rangle$  denotes one in which the Fermion at the Fermi level is in a bound state of the impurity. To accommodate the bound state, we insert its wavefunction into the Slater determinant instead of the last occupied mode of the final state Hamiltonian. The prefactor  $C_b$  is then obtained by evaluating the resulting overlap determinant for different system size and fitting the result to a power-law form.

#### 5.4.3 Prefactor of response at higher threshold

The prefactor of the singularity in the vicinity of the shadow band can also be similarly evaluated. One simply realizes that the overlap that dominates in this case is the one between the initial ground state and the final state where one electron is excited from the bottom of the final Fermi sea to just above the Fermi level. In performing the finite size analysis, we have to isolate the contribution from the Fermi level and the band bottom from Eq. (5.16) and expand the corresponding Fourier modes as

$$\sum_{\tilde{m}} |\langle FS|\tilde{m}\rangle|^2 e^{-iE_{\tilde{m}}t} = C_1(it+0)^{-(1-\frac{\delta_F}{\pi})^2} \times \frac{2}{R} \sum_{n'\geq 1} \frac{\pi^2 a^2(n')^2}{R^2} e^{in'^2\pi^2/R^2t}$$
$$= \frac{C_1 a^2}{4\pi} \sum_{n\geq 0,n'\geq 1} (-i)^{(1-\delta_F/\pi)^2} n'^2 B(n,(1-\delta_F/\pi)^2) \left(\frac{2\pi}{R}\right)^{3+(1-\delta_F/\pi)^2} \times e^{-i(n\omega_{min}-n'^2\pi^2/R^2)t},$$

and by comparing the terms on the right and left, we isolate the n = 0, n' = 1 term and relate it to the prefactor

$$C_{1} = \frac{4\pi}{a^{2}} \lim_{R \to \infty} \left(\frac{R}{2\pi}\right)^{3 + (1 - \frac{\delta_{F}}{\pi})^{2}} |\langle FS|n = 0, n' = 1 \rangle|^{2},$$
(5.32)

with  $|n = 0, n' = 1\rangle$  corresponding to the state of the final Hamiltonian with a fermion promoted from the band bottom to just above the Fermi level.

(5.31)

Figure 5.1 : (Color online) The prefactors that appear in the RF response near the thresholds at  $\omega_0, \omega_b$ , see Eqs. (5.8),(5.12). The prefactor C is depicted by the solid red line, while the prefactor  $C_b$  is depicted by the yellow solid line. The open squares and circles indicate agreement with the calculation of C and  $C_b$  in Ref. [78], respectively.

The prefactors calculated as described are plotted in Fig. 5.1, along with numerical data from Ref. [78].

# Chapter 6

# Correlation prefactors of 1D quantum liquids

### 6.1 Introduction

In the following two Chapters a general approach to calculating "nonuniversal" prefactors in static and dynamic correlation functions of 1D quantum liquids at zero temperature is presented. The present chapter deals with the general framework of the procedure, which involves relating the desired prefactors to the finite size scaling of certain matrix elements (form factors). This represents a new, powerful tool for extracting data valid in the thermodynamic limit from finite-size effects. As the main application, weakly interacting spinless fermions with an arbitrary pair interaction potential are considered, for which a few typical prefactors in static and dynamic correlation functions are calculated perturbatively.

## 6.2 Effective field theory in 1D

One-dimensional (1D) quantum liquids of bosons, fermions and spins are conventionally described using an effective hydrodynamic approach known as the Luttinger liquid theory [204, 205, 207, 208, 206]. This theory predicts the long-range behavior of equal-time correlation functions at zero temperature, which one obtains as a series expansion with power laws controlled by a dimensionless Luttinger liquid parameter K > 0, see Eqs. (7.1)-(7.3). While the "universal" parameter K is related to thermodynamic properties and can be easily extracted from numerical or exact solutions, the "nonuniversal" prefactors in the series expansion, e.g.  $A_m, B_m, C_m$ , see Eqs. (7.1)-(7.3) are usually not known except for a few cases [209, 210, 216, 215, 131]. At the same time, these prefactors set the actual scale of observable correlations, consequently determining them is an important theoretical challenge.

Here we first develop a general technique for calculating these nonuniversal prefactors by combining the Luttinger liquid Hamiltonian with the analysis of the finite-size properties of certain matrix elements (form factors). We then consider dynamic response functions such as the density structure factor and the spectral function, see Fig. 6.1. It has been shown recently [219, 220, 221, 224, 136, 231, 232, 234, 227] that dynamic response functions generically have singularities which can be described by effective Hamiltonians of impurities moving in Luttinger liquids. Analysis of the finite-size properties of these effective Hamiltonians allows us to extend the approach to various dynamic response functions. To demonstrate it, we perturbatively evaluate several prefactors of equal-time correlation functions and dynamic response functions for weakly-interacting fermions. We also calculate, non-perturbatively, various prefactors for the exactly solvable Lieb-Liniger model [242, 203] of 1D bosons with contact interactions. The latter model has been realized with ultracold atomic gases [253], and its correlation functions can be measured using interference [255, 257], analysis of particle losses [258], photoassociation [258], or Bragg and photoemission spectroscopy [259].

We will proceed as follows: In Sec. IIA, we use linear Luttinger liquid theory to work out the connection between prefactors of equal-time correlation functions and lowest energy form factors. In Sec. IIB, we show that the relative spectral weights of all low energy form factors can be fixed based on universal nonlinear Luttinger liquid theory [231]. In Sec IIC, we show that the effective field theory of impurities moving in Luttinger liquids allows to extend the relations between form factors and prefactors to dynamic response functions. In Sec. III we present the results of the perturbative calculations of various prefactors for weakly interacting spinless fermions. We summarize our results in Sec. IV. Some of the technical details are contained in the Appendices.

# 6.3 Results from effective field theory

The Luttinger liquid theory [204, 205, 207, 208, 206] predicts the behavior of the correlation functions for spinless bosons and fermions of density  $\rho_0$  at  $\rho_0 x \gg 1$  as (here  $k_F = \pi \rho_0$ )

$$\frac{\langle \hat{\rho}(x)\hat{\rho}(0)\rangle}{\rho_0^2} \approx 1 - \frac{K}{2(\pi\rho_0 x)^2} + \sum_{m\geq 1} \frac{A_m \cos(2mk_F x)}{(\rho_0 x)^{2m^2 K}},\tag{6.1}$$

$$\frac{\langle \hat{\psi}_B^{\dagger}(x)\hat{\psi}_B(0)\rangle}{\rho_0} \approx \sum_{m>0} \frac{B_m \cos(2mk_F x)}{(\rho_0 x)^{2m^2 K + 1/(2K)}},\tag{6.2}$$

$$\frac{\langle \hat{\psi}_F^{\dagger}(x)\hat{\psi}_F(0)\rangle}{\rho_0} \approx \sum_{m\geq 0} \frac{C_m \sin\left[(2m+1)k_F x\right]}{(\rho_0 x)^{(2m+1)^2 K/2 + 1/(2K)}}.$$
(6.3)

Here  $\hat{\rho}$  is the density operator, and  $\hat{\psi}_F(\hat{\psi}_B)$  is the fermionic (bosonic) annihilation operator. The Hamiltonian describing these correlations is written as (we follow notations of Ref. [208])

$$H_0 = \frac{v}{2\pi} \int dx \, \left( K(\nabla \theta)^2 + \frac{1}{K} (\nabla \phi)^2 \right), \tag{6.4}$$

where v is the sound velocity, the canonically conjugate fields  $\phi(x)$ ,  $\theta(x)$  have the commutation relation  $[\phi(x), \nabla \theta(x')] = i\pi \delta(x - x')$ , and the components of the fermionic (bosonic) fields with momenta  $(2m + 1/2 \pm 1/2)k_F$  are written as

$$\psi_{F(B)}(x,t) \sim \sum_{m} e^{i(2m+1/2\pm 1/2)[k_F x - \phi(x,t)] + i\theta(x,t)}.$$
 (6.5)

For repulsive bosons, one has K > 1, while for repulsive (attractive) fermions K < 1(> 1).

One of the reasons for the success of the Luttinger liquid theory is its ability to predict certain finite-size effects [148, 207] due to the conformal invariance of the Hamiltonian (7.4). Below we will show that conformal invariance can also be used to relate nonuniversal prefactors to the scaling of certain form factors [see Eqs. (7.11)-(7.12), (6.28)], which constitutes the main result of this Chapter. Form factors can be evaluated perturbatively or numerically for finite-size systems, and are known for certain integrable models such as the XXZ [149, 150], the Calogero-Sutherland [248], and the Lieb-Liniger [203, 249] models. Thus relations (7.11)-(7.12),(6.28) provide a powerful tool with which one may interpret finite-size effects and make predictions which are valid in the thermodynamic limit.

Let us start by considering interacting spinless fermions. Using the resolution of the identity in the expectation value  $\langle \hat{\psi}_F^{\dagger}(x,t)\hat{\psi}_F(0)\rangle$ , we get

$$\left\langle \hat{\psi}_{F}^{\dagger}(x,t)\hat{\psi}_{F}(0)\right\rangle = \sum_{k,\omega} e^{i(kx-\omega t)} \left| \left\langle k,\omega |\hat{\psi}_{F}|N \right\rangle \right|^{2}, \tag{6.6}$$

where  $\langle k, \omega | \hat{\psi}_F | N \rangle$  is a form factor of the annihilation operator,  $|k, \omega \rangle$  denotes an eigenstate of N-1 particles with momentum k and energy  $\omega$ , and  $|N\rangle$  is the ground state of N particles. For simplicity we assume N is odd so the ground state is nondegenerate. For a finite system, k and  $\omega$  are not continuous, but will be quantized and consequently the spectral function is a collection of delta functions in  $(k, \omega)$ . We will now obtain a similar representation from the Luttinger liquid theory and compare it with Eq. (7.6) to obtain the nonuniversal prefactors  $C_m$ . Hamiltonian (7.4) can be written using left- and right-moving components  $\varphi_{L(R)} = \theta \sqrt{K} \pm \varphi / \sqrt{K}$ , [207] which dictates the time dependence of the  $e^{i(2m+1)k_Fx}$  component of  $\langle \hat{\psi}_F^{\dagger}(x,t)\hat{\psi}_F(0,0)\rangle/\rho_0$  at  $\rho_0 |x \pm vt| \gg 1$  as

$$\frac{e^{i(2m+1)k_Fx}}{2i(-1)^m} \frac{C_m \rho_0^{-(2m+1)^2 K/2 - 1/2K}}{\left(i(vt+x)+0\right)^{\mu_{F,L}} \left(i(vt-x)+0\right)^{\mu_{F,R}}},\tag{6.7}$$

where

$$\mu_{F,L(R)} = (2m+1)^2 K/4 \pm (2m+1)/2 + 1/4K \ge 0.$$
(6.8)

The coefficients  $C_m$  appeared in Eq. (7.7) due to the comparison of the t = 0 limit of  $\langle \hat{\psi}_F^{\dagger}(x,t)\hat{\psi}_F(0,0)\rangle/\rho_0$  with the right hand side of Eq. (7.3). The two factors in the denominator of Eq. (7.7) describe contributions from left (right)-going excitations near the Fermi points which propagate with velocities  $\mp v$ . The signs of the infinitesimal shifts in the denominators ensure that only excitations with negative (positive) momenta can be created at the respective branches. For a finite system with periodic boundary conditions on a circle of length L, conformal invariance dictates (see e.g. Ref. [207]) that Eq. (7.7) gets modified as

$$\frac{e^{i(2m+1)k_Fx}C_m}{2i(-1)^m} \prod_{L,R} \left( \frac{\pi e^{i\pi(vt\pm x)/L}}{i\rho_0 L\sin\frac{\pi(vt\pm x)}{L} + 0} \right)^{\mu_{F,L(R)}}.$$
(6.9)

We can now expand the terms in the parentheses in a Fourier series

$$\left(\frac{\pi e^{i\pi(vt\pm x)/L}}{iL\sin\frac{\pi(vt\pm x)}{L}+0}\right)^{\mu} = \sum_{n_{\mp}\geq 0} C(n_{\pm},\mu) \frac{e^{\pm 2i\pi n_{\mp}\frac{x\mp vt}{L}}}{(L/2\pi)^{\mu}},$$
$$C(n_{\pm},\mu) = \frac{\Gamma(\mu+n_{\pm})}{\Gamma(\mu)\Gamma(n_{\pm}+1)}.$$
(6.10)

Comparing Eqs. (6.9)-(6.10) to the right hand side of Eq. (7.6), one can clearly identify contributions from low-energy and momenta particle-hole excitations at the right (left) Fermi branches with energies  $2\pi v n_{\pm}/L > 0$  and momenta  $\pm 2\pi n_{\pm}/L$ . Additionally, *m* inter-branch pairs of momentum  $2k_F$  each are formed by successively depleting discrete states below the left Fermi point (m > 0) and occupying the lowest-available states above the right one. On top of that, an additional hole is formed on the left branch, giving a total contribution of  $(2m + 1)k_F > 0$  to the momentum. The contribution from  $n_+ = n_- = 0$  gives the scaling of the "parent" form factor

$$\left| \langle m, N - 1 | \hat{\psi}_F | N \rangle \right|^2 \approx \frac{C_m \rho_0}{2(-1)^m} \left( \frac{2\pi}{\rho_0 L} \right)^{\frac{(2m+1)^2 K^2 + 1}{2K}}, \tag{6.11}$$

where  $|m, N-1\rangle$  is the lowest energy state of N-1 fermions with momentum  $(2m + 1)k_F$ . For Galilean invariant systems, states with different m can be obtained from the ground state by a center of mass Galilean boost. We see that as a consequence of the criticality of the Luttinger liquid, form factors of the annihilation operator have nontrivial scaling with the system size, and the prefactors in front of these nontrivial powers of L are directly related to the prefactors in the correlation functions. For density correlations and bosons, similar relations can be worked out, and are given by

$$\left| \langle m, N - 1 | \hat{\psi}_B | N \rangle \right|^2 \approx \frac{B_m \rho_0 (-1)^m}{(2 - \delta_{0,m})} \left( \frac{2\pi}{\rho_0 L} \right)^{\frac{4m^2 K^2 + 1}{2K}},$$
 (6.12)

$$\left|\langle m, N | \hat{\rho} | N \rangle\right|^2 \approx \frac{A_m \rho_0}{2} \left(\frac{2\pi}{\rho_0 L}\right)^{2m^2 K}.$$
(6.13)

Eqs. (7.11)-(7.12) allow one to evaluate the prefactors in Eqs. (7.1)-(7.3) by identifying a single, simplest "parent" form-factor for each of the operators  $\hat{\rho}$ ,  $\hat{\psi}_B$  and  $\hat{\psi}_F$ , respectively. Results for bosons are simply generalized to describe Luttinger liquids of spins on a lattice with standard substitutions [208], and in particular Eq. (7.12) explains the coincidence noticed in Refs. [131, 149] for the spin-1/2 XXZ model.

#### 6.3.1 Distribution of spectral weight among states

Let us now consider the spectral weights at finite energies and momenta in the vicinity of the Fermi points (for concreteness we will discuss fermions). In a finite-size system,

Figure 6.1: (Color online) (a) Spectral function  $A(k, \omega)$ , with shaded areas indicating the regions where it is nonzero, and notations for prefactors. (b) "Parent" state responsible for the singularity at  $\omega \approx -\varepsilon(k) > 0$  in spectral function: it contains a hole corresponding to a mobile "impurity" at  $k_h \approx -k$ , and one particle at each Fermi point. We also illustrate the finite size quantization of the momenta of the impurity and of excitations at the right Fermi point.
the spectral function is a collection of delta functions in  $(k, \omega)$ , weighted by form factors, see Eq. (7.6). From field theory, we not only determine the parent form factor, but also form factors associated with states containing low-energy excitations on top of the parent state, described by nonzero  $n_+$  and  $n_-$ . Within the linear spectrum approximation near the Fermi points, for  $n_{\pm} > 1$  certain particle-hole states are degenerate, thus within  $\propto 1/L$  accuracy, from Eq. (7.6) and Eqs. (6.9)-(6.10) the total spectral weight which falls into the degenerate subspace ("multiplet") with given  $n_+, n_-$  can be obtained from the parent form factor by multiplying it by  $C(n_+, \mu_{F,R})C(n_-, \mu_{F,L})$ . However, within  $\propto 1/L^2$  accuracy, states with sufficiently large  $n_+$  and  $n_-$  are not degenerate due to the nonlinearity of the generic fermionic spectrum, as can be illustrated by the case of weakly interacting fermions. Then  $C(n_+, \mu_{F,R})C(n_-, \mu_{F,L})$ gives only the total spectral weight within each multiplet, and the conventional linear Luttinger liquid theory doesn't distinguish the  $\propto 1/L^2$  splitting of the contributions within each multiplet. However, the splitting of the spectral weights within each multiplet is also universal, and can be understood based on the universal theory of nonlinear Luttinger liquids developed recently [231]. Below we will illustrate such splitting for the case of  $n_{-} = 0$ , i.e. when only excitations at the right branch are created.

Within the nonlinear Luttinger liquid theory, we evaluate various correlators (e.g. Eq. (7.1),(7.3)) by first expressing the fermionic creation and annihilation operators in terms of fermionic quasiparticle operators  $\tilde{\psi}_{R(L)}$ . The fermionic operators are related to the quasi particle operators using

$$\psi_R^{\dagger}(x) = e^{i \int_0^x dy (\delta_+ \tilde{\psi}_R^{\dagger}(y) \tilde{\psi}_R(y) + \delta_- \tilde{\psi}_L^{\dagger}(y) \tilde{\psi}_L(y))} \tilde{\psi}_R^{\dagger}(x).$$
(6.14)

Taking the nonlinearity in the spectrum of the original fermions into account [231],

we obtain the Hamiltonian  $H_R + H_L$  in terms of the quasiparticle operators with

$$H_{s=R,L} = \int dx \left( \mp iv : \tilde{\psi}_s^{\dagger} \nabla \tilde{\psi}_s : + \frac{1}{2m^*} : \nabla \tilde{\psi}_s^{\dagger} \nabla \tilde{\psi}_s : \right),$$
(6.15)

where  $m^*$  is the effective mass, characterizing the nonlinearity of  $\varepsilon(k)$ . Its inverse can be expressed through low energy parameters as [153]

$$\frac{1}{m^*} = \frac{\partial^2 \varepsilon}{\partial k^2} \bigg|_{k_F} = \frac{v}{\sqrt{K}} \frac{\partial v}{\partial h} + \frac{v^2}{2K\sqrt{K}} \frac{\partial K}{\partial h}, \tag{6.16}$$

with h denoting chemical potential and v the sound velocity. Expressions for correlators will include contributions from the left and right Fermi point with given  $\mu_{F,R(L)}$ , i.e. terms

$$\propto \left\langle \exp\left[-2\pi i\sqrt{\mu_{F,R}}\int_{-\infty}^{x} \mathrm{d}y:\tilde{\psi}_{R}^{\dagger}(y,t)\tilde{\psi}_{R}(y,t):\right]\times\right. \\\left. \exp\left[2\pi i\sqrt{\mu_{F,R}}\int_{-\infty}^{0} \mathrm{d}y:\tilde{\psi}_{R}^{\dagger}(y,0)\tilde{\psi}_{R}(y,0):\right]\right\rangle_{H_{R}}$$
(6.17)

where the average is taken over the infinite chiral Fermi sea  $|FS\rangle$  with all negative momenta occupied, and normal ordering is with respect to this vacuum. A similar contribution from the left-movers will also appear.

In a finite system, momenta of the fermionic quasiparticles are quantized near the Fermi point in increments of  $2\pi/L$ . We denote by  $p_1 > p_2 > .... > p_n \ge 0$  particle excitations carrying momenta  $2\pi p_i/L$ , and by  $q_1 < q_2 < ... < q_n < 0$  hole excitations carrying momenta  $-2\pi q_i/L$ . Then  $2\pi n_+/L = 2\pi/L \sum_i p_i - q_i$  is the total momentum of particle-hole excitations near the right Fermi point. Within the linear spectrum approximation, all states with the same  $n_+$  are degenerate, while due to nonlinearity each of them acquires an energy shift

$$\varepsilon(\{p_i, q_i\}) = \frac{2\pi^2}{m^* L^2} \sum_i \left(p_i^2 + q_i^2\right).$$
(6.18)

We can introduce a complete set of intermediate states in Eq. (6.17) between the two exponents and organize them by the momenta of particle-hole excitations as follows

$$\sum_{n_{+}=0}^{\infty} \sum_{p_{i}-q_{i}=n_{+}} e^{\frac{2\pi i n^{+}}{L}(x-vt)-i\varepsilon(\{p_{i},q_{i}\})t} \\ \left| \left\langle \{p_{i},q_{i}\} \left| e^{2\pi i \sqrt{\mu_{F,R}} \int_{-\infty}^{0} \mathrm{d}y:\tilde{\psi}_{R}^{\dagger}(y,0)\tilde{\psi}_{R}(y,0):} \right| \mathrm{FS} \right\rangle \right|^{2} \\ = \sum_{n_{+}=0}^{\infty} \sum_{p_{i}-q_{i}=n_{+}} e^{\frac{2\pi i n^{+}}{L}(x-vt)-i\varepsilon(\{p_{i},q_{i}\})t} \\ \left| \left\langle \{p_{i},q_{i}\} \left| e^{-\sum_{k\neq 0,l} \frac{\sqrt{\mu_{F,R}}}{k}} \tilde{\psi}_{R}^{\dagger}(k+l)\tilde{\psi}_{R}(l)} \right| \mathrm{FS} \right\rangle \right|^{2}, \tag{6.19}$$

where in the first line we have moved the position and time dependence of the operators over to the states, and in the second line we have Fourier transformed the creation and annihilation operators and performed the integral over y. The correlator above can be exactly evaluated using the methods of Ref. [267]. There they consider a "boundary state" exp  $\left[-(a+m)\sum_{k\neq 0} \left(\frac{e^{ikx}}{k}\sum_p \hat{\psi}_p^{\dagger'}_{p+k}\right)\right]|0\rangle$ , which we can identify as the one obtained by action of the string operator in Eq. (6.19) on the infinite chiral vacuum if we map  $m + a \rightarrow \sqrt{\mu_{F,R}}$ . Consequently we obtain the following result from Eqs.(59)-(61) of Ref. [267]:

$$= \frac{f(\lbrace p_i, q_i \rbrace)}{\left\langle \lbrace p_i, q_i \rbrace \left| e^{2\pi i \sqrt{\mu_{F,R}} \int_{-\infty}^{0} \mathrm{d}y: \tilde{\psi}_{R}^{\dagger}(y,0)\tilde{\psi}_{R}(y,0):} \right| \mathrm{FS} \right\rangle}{\left\langle \mathrm{FS} \left| e^{2\pi i \sqrt{\mu_{F,R}} \int_{-\infty}^{0} \mathrm{d}y: \tilde{\psi}_{R}^{\dagger}(y,0)\tilde{\psi}_{R}(y,0):} \right| \mathrm{FS} \right\rangle}$$

$$= \mathrm{Det}_{i,j \leq n} \left( \frac{1}{p_i - q_j} \right) \prod_{i \leq n} f^+(p_i) f^-(q_i), \qquad (6.20)$$

where

$$f^{+}(p) = \frac{\Gamma(p+1-\sqrt{\mu_{F,R}})}{\Gamma(-\sqrt{\mu_{F,R}})\Gamma(p+1)},$$
  
$$f^{-}(q) = \frac{\Gamma(-q+\sqrt{\mu_{F,R}})}{\Gamma(1+\sqrt{\mu_{F,R}})\Gamma(-q)}.$$
 (6.21)

Normalization of the spectral weight leads to the following "multiplet summation rule" (see Appendix A for an explicit demonstration)

$$\sum_{\sum p_i - q_i = n_+} |f(\{p_i, q_i\})|^2 = C(n_+, \mu_{F,R}).$$
(6.22)

Contributions from the left Fermi point are accounted for similarly, and the total form factor is a product of these two terms.

### 6.3.2 Prefactors of dynamic response functions

We now consider the dynamic response functions: the density structure factor

$$S(k,\omega) = \int dx dt^{i(\omega t - kx)} \langle \hat{\rho}(x,t) \hat{\rho}(0,0) \rangle, \qquad (6.23)$$

and spectral function  $A(k,\omega) = -\frac{1}{\pi} \text{Im}G(k,\omega) \text{sign}\omega$  where the Green's function  $G(k,\omega)$ is defined as [270]

$$G(k,\omega) = -i \int dx dt e^{i(\omega t - kx)} \langle T[\hat{\psi}(x,t)\hat{\psi}^{\dagger}(0,0)] \rangle.$$
(6.24)

To be specific let us consider the spectral function for  $\omega > 0$  and  $-k_F < k < k_F$ . In addition to the Fermi points, the field theoretical description of the singularity at  $-\varepsilon(k) > 0$  (see Ref. [232]; we follow the notations contained therein) involves a mobile "impurity" with momentum  $k_h \approx -k$  moving with velocity  $v_d = \partial \varepsilon(k_h) / \partial k_h$ , see Fig. 6.1. For non-interacting fermions, any spectral weight is absent at  $\omega > 0$  and  $-k_F < k < k_F$ , and for weakly interacting fermions the configuration responsible for a feature at  $\omega \approx -\varepsilon(k)$  is illustrated in Fig. 6.1; it has one particle at each Fermi points, and a hole corresponding to the impurity. While for stronger interactions such a simple interpretation of the impurity is absent, the field theoretical description still remains valid [232]. The Hamiltonian used in this approach takes the form

$$H_{d} = \int dx d^{\dagger}(x) \left[ \varepsilon(k) - iv_{d} \frac{\partial}{\partial x} \right] d(x),$$
  

$$H_{int} = \int dx \left[ V_{R} \rho_{R}(x) + V_{L} \rho_{L}(x) \right] \rho_{d}(x)$$
  

$$= \int dx \left( V_{R} \nabla \frac{\theta - \phi}{2\pi} - V_{L} \nabla \frac{\theta + \phi}{2\pi} \right) d(x) d^{\dagger}(x).$$
(6.25)

Here the operator d(x) creates a mobile hole with momentum k and velocity  $v_d = \partial \varepsilon(k)/\partial k$ . The interaction Hamiltonian describes the impurity interacting with the left and right movers of the Luttinger liquid.

The spectral function  $A(k,\omega)$  in the vicinity of  $-\varepsilon(k)$  is written as

$$A(k,\omega) \propto \int dx dt e^{i\omega t} \langle d^{\dagger}(x,t) d(0,0) \rangle_{H_{LL}+H_d+H_{int}}$$
  
=  $A_{0,+}(k) \int dx dt e^{i\delta\omega t} D(x,t) L(x,t) R(x,t),$   
(6.26)

where  $\delta \omega = \omega + \varepsilon(k), D(x,t) = \delta(x - v_d t)$  is the impurity correlator,  $L(R)(x,t) = (i(vt \pm x) + 0)^{-\mu_{0,+,L(R)}}$  [156], and we introduced a prefactor  $A_{0,+}(k)$  which will be determined by a comparison to the form factors. After the x, t integration, Eq. (6.26) results in

$$A(k,\omega) = \theta(\delta\omega) \frac{2\pi A_{0,+}(k)\delta\omega^{-\mu_{0,+}}}{\Gamma(1-\mu_{0,+})(v+v_d)^{\mu_{0,+,L}}(v-v_d)^{\mu_{0,+,R}}}$$

In finite-size systems, L(x,t) and R(x,t) get modified, see Eq. (6.10). The change of D(x,t) to  $\sum_{n_D} e^{2i\pi n_D (x-v_d t)/L}$  corresponds to the quantization of the impurity momentum. At fixed k, the shift of the momentum of the impurity can be expressed as  $n_D = n_- - n_+$ . Combining these terms, we get

$$A(k,\omega) = \sum_{n_{\pm}\geq 0} \delta\left(\delta\omega - \Delta E - \frac{2\pi n_{+}}{L}(v - v_{d}) - \frac{2\pi n_{-}}{L}(v + v_{d})\right) \times A_{0,+}(k) \frac{(2\pi)^{2-\mu_{0,+}}}{L^{1-\mu_{0,+}}} C(n_{+},\mu_{0,+,R}) C(n_{-},\mu_{0,+,L}),$$
(6.27)

where  $\Delta E$  is a universal  $\propto 1/L$  shift of the edge position [227]. Thus the finite size structure of the response function is given by the sum of two generically incommensurate frequency "ladders" at arbitrary k, in contrast to the vicinities of Fermi points. Analysis of the scaling of the parent form factor with  $n_{+} = n_{-} = 0$  then leads to

$$\left|\langle k; N+1|\hat{\psi}_F^{\dagger}|N\rangle\right|^2 \approx A_{0,+}(k) \left(\frac{2\pi}{L}\right)^{2-\mu_{0,+}},\tag{6.28}$$

where  $|k; N+1\rangle$  denotes the lowest energy state of N+1 fermions with total (discrete) momentum k. Similar relations can be derived for the density structure factor and the boson spectral function, and for each k, the left hand side consists of a single form factor which connects the ground state with the lowest energy state at total momentum k, while the right hand side shows scaling with the exponents of Ref. [232]:

$$\left|\langle k; N | \hat{\rho} | 0, N \rangle\right|^2 \approx \frac{S_0(k)}{L} \left(\frac{2\pi}{L}\right)^{1-\mu_0}, \qquad (6.29)$$

$$\left|\langle k; N+1 | \hat{\psi}_B^{\dagger} | N \rangle \right|^2 \approx A_{0,+}^B(k) \left(\frac{2\pi}{L}\right)^{2-\mu_{0,+}^b}, \qquad (6.30)$$

with [232, 156]

$$\mu_{0,+} = 1 - \mu_{0,+,L} - \mu_{0,+,R},$$
  

$$\mu_{0,+}^{b} = 1 - \mu_{0,+,L}^{b} - \mu_{0,+,R}^{b},$$
  

$$\mu_{0} = 1 - \mu_{0,L} - \mu_{0,R}.$$
(6.31)

We note that in Eqs. (6.28)-(6.30) k has to be fixed before taking the limit  $L \to \infty$ , since e.g. the  $k \to k_F$  and  $L \to \infty$  limits do not commute as has been shown in nonlinear Luttinger liquid theory [224, 231, 232].

Eqs. (7.11)-(7.12),(6.28)-(6.30) rely on the structure of the low-energy excitations at a given momentum, prescribed by the field theory; they are valid for all Luttinger liquids in 1D irrespective of microscopic interactions and can be used as a convenient tool to interpret the results of numerical studies. Below we illustrate their power by obtaining new nontrivial results for weakly interacting fermions and also present numerical data on some exact results [161] we obtained from the analysis of the finite size form factors of the Lieb-Liniger model.

## 6.4 Perturbative calculation of form factors

We use the non interacting Fermi gas in 1D as our unperturbed state. The ground state for a system of N non interacting fermions of mass M occupying a length L with density  $\rho_0 = N/L$  is characterized in momentum space by N real momenta  $\{-k_F, ..., k_F\}$ , increasing by increments of  $2\pi/L$ , with  $k_F = \pi(N-1)/L$ . Here we have assumed that N is odd so that the ground state is non-degenerate.

Defining the ground state  $|FS\rangle$  to have resulted from the action of N creation operators on an empty vacuum starting from the left-most momentum gives us a convention to specify the relative phases of various states that will be used in the calculations to follow. Moreover in the subsequent calculations it is only the relative phases between states that is pertinent since we are interested in absolute squared values of the form factors. To this system we add a weak four fermion interaction

$$\hat{V} = \frac{1}{2L} \sum_{q,p,p'} V(q) \hat{\psi}_{p+q}^{\dagger} \hat{\psi}_{p'-q'p'}^{\dagger} p'_{p},$$

where V(q) is the Fourier transform of the pair interaction potential V(r).

For weakly interacting fermions we may directly evaluate form factors in the left hand sides of Eqs. (7.11),(7.12), and (6.28) using conventional perturbation theory and extract prefactors. For example, since  $\mu_{0,+} = -1 + O(\hat{V}^2)$  [219, 232], one can expand the right hand side of Eq. (6.28) in powers of  $\hat{V}$  as

$$\frac{(2\pi)^3 A_{0,+}(k)}{L^3} \times [1 + (\mu_{0,+} + 1)\log(L/2\pi) + \dots].$$
(6.32)

While in an infinite size system this expansion is not convergent, for finite L it is well defined if one keeps L finite but large, and then takes the limit  $V(r) \rightarrow 0$ . We treat the interaction term perturbatively, and can e.g. write the expansion of the ground state as

$$|N\rangle = |\text{FS}\rangle + \sum_{|\alpha\rangle} \frac{\langle \alpha | \hat{V} | \text{FS} \rangle}{E_{\text{FS}} - E_{\alpha}} | \alpha \rangle + \dots, \qquad (6.33)$$

where  $|\text{FS}\rangle$  denotes a filled Fermi sea. Similar perturbative expressions can be written for the states on the left hand sides of Eqs. (7.11),(7.12), and (6.28), and one can then straightforwardly evaluate the scaling of form factors with integer powers of L. Due to momentum constraints, only few intermediate states contribute within lowest order perturbation theory. Eg. for  $A_{0,+}(k)$  (see Fig. 6.1 a), the only sequence of states which contributes is the following: first,  $\hat{V}$  creates two particles at the right and left Fermi points, and two holes at +k and -k; (see Fig. 6.2a), second the operator  $\hat{\psi}^{\dagger}(0) = \frac{1}{\sqrt{L}} \sum_{p} \hat{\psi}^{\dagger}(p)$  fills in a hole at +k, and we end up with the final state  $|k, N+1\rangle$ . Figure 6.2 : The states (a) - (c) shown above are the only intermediate states that give non-zero contributions in the perturbative calculation of the form factors used to determine the prefactors  $A_{0,+}(k), A_{1,-}(k)$  and  $A_{1,+}(k)$ , respectively.

## **6.4.1** Calculation of $A_{0,+}(k)$

We expect the spectral function in the region  $\omega > 0, k \in (-k_F, k_F)$  (see Fig. 6.1a) to behave as

$$A(k,\omega) \approx 2\pi A_{0,+}(k)\theta \left(\omega - \left(\frac{k_F^2 - k^2}{2m} + \Delta\varepsilon\right)\right)$$

$$\times \frac{(\omega - \left(\frac{k_F^2 - k^2}{2m} + \Delta\varepsilon\right))^{-\mu_{0,+}}}{\Gamma(1 - \mu_{0,+})(v + v_d)^{\mu_{0,+,L}}(v - v_d)^{\mu_{0,+,R}}},$$

$$\Delta\varepsilon = \int_{-k_F}^{k_F} \frac{dk'}{2\pi} \left(V(k' - k) - V(k' - k_F)\right) + O(\hat{V}^2),$$
(6.34)

where  $\Delta \varepsilon$  captures the shift in the dispersion curve of a non interacting fermionic system when interactions are introduced. To first order the shift is obtained by considering the Hartree-Fock corrections to the energy of eigenstates. The exponents  $\mu_{0,+}, \mu_{0,+,L}, \mu_{0,+,R}$  (see Eq. (6.31) and Ref. [156]) to leading order can be obtained using:

$$\mu_{0,+,L} = \left(\frac{1}{\sqrt{K}} - \frac{\delta_{-}}{2\pi}\right)^{2} = \left(1 + \frac{m(V(0) - V(2k_{F}))}{4\pi k_{F}} - \frac{m(V(k_{F} + k) - V(0))}{2\pi(k + k_{F})} + O(\hat{V}^{2})\right)^{2},$$

$$\mu_{0,+,R} = \left(\frac{1}{\sqrt{K}} + \frac{\delta_{+}}{2\pi}\right)^{2} = \left(1 + \frac{m(V(0) - V(2k_{F}))}{4\pi k_{F}} - \frac{m(V(k_{F} - k) - V(0))}{2\pi(k - k_{F})} + O(\hat{V}^{2})\right)^{2},$$

$$\mu_{0,+} = 1 - \mu_{0,+,L} - \mu_{0,+,R}$$

$$= -1 - \left(\frac{m(V(0) - V(2k_{F}))}{\pi k_{F}} + \frac{m(V(k - k_{F}) - V(0))}{\pi(k - k_{F})} - \frac{m(V(k + k_{F}) - V(0))}{\pi(k + k_{F})}\right)$$

$$+ O(\hat{V}^{2}).$$
(6.35)

$$\mu_{0,+} = -1 + O(\hat{V}). \tag{6.36}$$

Using Eq. (6.28) and the value of  $\mu_{0,+}$  in the limit of vanishing interactions from Eq. (6.36), we may obtain the prefactor  $A_{0,+}(k)$  from:

$$A_{0,+}(k) = \frac{L^3}{(8\pi^3)} |\langle k, N+1|\hat{\psi}^{\dagger}(0)|N\rangle|^2.$$
(6.37)

Thus we need to evaluate the form factor

$$\langle k, N+1|\hat{\psi}^{\dagger}(0)|N\rangle = \frac{1}{\sqrt{L}}\langle k, N+1|\sum_{p''}\hat{\psi}^{\dagger}_{p''}|N\rangle, \qquad (6.38)$$

where  $|k, N+1\rangle$  is the lowest energy eigenstate of the interacting system with N+1particles and total momentum k and  $|N\rangle$  is the N particle ground state. Since there is no exact answer for such a form factor for a generic interacting Fermi gas, we expand the ket vectors in Eq. (6.38) in terms of the eigenstates of the non interacting system perturbatively in  $\hat{V}$  in the following way:

$$|N\rangle = |FS\rangle + \sum_{|\alpha\rangle} \frac{\langle \alpha | \hat{V} | FS \rangle}{E_{FS} - E_{\alpha}} |\alpha\rangle + O(\hat{V}^2),$$
  
$$|k, N+1\rangle = |k, N+1\rangle^{(0)} + \sum_{|\alpha\rangle} \frac{\langle \alpha | \hat{V} | k, N+1 \rangle^{(0)}}{E_{k,N+1} - E_{\alpha}} |\alpha\rangle$$
  
$$+ O(\hat{V}^2), \qquad (6.39)$$

where, the state  $|\text{FS}\rangle$  is a filled Fermi sea of N particles, and the state  $|k, N + 1\rangle^{(0)}$ is an eigenstate of the N + 1 non interacting fermions, that has two particles with momenta  $-k_F - 2\pi/L$  and  $k_F + 2\pi/L$ , and a hole of momentum -k, on top of  $|\text{FS}\rangle$ . From now on we will specify various states of the non-interacting system by describing the configuration of the state with respect to  $|\text{FS}\rangle$ . The sum over  $|\alpha\rangle$  runs over the entire Hilbert space of the non interacting system except the zeroth order state on the right, and  $E_{\alpha}$  is the energy of the eigenstate  $|\alpha\rangle$  of the non interacting system.

When we use the expansions in Eq. (6.39) to linear order in expression (6.38) for the form factor, we obtain no contribution from terms that are zeroth order in  $\hat{V}$ since it is not possible to create the state  $|k, N + 1\rangle^{(0)}$  by acting on  $|\text{FS}\rangle$  with just a single creation operator. When we consider the two terms generated by taking the zeroth order term from one of the ket vector expansions and the first order term from the other it becomes possible to obtain non zero contributions. Thus we are left considering two terms:

$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{\rm FS} - E_{\alpha})} \langle k, N+1|^{(0)} \sum_{p''} \hat{\psi}^{\dagger}_{p''} |\alpha\rangle$$
$$\times \langle \alpha| \sum_{q,p,p'} V(q) \hat{\psi}^{\dagger}_{p+q} \hat{\psi}^{\dagger}_{p'-q'} \hat{p}'_{p'} |{\rm FS}\rangle$$
(6.40)

and

$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{k,N+1} - E_{\alpha})} \langle \alpha | \sum_{p''} \hat{\psi}_{p''}^{\dagger} | \text{FS} \rangle \\ \times \langle k, N+1 |^{(0)} \sum_{q,p,p'} V(q) \hat{\psi}_{p+q}^{\dagger} \hat{\psi}_{p'-q'}^{\dagger} p'_{p'} | \alpha \rangle.$$
(6.41)

We see that only the first term leaves a nonzero contribution for the following reasons. In term (6.40), the matrix element of the momentum conserving interaction  $\hat{V}$  limits the possibilities for  $|\alpha\rangle$  to be only states with zero momentum. On the other hand, for the matrix element of the creation operator to be non zero we require that the state  $|\alpha\rangle$  must have the same configuration as  $|k, N + 1\rangle^{(0)}$  but with one more hole. Since the state  $|k, N + 1\rangle^{(0)}$  already has a hole, the only admissible state is one with two particles of momenta  $k_F + 2\pi/L$  and  $-k_F + 2\pi/L$  and two holes of momenta k and -k and is shown in Fig. 6.2(a). When we consider term (6.41) we see that the states  $|\alpha\rangle$  which will give non zero contributions must have total momenta k and must contain one additional particle over the ground state. There can exist no such state since  $|k| < k_F$ , and consequently we may disregard term (6.41).

Thus the only contributions we are left with are due to the term in expression (6.40) for the state in Fig. 6.2(a):

$$E_{\rm FS} - E_{2a} = \frac{(k_F + 2\pi/L)^2}{M} - \frac{k^2}{M},$$
  

$$\langle k, N+1 | \hat{\psi}^{\dagger}(0) | N \rangle = \frac{M(V(k_F - k + 2\pi/L) - V(k_F + k + 2\pi/L))}{2L^{3/2}[(k_F + 2\pi/L)^2 - k^2]} - \frac{M(V(-k_F - k - 2\pi/L) - V(-k_F + k - 2\pi/L))}{2L^{3/2}[(k_F + 2\pi/L)^2 - k^2]} + O(\hat{V}^2).$$
(6.42)

Using the correspondence between the prefactor  $A_{0,+}(k)$  and the form factor given in Eq. (6.37) we obtain

$$A_{0,+}(k) = \frac{L^3}{(8\pi^3)} |\langle k, N+1 | \hat{\psi}^{\dagger}(0) | N \rangle|^2$$
  
=  $\frac{M^2 (V(k_F+k) - V(k_F-k))^2}{8\pi^3 (k_F^2 - k^2)^2},$  (6.43)

to leading order in  $\hat{V}$  and where we have used the fact that V(r) is real and symmetric, thus V(-q) = V(q). The divergence as  $k \to \pm k_F$  from the denominator of Eq. (6.43) still leads to a finite integral over  $\omega > 0$  when we substitute the expression for  $A_{0,+}$ in Eq. (6.34).

# **6.4.2** Calculation of $A_{1,-}(k)$

In the region  $\omega < 0, k \in (k_F, 3k_F)$  (see Fig.6.1a) the spectral function behaves as

$$\begin{aligned}
A(k,\omega) &\approx 2\pi A_{1,-}(k) \\
&\times \left(\omega + \left(\frac{k_F^2 - (k - 2k_F)^2}{2m} + \Delta\varepsilon\right)\right)^{-\mu_{1,-}} \\
&\times \frac{\theta\left(\omega + \left(\frac{k_F^2 - (k - 2k_F)^2}{2m} + \Delta\varepsilon\right)\right)}{\Gamma(1 - \mu_{1,-})(v + v_d)^{\mu_{1,-,L}}(v - v_d)^{\mu_{1,-,R}}}, \\
\Delta\varepsilon &= \int_{-k_F}^{k_F} \frac{dk'}{2\pi} \left(V(k' - k + 2k_F) - V(k' - k_F)\right) \\
&+ O(\hat{V}^2).
\end{aligned}$$
(6.44)

The exponents  $\mu_{1,-}, \mu_{1,-,L}, \mu_{1,-,R}$  are given by Eq. (6.31) and Ref. [156], and can be written to leading order as

$$\mu_{1,-,L} = \left(\sqrt{K} - \frac{\delta_{-}}{2\pi}\right)^{2} = \left(1 - \frac{m(V(0) - V(2k_{F}))}{4\pi k_{F}} + \frac{m(V(k_{F} + k) - V(0))}{2\pi(k + k_{F})} + O(\hat{V}^{2})\right)^{2},$$
  

$$\mu_{1,-,R} = \left(\sqrt{K} - \frac{\delta_{+}}{2\pi}\right)^{2} = \left(1 - \frac{m(V(0) - V(2k_{F}))}{4\pi k_{F}} + \frac{m(V(k_{F} - k) - V(0))}{2\pi(k - k_{F})} + O(\hat{V}^{2})\right)^{2},$$
  

$$\mu_{1,-} = 1 - \mu_{1,-,L} - \mu_{1,-,R}$$
  

$$= -1 + \left(\frac{m(V(0) - V(2k_{F}))}{\pi k_{F}} - \frac{m(V(k - k_{F}) - V(0))}{\pi(k - k_{F})} - \frac{m(V(k + k_{F}) - V(0))}{\pi(k + k_{F})}\right)$$
  

$$+ O(\hat{V}^{2}).$$
(6.45)

$$\mu_{1,-} = -1 + O(\hat{V}). \tag{6.46}$$

Using the value of the exponent in the absence of interactions and the finite size

version of Eq. (6.44) we may write

$$A_{1,-}(k) = \frac{L^3}{(8\pi^3)} |\langle k, N-1|\hat{\psi}(0)|N\rangle|^2.$$
(6.47)

Consequently we need the matrix element

$$\langle k, N-1|'(0)|N\rangle = \langle 2k_F + k_h, N-1|'(0)|N\rangle = \frac{1}{\sqrt{L}} \langle 2k_F + k_h| \sum_{p''} {}'_{p''}|N\rangle,$$
(6.48)

where  $k_h = k - 2k_F \in (-k_F, k_F)$ , and the state  $|2k_F + k_h, N - 1\rangle$  is the lowest energy eigenstate of momentum  $2k_F + k_h$  of N - 1 interacting fermions and  $|N\rangle$  is the Nparticle ground state of the system. Again we perform a perturbative expansion of the ket vectors in orders of V(q) in eigenstates of the free fermions as in Eq. (6.39). We note that the unperturbed version of the excited state,  $|2k_F + k_h, N - 1\rangle^{(0)}$ , will contain two holes with momenta  $k_F, k_h$  and a particle of momentum  $-k_F$ .

We find that there is no zeroth order contribution since the state  $|2k_F+k_h, N-1\rangle^{(0)}$ cannot be obtained by the action of a single annihilation operator on the ground state, since it contains two holes and a particle over the ground state. Thus we look to the first order terms of the form given in expressions (6.40) and (6.41). In order for the linear order terms to give a non-zero contribution we need the matrix elements of  $\hat{V}$ , which can only connect states of the same momentum, and that of the annihilation operator between  $\langle \alpha |$  and  $|\text{FS}\rangle$ , to simultaneously be non-zero. The first requirement automatically narrows down our choices to two subsets of intermediate states  $\{|\alpha\rangle\}$ . One subset contains states of zero momentum while the other contains states of momentum  $2k_F + k_h$ . For the matrix element of the annihilation operator to be nonzero, the states  $|\alpha\rangle$  of momentum  $2k_F + k_h$  must be identical to the filled Fermi sea but with a single additional hole - however this is impossible since the momentum of such a state can at most be  $k_F$ . Thus we must focus our attention on the term

$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{\rm FS} - E_{\alpha})} \langle 2k_F + k_h, N - 1 | \sum_{p''} {}^{'}_{p''} | \alpha \rangle$$
$$\times \quad \langle \alpha | \sum_{q,p,p'} V(q) \hat{\psi}^{\dagger}_{p+q} \hat{\psi}^{\dagger}_{p'-q'} {}^{'}_{p'} | {\rm FS} \rangle.$$

The only state  $|\alpha\rangle$  that gives a contribution to this term contains two holes of momenta  $k_F$  and  $k_h$  and two particles of momenta  $-k_F - 2\pi/L$  and  $2k_F + k_h + 2\pi/L$ , and is shown in Fig. 6.2(b). Consequently the matrix element to first order in  $\hat{V}$  can be calculated as follows:

$$E_{\rm FS} - E_{2b} = -\frac{(2k_F + k_h + 2\pi/L)^2}{2M} - \frac{(k_F + 2\pi/L)^2}{2M} + \frac{k_F^2}{2M} + \frac{k_h^2}{2M} = -\frac{2k_F}{M} (k_F + k_h) + O(1/L).$$

$$2k_F + k_h, N - 1|\hat{\psi}(0)|N\rangle = \frac{M(V(2k_F) - V(k_F + k_h))}{2k_F L^{3/2} (k_F + k_h)} + O(\hat{V}^2, 1/L). \quad (6.49)$$

We may then express the prefactor  $A_{1,-}(k)$  in terms of the matrix element using a similar correspondence to Eq. (6.43):

 $\langle$ 

$$A_{1,-}(k) = \frac{L^3}{(8\pi^3)} |\langle k, N-1|\hat{\psi}(0)|N\rangle|^2$$
  
=  $\frac{M^2(V(2k_F) - V(k_F - k))^2}{32\pi^3 k_F^2 (k_F - k)^2},$  (6.50)

where we have substituted  $k_h = k - 2k_F$  to obtain the final answer in terms of  $k_F \leq k \leq 3k_F$ .

As in the case of  $A_{0,+}(k)$ , we note again that the divergence as  $k \to k_F$  from the denominator of Eq. (6.50) still leads to a finite value when we substitute the expression for  $A_{1,-}(k)$  in Eq. (6.44) and integrate over  $\omega < 0$ .

# **6.4.3** Calculation of $A_{1,+}(k)$

When  $\omega > 0, k \in (k_F, 3k_F)$  (see Fig. 6.1a) the spectral function behaves as

$$\begin{aligned}
A(k,\omega) &\approx 2\pi A_{1,+}(k) \\
& \left(\omega - \left(\frac{k_F^2 - (k - 2k_F)^2}{2m} + \Delta\varepsilon\right)\right)^{-\mu_{1,+}} \\
& \times \frac{\theta\left(\omega - \left(\frac{k_F^2 - (k - 2k_F)^2}{2m} + \Delta\varepsilon\right)\right)}{\Gamma(1 - \mu_{1,+})(v + v_d)^{\mu_{1,+,L}}(v - v_d)^{\mu_{1,+,R}}}, \\
\Delta\varepsilon &= \int_{-k_F}^{k_F} \frac{dk'}{2\pi} \left(V(k' - k + 2k_F) - V(k' - k_F)\right) \\
& + O(\hat{V}^2).
\end{aligned}$$
(6.51)

Moreover we obtain perturbative expressions for the exponents  $\mu_{1,+,R}$ ,  $\mu_{1,+,L}$  and  $\mu_{1,+}$ from Eq. (6.31) and Ref. [156]:

$$\mu_{1,+,L} = \left(\sqrt{K} + \frac{1}{\sqrt{K}} - \frac{\delta_{-}}{2\pi}\right)^{2} = \left(2 - \frac{m(V(k_{F} + k) - V(0))}{2\pi(k + k_{F})} + O(\hat{V}^{2})\right)^{2},$$

$$\mu_{1,+,L} = \left(\sqrt{K} - \frac{1}{\sqrt{K}} - \frac{\delta_{+}}{2\pi}\right)^{2} = \left(\frac{m(V(0) - V(2k_{F}))}{4\pi k_{F}} + \frac{m(V(k_{F} - k) - V(0))}{2\pi(k - k_{F})} + O(\hat{V}^{2})\right)^{2},$$

$$\mu_{1,+} = 1 - \mu_{1,-,L} - \mu_{1,-,R}$$

$$= -3 + \frac{2m(V(k + k_{F}) - V(0))}{\pi(k + k_{F})} + O(\hat{V}^{2}).$$
(6.52)
$$\mu_{1,+} = -3 + O(\hat{V}).$$

Using the value of the exponent in the absence of interactions and the finite size version of Eq. (6.51) we may write

$$A_{1,+}(k) = \frac{L^5}{(32\pi^5)} |\langle k, N-1 | \hat{\psi}^{\dagger}(0) | N \rangle|^2.$$
(6.54)

Thus we first focus on the matrix element

$$\langle k, N+1 | \hat{\psi}^{\dagger}(0) | N \rangle = \langle 2k_F - k_h, N+1 | \hat{\psi}^{\dagger}(0) | N \rangle$$
$$= \frac{1}{\sqrt{L}} \langle 2k_F - k_h | \sum_{p''} \hat{\psi}^{\dagger}_{p''} | N \rangle, \qquad (6.55)$$

where  $k_h = 2k_F - k \in (-k_F, k_F)$ , and the state  $|2k_F - k_h, N + 1\rangle$  is the lowest energy eigenstate of the N + 1 particle interacting system with momentum  $2k_F - k_h$  and  $|N\rangle$ is the N particle ground state. We again expand the ket vectors in Eq. (6.55) as in Eq. (6.39). The corresponding eigenstate of the free fermions is  $|2k_F - k_h, N + 1\rangle^{(0)}$ , an N + 1 particle state with two particles with momenta  $k_F + 2\pi/L$  and  $k_F + 4\pi/L$ , and one hole with momentum  $k_h$ . Here too we must perturbatively expand in the states for which we calculate the above matrix element. There is no zeroth order contribution since the state  $|2k_F - k_h, N + 1\rangle^{(0)}$  cannot be created by the action of a single creation operator on the ground state.

Upon considering the first order terms of the form given in expressions (6.40), (6.41) we find the only non-zero contribution is to the term

$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{2k_F-k_h,N+1}-E_{\alpha})} \langle \alpha | \sum_{p''} \hat{\psi}^{\dagger}_{p''} | \text{FS} \rangle$$
$$\times \quad \langle 2k_F-k_h, N+1 | \sum_{q,p,p'} V(q) \hat{\psi}^{\dagger}_{p+q} \hat{\psi}^{\dagger}_{p'-q'} \overset{'}{p'}_{p} | \alpha \rangle,$$

from the state depicted in Fig. 6.2(c). Due to the kinematic constraint imposed by  $\hat{V}$ , the states that may contribute to the matrix element must either have zero momentum and must be connected to the state  $|2k_F - k_h, N + 1\rangle^{(0)}$  by the action of the creation operator, or have momentum  $2k_F - k_h$  and must be connected to the ground state by the action of the annihilation operator. The latter condition is the only kinematically feasible one, and the only allowed state is the one in Fig. 6.2(c). Thus we may collect all the terms that are linear order in  $\hat{V}$  as follows:

$$E_{2k_F-k_h,N+1} - E_{2c} = \frac{(k_F + 4\pi/L)^2}{2M} + \frac{(k_F + 2\pi/L)^2}{2M} - \frac{k_h^2}{2M} - \frac{(2k_F - k_h + 6\pi/L)^2}{2M} = -\frac{(k_F - k_h)^2}{M} + O(1/L),$$

$$\langle 2k_F - k_h, N + 1 | \hat{\psi}^{\dagger}(0) | N \rangle = \frac{M(V(k_F - k_h + 4\pi/L) - V(k_F - k_h + 2\pi/L))}{L^{3/2}(k_F - k_h)^2} = \frac{2\pi M V'(k_F - k_h)^2}{L^{5/2}(k_F - k_h)^2}.$$
(6.56)

Note that in the above expression, the appearance of the derivative is essential to give the correct power of 1/L, which is evident when one considers the correspondence between the prefactor  $A_{1,+}(k)$  and the form factor (6.55) given below.

From finite size scaling the prefactor  $A_{1,+}(k)$  can be obtained using the matrix element above:

$$A_{1,+}(k) = \frac{L^5}{32\pi^5} |\langle k, N+1 | \hat{\psi}^{\dagger}(0) | N \rangle|^2 = \frac{M^2 V'(k-k_F)^2}{8\pi^3 (k-k_F)^4}, \tag{6.57}$$

where we have substituted  $k_h = 2k_F - k$  to obtain the final answer in terms of  $k_F \leq k \leq 3k_F$ . We note that the divergence of Eq. (6.57) as  $k \to k_F$  is generically the same  $\propto (k - k_F)^{-2}$  divergence seen in  $A_{1,-}(k \to k_F)$ . Yet again the integral of the spectral weight over  $\omega > 0$  remains finite as can be seen from Eq. (6.51).

The procedure to obtain the prefactors  $A_{n\geq 1,\pm}(k)$  is similar to the one used so far. In general, to lowest non-vanishing order  $A_{n\geq 1,\pm}(k)$  will be  $\propto V^{2n}$ , but one needs to sum contributions to the form factor expansion from a rapidly growing number of intermediate states. Moreover terms appearing with higher orders of  $\hat{V}$ need to be carefully separated from terms  $\propto (\log(L))^n$  that generate corrections to the exponent (see Eq. (6.32)). The latter procedure is demonstrated in Sec. IIIF where we calculated  $A_{0,-}(k)$  to the lowest non-vanishing order in  $\hat{V}$ . Figure 6.3 : The state in (a) depicts the parent state with respect to which we calculate the annihilation operator form factor to obtain prefactor  $C_1$ . That state in (b) depicts the only intermediate state which gives non-zero contribution to the form factor in the perturbative expansion to first order in  $\hat{V}$ .

### 6.4.4 Calculation of prefactor $C_1$

We now consider the prefactor  $C_1$  defined in Eq. (7.3). We denote by  $|m = 1, N - 1\rangle$ the lowest energy N - 1 particle eigenstate of the interacting fermion system of momentum  $3k_F$ . The corresponding state of the free fermion system (zeroth order term of the perturbative expansion) has two holes at the left Fermi point and one particle at the right Fermi point and is depicted in Fig. 6.3(a). We wish to calculate the annihilation operator form factor for this state and the N particle ground state  $|N\rangle$ :

$$\langle m = 1, N - 1 | \hat{\psi}(0) | N \rangle = \frac{1}{\sqrt{L}} \langle m = 1, N - 1 | \sum_{p''} {}^{'}{}_{p''} | N \rangle.$$
 (6.58)

We may again expand the states above like Eq. (6.39). We find that the first non-zero contributions in the perturbative expansion appear at the first order in  $\hat{V}$ . To this order we obtain the following two terms by expanding the states in the braand the ket vector perturbatively in  $\hat{V}$ :

$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{\rm FS} - E_{\alpha})} \langle m = 1, N - 1 | \sum_{p''} {}^{'}_{p''} | \alpha \rangle$$

$$\langle \alpha | \sum_{q,p,p'} V(q)'_{p+q p'-q' p'} {}^{'}_{p} | {\rm FS} \rangle, \qquad (6.59)$$
and
$$\sum_{|\alpha\rangle} \frac{1}{2L^{3/2}(E_{m=1,N-1} - E_{\alpha})} \langle \alpha | \sum_{p''} {}^{'}_{p''} | {\rm FS} \rangle$$

$$\langle m = 1, N - 1 | \sum_{q,p,p'} V(-q)'_{p+q p'-q' p'} {}^{'}_{p} | \alpha \rangle. \qquad (6.60)$$

The states which give non-zero contributions to the term (6.59) must have 0 momentum. Furthermore we must be able to transform them into the state  $|m = 1, N-1\rangle$ by the action of a single annihilation operator. This leaves only one possibility shown in Fig. 6.3(b). While for the term (6.60) to be non-zero we require states which have momentum  $3k_F$  which can be obtained from the ground state by the action of a single annihilation operator, i.e. a state with one hole of momentum  $-3k_F$ , which is impossible to achieve.

Thus we find the form factor as follows:

$$E_{\rm FS} - E_{3b} = \frac{k_F^2}{2M} + \frac{(k_F - 2\pi/L)^2}{2M} - \frac{(k_F + 2\pi/L)^2}{2M} - \frac{(3k_F)^2}{2M}$$
$$= -\frac{4k_F}{M} \left(k_F + \frac{\pi}{L}\right),$$
$$\langle m = 1, N - 1|\hat{\psi}(0)|\text{FS}\rangle = \frac{M(V(2k_F + 2\pi/L) - V(2k_F))}{4L^{3/2}k_F^2} = \frac{M\pi V'(2k_F)}{2L^{5/2}k_F^2} (6.61)$$

We may express  $C_1$  in terms of this form factor using the correspondence we have derived between the form factor calculated above and our desired prefactor:

$$C_1 = \frac{2(\rho_0 L)^5}{(2\pi)^5} |\langle m = 1, N - 1 | \hat{\psi}(0) | N \rangle|^2 = \frac{M^2 \rho_0 V'(2k_F)^2}{64\pi^7}.$$
 (6.62)

#### 6.4.5 Calculation of prefactor $A_2$

To obtain the prefactor  $A_2$  in Eq. (7.1) we must calculate the following matrix element:

$$\langle m = 2, N | \hat{\rho}(0) | N \rangle = \langle m = 2, N | \frac{1}{L} \sum_{q',k'} \hat{\psi}^{\dagger}_{k'+q'} {}'_{k'} | N \rangle,$$
 (6.63)

where  $|m = 2, N\rangle$  is the lowest energy eigenstate of the interacting system with momentum  $4k_F$ . The unperturbed version of this state, for N free fermions, contains two adjacent holes in the vicinity of the left Fermi point and two adjacent particles in the vicinity of the right Fermi point.

We evaluate the form factor in Eq. (6.63) by again perturbatively expanding the ket vectors in the free fermion basis, in powers of  $\hat{V}$  as in Eq. (6.39). We again disregard the terms that are zeroth order in  $\hat{V}$  since the density operator cannot create the m = 2 Umklapp state from the ground state, and consider the first order terms for the first non vanishing contributions.

The first term of  $O(\hat{V})$  is

$$\sum_{|\alpha\rangle} \frac{1}{2L^2 (E_{\rm FS} - E_{\alpha})} \langle m = 2, N | \sum_{q',k'} \hat{\psi}^{\dagger}_{k'+q'} {}^{\prime}_{k'} | \alpha \rangle$$
$$\langle \alpha | \sum_{q,p,p'} V(q) \hat{\psi}^{\dagger}_{p+q} \hat{\psi}^{\dagger}_{p'-q'} {}^{\prime}_{p'} | {\rm FS} \rangle.$$
(6.64)

The constraint from the first matrix element tells us that the intermediate state can differ from the Umklapp state  $|m = 2, N\rangle$  in only two ways since the density operator can either create a new particle-hole pair, or move an existing hole or particle to a different 'spot' in momentum space.

At this stage there are two possible types of intermediate states  $|\alpha\rangle$ . One possibility is a state with only one particle-hole pair on top of the ground state such that this pair is one of the ones contained in the configuration  $|m = 2, N\rangle$ . In this case the density operator creates the second excitation of roughly  $p \approx 2k_F$ . The second

Figure 6.4 : The states (a)-(d) indicated above are the only intermediate states that give non-zero contribution to the first order in  $\hat{V}$  in the perturbative expansion of the form factor in Eq. (6.63). This form factor is used to determine  $A_2$  to leading oder in  $\hat{V}$ . Contributions to the form factor from the states (a) and (b) pictured above are calculated in Eq. (6.65) and the contributions from states (c) and (d) in Eq. (6.67).

possible type is an intermediate state which contains two particle-hole pairs. Such a state can at most differ by one particle or hole from the configuration  $|m = 2, N\rangle$ since we can use the density operator to move this particle or hole to give the correct final configuration.

In the case where  $|\alpha\rangle$  contains only a single particle-hole pair, the only way the second matrix element can be non zero is if the action of the  $\hat{V}$  creates one particle hole pair of momentum  $p \approx 2k_F$  and the other of momentum 0. This cannot be done since the operator is explicitly momentum conserving. Thus we must only consider intermediate states with two particle hole pairs where one particle or hole may differ from the configuration of  $|m = 2, N\rangle$ .

We can further narrow down the intermediate state  $|\alpha\rangle$  to the two shown in

Fig. 6.4(a), (b). The reasoning is the following; let us try to generate a state that differs by one particle from the desired Umklapp state. To do so we use one of the creation-annihilation pairs to generate a hole at either  $-k_F$  or  $-k_F + 2\pi/L$  and a particle at either  $k_F + 2\pi/L$  or  $k_F + 4\pi/L$ . The second annihilation operator must then make the hole that was not made by the first. This choice along with the momentum conserving constraint fixes the last particle to be at approximately  $-3k_F$ . The above procedure will generate eight terms - for each of the states in Fig. 6.4(a), (b), there are two choices for where one of the creation operators can act and two independent choices for where one of the annihilation operators can act. The second creation and annihilation operators are fixed. This corresponds to a total of four ways to connect the ground state to each of the two states, giving a total of eight terms.

If on the other hand we try to generate a state that differs by one hole from the Umklapp state, we find that there is no way to do so given the kinematic constraints imposed by the interaction term, i.e. using a similar argument to the case of the deviant particle, we find for the state differing by one hole the only way to conserve momentum is to have the annihilation operator act outside the Fermi sea. Thus we exhaust all the possible intermediate states that give non zero contributions for both the matrix elements.

We may collect the various contributions to Eq. (6.64) for the states shown in Fig. 6.4 (a) and (b):

$$E_{\rm FS} - E_{4a} = \frac{-k_F^2}{2M} + \frac{(-k_F + 2\pi/L)^2}{2M} - \frac{(k_F + 2\pi/L)^2}{2M} - \frac{(-3k_F)^2}{2M}$$
  

$$= -\frac{4k_F}{M} \left(k_F + \frac{\pi}{L}\right),$$
  

$$M_{4a} = -\frac{M(V(2k_F + \frac{2\pi}{L}) - V(2k_F))}{8L^2k_F(k_F + \frac{\pi}{L})} - \frac{M(V(-2k_F - \frac{2\pi}{L}) - V(-2k_F))}{8L^2k_F(k_F + \frac{\pi}{L})},$$
  

$$E_{\rm FS} - E4b = \frac{(-k_F)^2}{2M} + \frac{(-k_F + 2\pi/L)^2}{2M} - \frac{(k_F + 4\pi/L)^2}{2M} - \frac{(-3k_F - 2\pi/L)^2}{2M}$$
  

$$= -\frac{4k_F}{M} \left(k_F + \frac{3\pi}{L} + \frac{2\pi}{k_FL^2}\right),$$
  

$$M_{4b} = -\frac{M(V(2k_F + \frac{2\pi}{L}) - V(2k_F + \frac{4\pi}{L}))}{8L^2k_F \left(k_F + \frac{3\pi}{L} + \frac{2\pi^2}{k_FL^2}\right)} - \frac{M(V(-2k_F - \frac{2\pi}{L}) - V(-2k_F - \frac{4\pi}{k_FL^2}))}{8L^2k_F \left(k_F + \frac{3\pi}{L} + \frac{2\pi^2}{k_FL^2}\right)}$$

Next we consider the second term that is linear order in V(q):

$$\sum_{|\alpha\rangle} \frac{1}{2L^2(E_{m=2,N} - E_{\alpha})} \langle \alpha | \sum_{q',k'} \hat{\psi}_{k'+q'}^{\dagger} | FS \rangle$$
$$\langle m = 2, N | \sum_{q,p,p'} V(-q) \hat{\psi}_{p+q}^{\dagger} \hat{\psi}_{p'-q'p'}^{\dagger} | \alpha \rangle.$$
(6.66)

We find that for the first matrix element to be non zero,  $|\alpha\rangle$  must contain only one particle hole excitation over the ground state which the density operator will remove. Furthermore, because  $\hat{V}$  conserves momentum,  $|\alpha\rangle$  must have momentum  $4k_F$ . The interaction term must act on the state  $|\alpha\rangle$  in the following way; one of the pairs of creation-annihilation operators must create one of the paired particle-hole excitations of momentum  $\approx 2k_F$  as found in  $|m = 2, N\rangle$ . The other is automatically constrained to change the momentum of a particle by  $\approx 2k_F$ . The combined action of the four fermion operators on  $|\alpha\rangle$  must generate  $|m = 2, N\rangle$  in order for the matrix element to be non zero. The allowed intermediate states that give a non zero contribution from the term (6.66) are illustrated in Fig. 6.4 (c), (d), and give the following contributions:

$$E_{m=2,N} - E_{4c} = \frac{(k_F + 2\pi/L)^2}{2M} + \frac{(k_F + 4\pi/L)^2}{2M} - \frac{(-k_F)^2}{2M} - \frac{(-k_F + 2\pi/L)^2}{2M} + \frac{(-k_F)^2}{2M} - \frac{(3k_F + 4\pi/L)^2}{2M} \\ = -\frac{4k_F}{M} \left( k_F + \frac{\pi}{L} \right), \\ M_{4c} = -\frac{M(V(2k_F + \frac{2\pi}{L}) - V(2k_F))}{8L^2k_F(k_F + \frac{\pi}{L})} - \frac{M(V(-2k_F - \frac{2\pi}{L}) - V(-2k_F))}{8L^2k_F(k_F + \frac{\pi}{L})}, \\ E_{m=2,N} - E_{1d} = \frac{(k_F + 2\pi/L)^2}{2M} + \frac{(k_F + 4\pi/L)^2}{2M} - \frac{(-k_F)^2}{2M} - \frac{(-k_F + 2\pi/L)^2}{2M} \\ + \frac{(-k_F + 2\pi/L)^2}{2M} - \frac{(3k_F + 6\pi/L)^2}{2M} \\ = -\frac{4k_F}{M} \left( k_F + \frac{3\pi}{L} + \frac{2\pi^2}{k_FL^2} \right), \\ M_{4d} = -\frac{M(V(2k_F + \frac{2\pi}{L}) - V(2k_F + \frac{4\pi}{L}))}{8L^2k_F(k_F + \frac{3\pi}{L} + \frac{2\pi^2}{k_FL^2})} - \frac{M(V(-2k_F - \frac{2\pi}{L}) + V(-2k_F - \frac{4\pi}{L}))}{8L^2k_F(k_F + \frac{3\pi}{L} + \frac{2\pi^2}{k_FL^2})}.$$

$$(6.67)$$

Collecting these terms gives the following result to leading order in  $1/L, \hat{V}$ 

$$\langle m = 2, N | \hat{\rho}(0) | GS \rangle = -\frac{2M\pi^2}{k_F^3 L^4} \left[ V'(2k_F) - k_F V''(2k_F) \right].$$

This means that for  $A_2$  we have

$$A_{2} = \frac{2(\rho_{0}L)^{8}}{(2\pi)^{8}\rho_{0}} |\langle m = 2, N|\hat{\rho}(0)|GS\rangle|^{2} = \frac{M^{2}\rho_{0}}{32\pi^{10}} [V'(2k_{F}) - k_{F}V''(2k_{F})]^{2}.$$
(6.68)

# **6.4.6** Calculation of prefactor $A_{0,-}(k)$

We can identify the prefactor  $A_{0,-}(k)$  using:

$$\begin{split} |\langle k, N-1|'(0)|N\rangle|^2 &= \frac{2\pi A_{0,-}(k)}{L} \left(\frac{2\pi}{L}\right)^{1-\mu_{0,-}} = \frac{2\pi A_{0,-}}{L} \left(1 + (1-\mu_{0,-})\log\left(\frac{2\pi}{L}\right) + \ldots\right) \\ &= \frac{2\pi}{L} \left(1 + A_{0,-}^{(2)} + O(\hat{V}^4)\right) \left(1 + (1-\mu_{0,-}^{(2)})\log\left(\frac{2\pi}{L}\right) + O(\log^2, \hat{V}^4)\right) \\ &= \frac{2\pi}{L} \left(1 + A_{0,-}^{(2)} + (1-\mu_{0,-}^{(2)})\log\left(\frac{2\pi}{L}\right) + O(\log^2, \hat{V}^4)\right), \\ \mu_{0,-}^{(2)} &= 1 - \frac{m^2}{4\pi^2} \frac{[V(0) - V(k_F + k)]^2}{(k_F + k)^2} - \frac{m^2}{4\pi^2} \frac{[V(0) - V(k_F - k)]^2}{(k_F - k)^2}, \quad (6.69) \end{split}$$

where in the second line of the above expression the first pair of parentheses contains the perturbative expansion of the prefactor and the second contains the expansion of the power law. The superscript (2) on a term indicates that the term is of  $O(\hat{V}^2)$  accuracy.

Similarly to Eq. (6.28), the form factor required to obtain  $A_{0,-}(k)$  is

$$\langle k, N-1|'(0)|N\rangle = \frac{1}{L^{1/2}} \langle k, N-1|\sum_{p''} p''|N\rangle.$$
 (6.70)

The state  $|k, N - 1\rangle$  contains a single hole of momentum k. The perturbative calculation of the form factor in Eq. (6.70) is complicated by the fact that at the zeroth order, i.e. for the non-interacting Fermi gas, the form factor is already non-zero. Consequently any dependence on the pair potential  $\hat{V}$  enters as a term beyond leading order. This is problematic because terms that arise after the first non-vanishing order in the expansion of a generic parent form factor make two types of contributions. They not only contribute sub-leading corrections to the prefactor, which we require, but also generate powers of  $\log(L)$  which give rise to the non-trivial power law in L.

Let us first expand the ket vectors in Eq. (6.70) up to second order in  $\hat{V}$  and then show that this is required because there are no  $O(\hat{V})$  contributions to the form factor.

$$k, N-1 \rangle = |k, N-1\rangle^{(0)} + \sum_{|\alpha\rangle} \frac{\langle \alpha | \hat{V} | k, N-1\rangle^{(0)}}{E_{k,N-1} - E_{\alpha}} |\alpha\rangle + \sum_{|\alpha\rangle,|\beta\rangle} \frac{\langle \alpha | \hat{V} | \beta\rangle \langle \beta | \hat{V} | k, N-1\rangle^{(0)}}{(E_{k,N-1} - E_{\alpha})(E_{k,N-1} - E_{\beta})} |\alpha\rangle$$

$$- \sum_{|\alpha\rangle} \frac{\langle k, N-1|^{(0)} \hat{V} | k, N-1\rangle^{(0)} \langle \alpha | \hat{V} | k, N-1\rangle^{(0)}}{(E_{k,N-1} - E_{\alpha})^2} |\alpha\rangle$$

$$- |k, N-1\rangle^{(0)} \sum_{|\alpha\rangle} \frac{|\langle \alpha | \hat{V} | k, N-1\rangle^{(0)}|^2}{2(E_{k,N-1} - E_{\alpha})^2},$$

$$|N\rangle = |FS\rangle + \sum_{|\alpha\rangle} \frac{\langle \alpha | \hat{V} | FS\rangle}{E_{FS} - E_{\alpha}} |\alpha\rangle + \sum_{|\alpha\rangle,|\beta\rangle} \frac{\langle \alpha | \hat{V} | \beta\rangle \langle \beta | \hat{V} | FS\rangle}{(E_{FS} - E_{\alpha})(E_{FS} - E_{\beta})} |\alpha\rangle$$

$$- \sum_{|\alpha\rangle} \frac{\langle FS | \hat{V} | FS \rangle \langle \alpha | \hat{V} | FS \rangle}{(E_{k,N-1} - E_{\alpha})^2} |\alpha\rangle$$

$$- |FS\rangle \sum_{|\alpha\rangle} \frac{|\langle \alpha | \hat{V} | FS \rangle|^2}{2(E_{FS} - E_{\alpha})^2}.$$

$$(6.71)$$

Clearly there is a trivial zeroth order contribution,

$$\frac{1}{L^{1/2}} \langle k, N - 1 |^{(0)'}{}_{k} | \text{FS} \rangle = \frac{1}{L^{1/2}}, \qquad (6.72)$$

where the annihilation operator removes the particle of momentum k from the ground state to connect it to  $|k, N-1\rangle^{(0)}$ .

Furthermore there can be no  $O(\hat{V})$  terms. There are two sources of first order terms corresponding to keeping a first order term in one of the ket vector expansions and the zeroth order term in the other. Moreover, due to the momentum conservation constraint imposed by  $\hat{V}$  the intermediate states corresponding to these two groups of terms will have a total momentum of either 0 (same as  $|FS\rangle$ ) or -k (same as  $|k, N - 1\rangle^{(0)}$ ). Finally, these intermediate states must be connected to  $|k, N - 1\rangle^{(0)}$  or  $|FS\rangle$ respectively, by the action of a single annihilation operator. The only zero momentum state that can be connected to  $|k, N - 1\rangle^{(0)}$  by a single annihilation operator is  $|FS\rangle$ since the annihilation operator has to remove momentum  $|k| < k_F$  by creating a single hole, necessarily carrying momentum k. On the other hand the same argument holds for intermediate states of momentum -k connecting the ground state by the action of ' on the left, i.e. the only state that can be connected to  $|FS\rangle$  in this way is  $|k, N - 1\rangle^{(0)}$ . Since the sum over intermediate states specifically forbids them from being identical to the unperturbed state, we obtain no contribution of  $O(\hat{V})$  to the form factor.

There are three ways of generating  $O(\hat{V}^2)$  terms: we may either pick  $O(\hat{V})$  terms in the ket vector expansions of both states in Eq. (6.70), or pick an  $O(\hat{V}^2)$  term from one ket vector and an unperturbed term from the other (there are two ways of doing this). However not every term will give a contribution. Some terms can be discarded for the same reason the  $O(\hat{V})$  terms drop out. This is because the structure of the matrix elements appearing in these terms is the same as in the  $O(\hat{V})$  terms i.e. they require the matrix element of the annihilation operator between either  $|FS\rangle$ or  $|k, N - 1\rangle^{(0)}$  and an intermediate state to be zero with the constraint that the intermediate state must have the same momentum as, but cannot be equal to either of those states. Thus we need only consider the following terms:

$$F_{1} = \frac{\sum_{|\alpha\rangle,|\beta\rangle} \sum_{p''} \sum_{p_{1},p_{1}',q_{1}} \sum_{p_{2},p_{2}',q_{2}} \langle \alpha |'_{p''} |\beta\rangle \langle k, N-1|^{(0)} V(q_{1}) \hat{\psi}_{p_{1}+q_{1}}^{\dagger} \hat{\psi}_{p'-q_{1}}^{\dagger} \hat{\psi}_{p_{1}'}^{\dagger} |\alpha\rangle}{4L^{5/2} (E_{k,N-1} - E_{\alpha}) (E_{\text{FS}} - E_{\beta})} \times \langle \beta | V(q_{2}) \hat{\psi}_{p_{2}+q_{2}}^{\dagger} \hat{\psi}_{p_{2}'-q_{2}}^{\dagger} |p_{2}'| \text{FS} \rangle,$$

$$F_{2} = -\frac{\sum_{|\alpha\rangle} \sum_{p''} \sum_{p_{1}, p'_{1}, q_{1}} \langle k, N-1|^{(0)'}{}_{p''}|FS\rangle |\langle FS|V(q_{1})\hat{\psi}^{\dagger}_{p_{1}+q_{1}}\hat{\psi}^{\dagger}_{p'-q_{1}}\hat{p}^{\prime}_{1}|\alpha\rangle|^{2}}{8L^{5/2}(E_{FS}-E_{\alpha})^{2}}, \quad (6.74)$$

$$F_{3} = -\frac{\sum_{|\alpha\rangle} \sum_{p''} \sum_{p_{1}, p'_{1}, q_{1}} \langle k, N-1|^{(0)'} |FS\rangle |\langle k, N-1|^{(0)} V(q_{1}) \hat{\psi}^{\dagger}_{p_{1}+q_{1}} \hat{\psi}^{\dagger}_{p'-q_{1}} |\alpha\rangle|^{2}}{8L^{5/2} (E_{k,N-1} - E_{\alpha})^{2}},$$
(6.75)

where

$$\langle k, N-1|^{(0)'}{}_{k}|\mathrm{FS}\rangle = \frac{1}{L^{1/2}} + F_{1} + F_{2} + F_{3} + O(\hat{V}^{4}).$$
 (6.76)

Let us now consider each of the terms in Eqs. (6.73) - (6.75) on the basis of allowed intermediate states. We observe that the only admissible states  $|\alpha\rangle$  in Eq. (6.73) are ones containing a net zero momentum pair of particle-hole pairs and a hole of momentum k. This is because the third matrix element in Eq. (6.73) will lead to states  $|\beta\rangle$  with two net-zero momentum particle-hole pairs, while the second matrix element can indeed admit two kinds of states. However, the matrix element of the annihilation operator will only connect  $|\alpha\rangle$  and  $|\beta\rangle$  that have identical pairs of net zero momentum particle-hole pairs, since the annihilation operator can then create the additional hole at k in  $\beta$ . Thus we may write the total contribution due to  $F_1$  as

$$F_{1} = \sum_{\substack{k_{F} \ p \ge -k_{F} \ q > k_{F} - p \ p' \neq k, p, p' \ge -k_{F}}}^{\infty} \sum_{\substack{p \neq k, p, p' \ge -k_{F}}}^{\min[k_{F}, q - k_{F}]} \frac{2[V(q) - V(p - p' + q)]^{2}}{4L^{5/2}(\Delta E)^{2}},$$
$$\Delta E = -\frac{q}{m}(q + (p - p')).$$
(6.77)

(6.73)

In Eq. (6.77) we enumerate all possible ways to generate an intermediate state with two net zero momentum particle-hole pairs. We can understand the limits on the sums in the following way: the first hole can be placed anywhere in the filled Fermi sea (except at the pre-existing hole of momentum k). With this hole in place, the momentum transfer to the corresponding particle (total momentum of p+q) needs to be large enough that the particle is created "outside" the filled Fermi sea. We first consider a positive momentum transfer and have that the transfer q must be larger than  $k_F - p$ . This sets the lower limit on the second sum. Finally we consider the second particle-hole pair. For the hole of momentum p' to lie within the Fermi sea and simultaneously have its corresponding particle of momentum p' - q outside the sea, we note that p' can have at most a momentum of  $q - k_F$  provided that  $q - k_F \leq k_F$ . If q exceeds this latter condition then p' may lie anywhere in the sea as long as it is not equal to p or k. If we then consider how the intermediate state corresponding to some allowed choice of p, p', q can be created with a negative momentum transfer we find that setting  $q \rightarrow p' - p - q$  also generates the same state. Moreover we may also relabel  $p \to p', p' \to p$  and repeat the same argument above, leading to an additional factor of 2 multiplying the sums. The relative signs of these terms is fixed by the canonical anti-commutation relations of the fermionic operators. Furthermore the only way to connect states  $\alpha$  and  $\beta$  in Eq. (6.73) with the annihilation operator matrix product is if the particle-hole pairs in the two states are identical, leading to the appearance of the square in Eq. (6.77).

A very similar argument to the one above allows us to write down an expression for  $F_2$ . The key difference is there is no restriction disallowing the holes from having a momentum k since the intermediate states are not involved in the annihilation operator matrix element. Thus we have

$$F_{2} = -\sum_{p \geq -k_{F}}^{k_{F}} \sum_{q > k_{F}-p}^{\infty} \sum_{\substack{p' \neq p, \\ p' \geq -k_{F}}}^{\min[k_{F}, q-k_{F}]} \frac{2[V(q) - V(p - p' + q)]^{2}}{8L^{5/2}(\Delta E)^{2}},$$
$$\Delta E = -\frac{q}{m}(q + (p - p')).$$
(6.78)

Lastly, for  $F_3$  we have two groups of terms. On the one hand akin to Eq. (6.77) we may have intermediate states with two particle-hole pairs. Here too there is a restriction on where the holes can be since there is a pre-existing hole of momentum k. On the other hand, we may also have states where the hole of momentum k has been 'moved', followed by the creation of an additional particle-hole pair.

$$F_{3} = -\sum_{\substack{p \neq k, \\ p \geq -k_{F}}}^{k_{F}} \sum_{q > k_{F}-p}^{\infty} \sum_{\substack{p' \neq k, p, \\ p' \geq -k_{F}}}^{\min[k_{F}, q-k_{F}]} \frac{2[V(q) - V(p - p' + q)]^{2}}{8L^{5/2}(\Delta E)^{2}} - \sum_{p=-k_{F}}^{p < k} \sum_{p'=-k_{F}}^{-k_{F}-p+k} \frac{2[V(k - p) - V(k - p')]^{2}}{8L^{5/2}(\Delta \tilde{E})^{2}} - \sum_{p>k}^{k_{F}} \sum_{p'>k_{F}-p+k}^{k_{F}} \frac{2[V(k - p) - V(k - p')]^{2}}{8L^{5/2}(\Delta \tilde{E})^{2}}, \Delta E = -\frac{q}{m}(q + (p - p')), \Delta \tilde{E} = \frac{k}{m}(p + p' - k) - \frac{pp'}{m}.$$
(6.79)

Thus upon summing these contributions we are left with the following terms:

$$\sum_{i} F_{i} = -(T_{4ex} + T_{3ex}^{(1)} + T_{3ex}^{(2)}),$$

$$T_{3ex}^{(1)} = \sum_{p=-k_{F}}^{p < k} \sum_{p'=-k_{F}}^{-k_{F}-p+k} \frac{[V(k-p) - V(k-p')]^{2}}{4L^{5/2}(\Delta \tilde{E})^{2}},$$

$$T_{3ex}^{(2)} = \sum_{p>k}^{k_{F}} \sum_{p'>k_{F}-p+k}^{k_{F}} \frac{[V(k-p) - V(k-p')]^{2}}{4L^{5/2}(\Delta \tilde{E})^{2}},$$

$$T_{4ex} = \sum_{q>k_{F}-k}^{\infty} \sum_{\substack{p' \neq k, \\ p' \geq -k_{F}}}^{\min[q-k_{F},k_{F}]} \frac{[V(q) - V(k-p'+q)]^{2}}{4L^{5/2}(\Delta E)^{2}},$$

$$\Delta E = -\frac{q}{m}(q + (k-p')),$$

$$\Delta \tilde{E} = \frac{k}{m}(p+p'-k) - \frac{pp'}{m}.$$
(6.80)

The notation above is suggestive of the fact that we are considering contributions to the form factor due to intermediate states with 4 excitations (2 particle-hole pairs) and 3 excitations (a particle-hole pair and an unpaired hole) separately.

Let us consider first:

$$\begin{split} T_{3\mathrm{ex}}^{(1)} &= \frac{m^2}{4L^{5/2}} \sum_{p=-k_F}^{p$$

Starting from the initial sum, we have separated the contributions from three different regions over which we need to sum the right side of the above equation.

Figure 6.5 : The various regions of integration corresponding to summing up the contribution to the form factor from states that have two holes and one particle excitation.

We have taken the continuum limit to express the sums as integrals in these regions, however, we have separated the contributions in regions (1) and (2) when one of the holes is within the region of momentum space,  $(k - \Delta, k)$  (corresponding to the lightly shaded triangles in Fig. (6.5)), and maintained these contributions as discrete sums. This is because the energy denominator will become badly behaved in this region and upon integration yield a logarithm of L; however we require more than logarithmic accuracy since such corrections may enter the prefactor.

While our expressions are formally correct for a fixed  $\Delta$ . We wish to demonstrate that the limit as  $\Delta \to 0$  of the above expression exists and subsequently obtain an analytic expression for it. In order to do this we will approximate the integral when the range of p nears  $k - \Delta$  and obtain the leading order  $\Delta$  dependent contribution. We will then carry out the discrete sums and obtain the leading order  $\Delta$  dependent contribution as well as any non-vanishing constants. We will show the existence of the  $\Delta \to 0$  limit by demonstrating that all divergent  $\Delta$  dependent contributions vanish. After approximating the behavior of the divergent integral in Eq. (6.81) at the upper bound we are left with

$$\frac{m^2}{16\pi^2 k^2 L^{1/2}} \mathcal{P}_+ \int_{\frac{1-k_F/k}{2}}^{1} dx \int_{-k_F/k}^{1-k_F/k-x} dy \left( \frac{[V(k(1-x)) - V(k(1-y))]^2}{(1-x)^2(y-1)^2} - \frac{m^2 [V(0) - V(k+k_F)]^2}{4\pi^2 L^{1/2}(k+k_F)^2} \left(\log(\Delta)\right) \right), \quad (6.81)$$

where the notation and meaning of the special principal value integration denoted by  $\mathcal{P}_+$  is defined in the appendix, see Eqs.(B.-4)-(B.-7).

Meanwhile we may evaluate the sum in Eq. (6.81) explicitly using the identities and expansions of the poly-gamma functions, Eqs (B.-5)-(B.-4):

$$\frac{m^2}{2L^{5/2}} \sum_{p=k-\Delta}^{p=k-2\pi/L} \sum_{p'=-k_F}^{p'=-k_F+k-p-2\pi/L} \frac{[V(k-p)-V(k-p')]^2}{(k-p)^2(p'-k)^2} \\
= \frac{m^2[V(0)-V(k+k_F)]^2L^{3/2}}{32\pi^4((N-1)/2+n_k)^2} \left(\log\left(\frac{2\pi\delta}{L}\right) - \log\left(\frac{2\pi}{L}\right) + \gamma_E\right) \\
= \frac{m^2[V(0)-V(k+k_F)]^2}{8\pi^2L^{1/2}(k_F+k)^2} \left(\log(\Delta) - \log\left(\frac{2\pi}{L}\right) + \gamma_E\right), \quad (6.82)$$

where  $\gamma_E \approx 0.5772$  is the Euler-Mascheroni constant.

We note how the logarithmic divergence appears with opposite sign in the finite sum and the boundary of the integral and thus drops out of the final answer. We therefore obtain an expression for the term

$$T_{3ex}^{(1)} = \frac{m^2}{4L^{1/2}} \mathcal{P}_+ \int_{\frac{1-k_F/k}{2}}^{1} \frac{dx}{2\pi} \int_{-k_F/k}^{-k_F/k+1-x} \frac{dy}{2\pi} \frac{[V(k(1-x)) - V(k(1-y))]^2}{k^2(1-x)^2(y-1)^2} \\ + \frac{m^2}{4L^{1/2}} \int_{-k_F}^{\frac{-k_F+k}{2}} \frac{dp}{2\pi} \int_{-k_F}^{\frac{-k_F+k}{2}} \frac{dp'}{2\pi} \frac{[V(k-p) - V(k-p')]^2}{(k-p)^2(p'-k)^2} \\ - \frac{m^2[V(0) - V(k+k_F)]^2}{8\pi^2L^{1/2}(k+k_F)^2} \left(\log\left(\frac{2\pi}{L}\right) - \gamma_E\right).$$
(6.83)

A similar calculation yields for the second term summing contributions from intermediate states with three excitations

$$T_{3ex}^{(2)} = \frac{m^2}{4L^{1/2}} \mathcal{P}_{-} \int_{1}^{\frac{1+k_F/k}{2}} \frac{dx}{2\pi} \int_{k_F/k+1-x}^{k_F/k} \frac{dy}{2\pi} \frac{[V(k(x-1)) - V(k(y-1))]^2}{k^2(1-x)^2(y-1)^2} + \frac{m^2}{4L^{1/2}} \int_{\frac{k_F+k}{2}}^{k_F} \frac{dp}{2\pi} \int_{\frac{k_F+k}{2}}^{k_F} \frac{dp'}{2\pi} \frac{[V(p-k) - V(p'-k)]^2}{(k-p)^2(p'-k)^2} - \frac{m^2[V(0) - V(k_F-k)]^2}{8\pi^2 L^{1/2}(k_F-k)^2} \left(\log\left(\frac{2\pi}{L}\right) - \gamma_E\right).$$
(6.84)

The sums from the contribution of intermediate states with two pairs of particlehole excitations are well behaved and can be immediately interpreted as integrals:

$$T_{4\text{ex}} = \frac{m^2}{4L^{5/2}} \sum_{q>k_F-k}^{\infty} \sum_{p'>-k_F}^{\min[-k_F+q,k_F]} \frac{[V(q) - V(k-p'+q)]^2}{q^2(k-p'+q)^2} = \frac{m^2}{16\pi^2 L^{1/2}} \left[ \int_{k_F-k}^{2k_F} dq \int_{-k_F}^{-k_F+q} dp' \frac{[V(q) - V(k-p'+q)]^2}{q^2(q+k-p')^2} \right] + \int_{2k_F}^{\infty} dq \int_{-k_F}^{-k_F} dp' \frac{[V(q) - V(k-p'+q)]^2}{q^2(q+k-p')^2} \right]$$
(6.85)

Thus we obtain the full contribution to the form factor up to order  $\hat{V}^2$ :

$$\begin{split} \langle k, N-1|'(0)|N \rangle \\ &= \frac{1}{2L^{1/2}} \bigg[ 2 - \frac{m^2}{4\pi^2} \bigg\{ \mathcal{P}_+ \int_{\frac{1-k_F/k}{2}}^{1} dx \int_{-k_F/k}^{-k_F/k+1-x} dy \frac{[V(k(1-x)) - V(k(1-y))]^2}{k^2(1-x)^2(y-1)^2} \\ &+ \mathcal{P}_- \int_{1}^{\frac{1+k_F/k}{2}} dx \int_{k_F/k+1-x}^{k_F/k} dy \frac{[V(k(x-1)) - V(k(y-1))]^2}{k^2(1-x)^2(y-1)^2} \\ &+ \int_{-k_F}^{-\frac{k_F+k}{2}} dp \int_{-k_F}^{-\frac{k_F+k}{2}} dp' \frac{[V(k-p) - V(k-p')]^2}{2(k-p)^2(p'-k)^2} \\ &+ \int_{k_F-k}^{2k_F} dp \int_{-k_F}^{k_F} dp' \frac{[V(p-k) - V(p'-k)]^2}{2(k-p)^2(p'-k)^2} \\ &+ \int_{2k_F}^{2k_F} dq \int_{-k_F}^{-k_F+q} dp' \frac{[V(q) - V(k-p'+q)]^2}{2q^2(q+k-p')^2} \\ &+ \int_{2k_F}^{\infty} dq \int_{-k_F}^{-k_F+q} dp' \frac{[V(q) - V(k-p'+q)]^2}{2q^2(q+k-p')^2} \\ &+ \left( \frac{[V(0) - V(k_F+k)]^2}{(k_F+k)^2} + \frac{[V(0) - V(k_F-k)]^2}{(k_F-k)^2} \right) \gamma_E \bigg\} \\ &+ \frac{m^2}{4\pi^2} \bigg( \frac{[V(0) - V(k_F+k)]^2}{(k_F+k)^2} + \frac{[V(0) - V(k_F-k)]^2}{(k_F-k)^2} \bigg) \log\bigg(\frac{2\pi}{L}\bigg) \bigg]. \end{split}$$

$$(6.86)$$

Comparing Eq. (6.86) with the field theory prediction, we obtain the leading correction to the prefactor  $A_{0,-}(k)$ :
$$A_{0,-}(k) = \frac{1}{2\pi} - \frac{m^2}{8\pi^3} \bigg\{ \mathcal{P}_+ \int_{\frac{1-k_F/k}{2}}^{1} dx \int_{-k_F/k}^{-k_F/k+1-x} dy \frac{[V(k(1-x)) - V(k(1-y))]^2}{k^2(1-x)^2(y-1)^2} \\ + \mathcal{P}_- \int_{1}^{\frac{1+k_F/k}{2}} dx \int_{k_F/k+1-x}^{k_F/k} dy \frac{[V(k(x-1)) - V(k(y-1))]^2}{k^2(1-x)^2(y-1)^2} \\ + \int_{-k_F}^{\frac{-k_F+k}{2}} dp \int_{-k_F}^{\frac{-k_F+k}{2}} dp' \frac{[V(k-p) - V(k-p')]^2}{2(k-p)^2(p'-k)^2} \\ + \int_{k_F-k}^{k_F} dp \int_{-k_F}^{k_F} dp' \frac{[V(p-k) - V(p'-k)]^2}{2(k-p)^2(p'-k)^2} \\ + \int_{k_F-k}^{2k_F} dq \int_{-k_F}^{-k_F+q} dp' \frac{[V(q) - V(k-p'+q)]^2}{2q^2(q+k-p')^2} \\ + \int_{2k_F}^{\infty} dq \int_{-k_F}^{-k_F+q} dp' \frac{[V(q) - V(k-p'+q)]^2}{2q^2(q+k-p')^2} \\ + \left(\frac{[V(0) - V(k_F+k)]^2}{(k_F+k)^2} + \frac{[V(0) - V(k_F-k)]^2}{(k_F-k)^2}\right) \gamma_E \bigg\}.$$
(6.87)

## 6.5 Summary

We present below a few results for the nonuniversal prefactors of correlation functions and dynamic response functions (see Eqs. (7.1)-(7.3) and Eq. (6.26)). The results of the perturbative calculations described in the previous section produce the following leading order results for the prefactors (see Eqs. (6.26), (6.34), (6.44), (7.1), (7.3)respectively):

$$A_{0,+}(k) = \frac{M^2 (V(k_F + k) - V(k_F - k))^2}{8\pi^3 (k_F^2 - k^2)^2}, \qquad (6.88)$$

$$A_{1,-}(k) = \frac{M^2 (V(2k_F) - V(k_F - k))^2}{32\pi^3 k_F^2 (k - k_F)^2},$$
(6.89)

$$A_{1,+}(k) = \frac{M^2 V'(k-k_F)^2}{8\pi^3 (k-k_F)^4}, \qquad (6.90)$$

$$C_1 = \frac{M^2 \rho_0 V'(2k_F)^2}{64\pi^7}, \qquad (6.91)$$

$$A_2 = \frac{M^2 \rho_0 (V'(2k_F) - k_F V''(2k_F))^2}{32\pi^{10}}.$$
 (6.92)

We see that all the prefactors above vanish when V(k) is constant, satisfying the expectation that a contact interaction  $V(r) \propto \delta(r)$  between the spinless fermions should not affect any observables. We were also able to reproduce the known values of the prefactors  $C_1, A_2$  [215] for the Calogero-Sutherland model, with our perturbative fermionic results, Eqs. (22), (23). We note that the results above would be hard to obtain using the conventional infinite size diagrammatic technique due to logarithmic divergences [219, 221], but the consideration of finite size scaling allows us to obtain these answers using essentially only undergraduate quantum mechanics tools. To lowest non-vanishing order, we see that the prefactors  $A_{0,+}(k), A_{1,\pm}(k)$  are  $\propto V^2$ . In general, to lowest non-vanishing order  $A_{n\geq 1,\pm}(k)$  will be  $\propto V^{2n}$ , although the complexity of the expressions grows. To obtain corrections beyond leading order to  $A_{n,\pm}(k)$  (and the first non-trivial correction to  $A_{0,-}(k), A_1$  and  $C_0$ ), one needs to carefully separate terms in the perturbation series that diverge as powers of  $\log(L)$  from the relevant correction to the prefactors, which we have demonstrated in Section IIIF above.

For the Lieb-Liniger model, we obtain analytic expressions for the prefactors of correlation functions non-perturbatively. We relate them to the exactly known form factors [249] which have been used recently for numerical evaluation of dynamic response functions [269]. In Fig. 7.4 we show results for a few prefactors for different interaction strengths (details will be presented elsewhere [158]), and some known limits are also plotted for comparison. As a further check we have also successfully reproduced the perturbative fermionic result for the prefactor  $A_2$  [see Eq. (6.92)] of the Cheon-Shigehara model [159], which is dual to the Lieb-Liniger model and has the same density correlations. It should be noted that recently the correlation functions for the Lieb-Liniger model have been treated without field theoretical considerations but rather by directly working with the microscopic details of the theory (see Ref. [214]), and the results of this work coincide with ours.

To summarize, we developed a general approach to calculating nonuniversal prefactors in static and dynamic correlation functions of 1D quantum liquids, by relating them to the finite-size scaling of the matrix elements of the corresponding operators. To find a given prefactor, only a single matrix element (form factor) between the lowest energy states needs to be evaluated, see Eqs. (7.11)-(7.12), (6.28). Moreover, the method does not rely on the integrability of a model. To demonstrate our approach, we calculated some prefactors in static and dynamic correlation functions for weakly interacting spinless fermions with an arbitrary pair interaction potential, see Eqs. (6.88)-(6.92).

Methods of Section II applied to an integrable model, allow one to obtain exact

Figure 6.6 : (Color online) Non-perturbative results for the Lieb-Liniger model of 1D bosons:  $2\pi^2 A_1$  (dashed black),  $512\pi^{10}A_2$  (solid green) and  $B_0$  (dot-dashed blue),  $-8\pi^2 B_1$  (dotted red) as functions of the Luttinger liquid parameter K. In the limit of strong interaction  $(K \to 1)$  our expressions for  $B_0$  and  $B_1$  agree with the known values [210], while  $A_1 \to 1/2\pi^2$ ,  $A_2 \to 0$  are in accordance with the density correlator of the free Fermi gas. We also match  $B_0$  in the weakly interacting regime  $(K \gg 1)$  to Popov's result (dashed line) [209], and show some numerical results (crosses) [161].

expressions for prefactors of the response functions, at arbitrary interaction strength. The results of the perturbative calculation detailed in Section III agree, in the proper limit, with the results [158] obtained by the methods of Section II for the exactly solvable Lieb-Liniger model, see Fig. 7.4.

# Chapter 7

# Correlation prefactors: exactly solvable models

### 7.1 Introduction

The following Chapter extends the framework developed in the previous chapter which addressed problem of obtaining non-universal prefactors of the correlation functions of 1D systems at zero temperature. The approach, which combined the effective field theory description of generic 1D quantum liquids with the finite size scaling of form factors (matrix elements), is used here to obtain prefactors of the long-distance behavior of equal time correlation functions as well as prefactors of singularities of dynamic response functions for two specific integrable models: the Calogero-Sutherland, and Lieb-Liniger models. The bulk of this chapter is devoted to the details of calculation of finite size form factors using microscopic techniques developed in the context of integrable models.

## 7.2 Overview

It was shown in the previous Chapter, as well as in Refs. [121, 122], that by combining the analysis of the Luttinger liquid Hamiltonian with the finite-size properties of certain matrix elements (form factors), a general technique for calculating these nonuniversal prefactors was developed for a generic 1D quantum liquid. Moreover, it has been shown recently [218]-[237] that dynamic response functions generically have singularities which can be described by effective Hamiltonians of impurities moving in Luttinger liquids. Analysis of the finite-size properties of these effective Hamiltonians can also be used to obtain prefactors of various dynamic response functions.

In what follows, we apply this technique to the calculation of prefactors of the correlation functions of integrable models, focusing specifically on two integrable models: the Calogero-Sutherland model (CSM) [239, 5, 241] of fermions interacting via a long range inverse-squared-distance potential, and the Lieb-Liniger model [242] of bosons with pairwise contact interactions. These models have the advantage of being solvable [241, 242] and additionally have readily available expressions for finite size form factors [203, 248, 249], which we will investigate to obtain analytic expressions for prefactors of their correlation functions valid in the thermodynamic limit. Furthermore, the Lieb-Liniger model has been realized with ultracold atomic gases [254, 253], and its correlation functions can be measured using interference [255, 256, 257], analysis of particle losses [258], photoassociation [258], or Bragg and photoemission spectroscopy [259], and density fluctuation statistics [260].

The presentation is organized as follows: In Sec. ?? we recapitulate the general results, obtained previously in [] and in Chapter , with the aim of setting up the notation and presenting a self-contained study. Sec. 7.4 we present details of the calculation of the prefactor in the dynamic structure factor (DSF) in the vicinity of the threshold singularity for the CSM, by working out the thermodynamic limit of form factors. This is to serve as an introduction to the more technically involved calculations presented in Sec. 7.5 where we obtain several prefactors of static and dynamic correlation functions of the Lieb-Liniger model, with details on the calculation of thermodynamic limits of form factors of this model. Additional technical details are contained in the Appendix.

## 7.3 Results from effective field theory

The Luttinger liquid theory [204, 205, 207, 208, 206] predicts the behavior of the correlation functions for spinless bosons and fermions of density  $\rho_0$ , when  $\rho_0 x \gg 1$  as (here  $k_F = \pi \rho_0$ )

$$\frac{\langle \hat{\rho}(x)\hat{\rho}(0)\rangle}{\rho_0^2} \approx 1 - \frac{K}{2(\pi\rho_0 x)^2} + \sum_{m\geq 1} \frac{A_m \cos(2mk_F x)}{(\rho_0 x)^{2m^2 K}},\tag{7.1}$$

$$\frac{\langle \hat{\psi}_B^{\dagger}(x)\hat{\psi}_B(0)\rangle}{\rho_0} \approx \sum_{m\geq 0} \frac{B_m \cos(2mk_F x)}{(\rho_0 x)^{2m^2 K + 1/(2K)}},\tag{7.2}$$

$$\frac{\langle \hat{\psi}_F^{\dagger}(x)\hat{\psi}_F(0)\rangle}{\rho_0} \approx \sum_{m\geq 0} \frac{C_m \sin\left[(2m+1)k_F x\right]}{(\rho_0 x)^{(2m+1)^2 K/2 + 1/(2K)}},\tag{7.3}$$

Here  $\hat{\rho}$  is the density operator,  $\hat{\psi}_B(\hat{\psi}_F)$  is the bosonic (fermionic) annihilation operator. The Hamiltonian describing these correlations is written as (we follow notations of Ref. [208])

$$H_0 = \frac{v}{2\pi} \int dx \, \left( K(\nabla \theta)^2 + \frac{1}{K} (\nabla \phi)^2 \right), \tag{7.4}$$

where v is the sound velocity, the canonically conjugate fields  $\phi(x)$ ,  $\theta(x)$  have the commutation relation  $[\phi(x), \nabla \theta(x')] = i\pi \delta(x - x')$ , and the components of the fermionic (bosonic) fields with momenta  $(2m + 1/2 \pm 1/2)k_F$  are written as

$$\psi_{F(B)}(x,t) \sim e^{i(2m+1/2\pm 1/2)[k_F x - \phi(x,t)] + i\theta(x,t)},$$
(7.5)

where each component is defined up to a non-universal prefactor. For repulsive bosons, one has K > 1, while for repulsive (attractive) fermions K < 1(> 1). In Eqs. (7.1)-(7.3), we included only slowest decaying power laws for each oscillating component. In principle, irrelevant corrections (see e.g. Ref. [265]) to Hamiltonian (7.4) and operators (7.5) generate various faster decaying power-law terms for each oscillating component in addition to the one presented above [266]. Here we are interested in prefactors of the leading decay in each oscillating component, however we can in principle track down further corrections by extending the method, though we expect such an extension to be quite non-trivial and potentially tedious.

#### 7.3.1 Prefactors of equal-time correlators

Let us consider a system of interacting bosons. Using the resolution of the identity in the expectation value  $\langle \hat{\psi}_B^{\dagger}(x,t)\hat{\psi}_B(0)\rangle$ , we get

$$\left\langle \hat{\psi}_{B}^{\dagger}(x,t)\hat{\psi}_{B}(0)\right\rangle = \sum_{k,\omega} e^{i(kx-\omega t)} \left| \langle k,\omega | \hat{\psi}_{B} | N \rangle \right|^{2},$$
(7.6)

where  $\langle k, \omega | \hat{\psi}_B | N \rangle$  is a form factor of the annihilation operator,  $|k, \omega \rangle$  denotes an eigenstate of N - 1 particles with momentum k and energy  $\omega$ , and  $|N\rangle$  is the ground state of N particles. For a finite system, k and  $\omega$  are not continuous, but will be quantized and consequently the spectral function is a collection of delta functions in  $(k, \omega)$ . We will now obtain a similar representation from the Luttinger liquid theory and compare it with Eq. (7.6) to obtain the non-universal prefactors  $B_m$ . Hamiltonian (7.4) can be written using left- and right-moving components  $\varphi_{L(R)} = \theta \sqrt{K} \pm \varphi / \sqrt{K}$ , [207] which dictates the time dependence of the  $\cos(2mk_F x)$ component of  $\langle \hat{\psi}_B(x,t) \psi_B(0,0) \rangle / \rho_0$ , at  $\rho_0 | x \pm vt | \gg 1$  as

$$\frac{(-1)^m B_m \rho_0^{-2m^2 K - 1/2K} \cos\left(2m k_F x\right)}{\left(i(vt+x)+0\right)^{\mu_L} \left(i(vt-x)+0\right)^{\mu_R}},\tag{7.7}$$

where  $\mu_{L(R)} = m^2 K \pm m + 1/4K > 0$ . The coefficients  $B_m$  appeared in Eq. (7.7) because we relate the t = 0 limit of  $\langle \hat{\psi}_B^{\dagger}(x,t)\hat{\psi}_B(0,0)\rangle/\rho_0$  to the right hand side of Eq. (7.2). The two factors in the denominator describe contributions from left (right)going excitations which propagate with velocities  $\mp v$ , and signs of the infinitesimal shifts in the denominators ensure that only excitations with negative (positive) momenta can be created at the respective branches. For a finite system with periodic boundary conditions on a circle of length L, conformal invariance dictates (see e.g. Ref. [207]), the right-going component  $(i(vt - x) + 0)^{-\mu_R}$  is replaced by

$$\left(\frac{\pi e^{i\pi(vt-x)/L}}{iL\sin\frac{\pi(vt-x)}{L}+0}\right)^{\mu_R} = \sum_{n_r \ge 0} C(n_r,\mu_R) \frac{e^{2i\pi n_r(x-vt)/L}}{(L/2\pi)^{\mu_R}},\tag{7.8}$$

$$C(n_r, \mu_R) = \frac{\Gamma(\mu_R + n_r)}{\Gamma(\mu_R)\Gamma(n_r + 1)},$$
(7.9)

and similarly for left-going components with  $\mu_R$ ,  $n_r$  substituted by  $\mu_L$ ,  $n_l$ . These equations lead to nontrivial predictions for the exact scaling of the form factors of a model describing interacting 1D bosons, e.g. the Lieb-Liniger model. By comparing the finite size excitation spectrum of  $H_0$  with the exact solution of the Lieb-Liniger model, up to  $\propto 1/L$  terms, we identify  $\mp 2\pi n_{l(r)}/L$  as the total momenta of excitations created near the left (right) quasi-Fermi points, i.e. the edges of the distribution of quasimomenta characterizing an eigenstate of the model. Considering  $n_r = n_l = 0$ then leads to the scaling law

$$\left| \langle m, N-1 | \hat{\psi}_B | 0, N \rangle \right|^2 = \frac{(-1)^m B_m \rho_0}{2 - \delta_{0,m}} \left( \frac{2\pi}{\rho_0 L} \right)^{\frac{4m^2 K^2 + 1}{2K}},$$
(7.10)

where  $|m, N\rangle$  denotes an eigenstate of N bosons having center of mass momentum  $2mk_F$ . We see that as a consequence of the criticality of the Luttinger liquid, form factors of the annihilation operator have nontrivial scaling with the system size, and the prefactors of these nontrivial powers of L are directly related to the prefactors of the correlation functions.

For density correlations, field correlation functions for fermions and correlators of spins, similar relations can be worked out as long as we represent the relevant operators in the bosonized language, and are given by

$$\left| \langle m, N-1 | \hat{\psi}_F | N \rangle \right|^2 \approx \frac{C_m \rho_0}{2(-1)^m} \left( \frac{2\pi}{\rho_0 L} \right)^{\frac{(2m+1)^2 K^2 + 1}{2K}},$$
(7.11)

$$|\langle m, N | \hat{\rho} | N \rangle|^2 \approx \frac{A_m \rho_0}{2} \left(\frac{2\pi}{\rho_0 L}\right)^{2m^2 K}.$$
(7.12)

Eqs. (7.10)-(??) allow one to evaluate the prefactors in Eqs. (7.1)-(7.3) by identifying a single, simplest "parent" form factor for each of the operators  $\hat{\rho}, \hat{\psi}_B, \hat{\psi}_F$ .

Field theoretical considerations allow to fix not only the form factor with  $n_r = n_l = 0$ , but also the form factors for all low-energy states. However, since for  $n_{r(l)} > 1$  states can be degenerate, one needs to understand how the spectral weight  $C(n_r, \mu_R)$  is split between different form factors. This question can be answered by matching contributions from each form factor with the free fermionic quasiparticle representation of the Luttinger Liquid [231]. Such representation has the same degeneracies as the exact solution, and we calculated [218] its form factors using the results of Ref. [267]. For a state with k particle-hole excitations near the right quasi-Fermi point specified by integers  $p_1 > ... > p_k \ge 0$  (particles) and  $q_1 < ... < q_k < 0$  (holes), with total momentum  $(2\pi/L) \sum_i (p_i - q_i) = 2\pi n_r/L$ , we obtain that the ratio of its form factor to the one with  $n_r = n_l = 0$  equals

$$f(\{p_i, q_i\}) = \text{Det}_{i,j \le k} \left(\frac{1}{p_i - q_j}\right) \prod_{i \le k} f^+(p_i) f^-(q_i),$$
(7.13)

where

$$f^+(p) = \frac{\Gamma(p+1-\sqrt{\mu_R})}{\Gamma(-\sqrt{\mu_R})\Gamma(p+1)}, f^-(q) = \frac{\Gamma(-q+\sqrt{\mu_R})}{\Gamma(1+\sqrt{\mu_R})\Gamma(-q)}$$

Normalization of the spectral weight leads to the following "multiplet summation rule" (see Ref. [218] and appendix of the same for details):

$$\sum_{\sum p_i - q_i = n_r} |f(\{p_i, q_i\})|^2 = C(n_r, \mu_R).$$
(7.14)

When  $n_l \neq 0$ , contributions from the left quasi-Fermi point are accounted for similarly, and the total form factor is a product of these two terms.

#### 7.3.2 Prefactors of singularities in dynamic response

We now apply the techniques described above to the prefactors of singularities in dynamic response functions [218]. For more comprehensive discussions of singularities in the response functions of 1D quantum liquids as well as the field theoretical description which captures these phenomena, see Refs. [219]-[237]. For concreteness we focus here on the Lieb-Liniger model of bosons. We will consider the dynamic structure factor

$$S(k,\omega) = \int dx dt^{i(\omega t - kx)} \langle \hat{\rho}(x,t) \hat{\rho}(0,0) \rangle, \qquad (7.15)$$

and the spectral function  $A(k,\omega) = -\frac{1}{\pi} \text{Im}G(k,\omega) \text{sign}\omega$  where the Green's function  $G(k,\omega)$  is defined as [270]

$$G(k,\omega) = -i \int dx dt e^{i(\omega t - kx)} \langle T[\hat{\psi}(x,t)\hat{\psi}^{\dagger}(0,0)] \rangle.$$
(7.16)

We consider the dynamic structure factor  $S(k, \omega)$  in more detail below, and present only final results for the spectral function  $A(k, \omega)$ . The exponents of  $S(k, \omega)$ ,  $\mu_{1,2}$  at Lieb's collective modes [242, 203]  $\varepsilon_{1,2}(k)$  can be written as  $\mu_{1,2} = 1 - \tilde{\mu}_R - \tilde{\mu}_L$ , where  $\tilde{\mu}_{R(L)}$  denote contributions from right (left) branches and are given by [232].

$$\tilde{\mu}_{R(L)} = \left(\frac{\sqrt{K}}{2} \pm \frac{1}{2\sqrt{K}} + \frac{\delta_{\pm}(k)}{2\pi}\right)^2.$$
(7.17)

The phases  $\delta_{\pm}$  can be obtained explicitly by knowing the analytic form of the dispersion curve, the Luttinger parameter K and momentum k [232], or by directly extracting them from the microscopic model (see Ref. [224] for the calculation of the phase shifts for bosons using the Bethe ansatz for the Lieb-Liniger model). Figure 7.1 : (a) Dynamic structure factor  $S(k,\omega)$  and (b) spectral function  $A(k,\omega)$ . Shaded areas indicate the regions where they are non-vanishing. Liebs particle mode  $\varepsilon_1(k)$  and hole excitation mode  $\varepsilon_2(k)$  are indicated. For spectral function  $A(k,\omega)$  region with  $\omega > 0(\omega < 0)$  corresponds to the particle (hole) part of the spectrum. The figure above indicates the notation for the prefactor of the singularity in the response functions at a given edge of support.

In addition to the quasi-Fermi points, the field theoretical description of the singularities [232] involves an impurity moving with velocity  $v_d = \partial \varepsilon_{1,2}(k)/\partial k$ , and  $S(k,\omega)$ in the vicinities of collective modes are written as

$$S(k,\omega) = S_{1,2}(k) \int dx dt e^{i\delta\omega t} D(x,t) L(x,t) R(x,t), \qquad (7.18)$$

where  $\delta \omega = \omega - \varepsilon_{1,2}(k)$ ,  $D(x,t) = \delta(x - v_d t)$  is the impurity correlator,  $L(R)(x,t) = (i(vt \pm x) + 0)^{-\tilde{\mu}_{L(R)}}$ , and we introduced prefactors  $S_{1,2}(k)$  which will be fixed from the comparison with form factors. In the vicinity of  $\varepsilon_2(k)$ , Eq. (7.18) results in

$$S(k,\omega) = \theta(\delta\omega) \frac{2\pi S_2(k)\delta\omega^{\tilde{\mu}_R + \tilde{\mu}_L - 1}}{\Gamma(\tilde{\mu}_R + \tilde{\mu}_L)(v + v_d)^{\tilde{\mu}_L}|v - v_d|^{\tilde{\mu}_R}},$$
(7.19)

while in the vicinity of  $\varepsilon_1(k)$  one has a two-sided singularity,

$$S(k,\omega) = \frac{\sin \pi \tilde{\mu}_L \theta(\delta\omega) + \sin \pi \tilde{\mu}_R \theta(-\delta\omega)}{\sin \pi (\tilde{\mu}_L + \tilde{\mu}_R)} \times \frac{2\pi S_1(k) \delta \omega^{\tilde{\mu}_R + \tilde{\mu}_L - 1}}{\Gamma(\tilde{\mu}_R + \tilde{\mu}_L)(v + v_d)^{\tilde{\mu}_L} |v - v_d|^{\tilde{\mu}_R}},$$
(7.20)

In finite size systems, L(x,t) and R(x,t) get modified, see Eq. (7.8). The change of D(x,t) to  $\sum_{n_D} e^{2i\pi n_D (x-v_d t)/L}$  corresponds to the quantization of the impurity momentum. Analysis of the scaling of the form factor with  $n_r = n_l = 0$  then leads to

$$|\langle k; N | \hat{\rho} | N \rangle|^2 \approx \frac{S_{1(2)}(k)}{L} \left(\frac{2\pi}{L}\right)^{\tilde{\mu}_R + \tilde{\mu}_L}, \qquad (7.21)$$

where the exponents are specified in Eq. (7.17), and  $|k; N\rangle$  denotes a state of N bosons with a single particle (hole) with high momentum, and a hole (particle) at the right quasi-Fermi point, such that the total momentum is k. The state on the right is the full N particle ground state (in this case that of the bosons). We note that in Eq. (7.21) k has to be fixed before taking the limit  $L \to \infty$ , since the  $k \to 0$  and  $L \to \infty$  limits do not commute in the nonlinear Luttinger Liquid theory [224, 231, 232]. It should also be noted that while our discussion focused on bosons in the Lieb-Liniger model, the relation in Eq. (7.21) is general and will apply equally well to the dynamic structure factor of the CSM, albeit with different exponents  $\tilde{\mu}_{R,L}$ .

Similar to the dynamic structure factor, the spectral function also displays singular behavior near the Lieb modes [224, 232] and we find relations for the prefactors of the spectral function in terms of form factors of the creation/annihilation operators. We set the following notation before presenting equations similar to Eq. (7.21) for the prefactors of the spectral function. In the vicinities of  $\varepsilon_1(k)$  and  $-\varepsilon_2(k)$ , respectively, the spectral function behaves like

$$A(k,\omega) = \theta(\omega \mp \varepsilon_{1(2)}(k)) \frac{2\pi \overline{A_{\pm}(k)}(\omega \mp \varepsilon_{1(2)}(k))^{\overline{\mu_R} + \overline{\mu_L} - 1}}{\Gamma(\overline{\mu_R} + \overline{\mu_L})(v + v_d)^{\overline{\mu_L}} |v - v_d|^{\overline{\mu_R}}},$$
(7.22)

with exponents [232]

$$\overline{\mu_{\pm}} = 1 - \overline{\mu_R} - \overline{\mu_L},$$

$$\overline{\mu_{R(L)}} = \left(\frac{\sqrt{K}}{2} - \frac{\delta_{\pm}(k)}{2\pi}\right)^2.$$
(7.23)

Note that in the above the phase shifts  $\delta_{\pm}$  can be calculated by knowing the dispersion curve and k [232] or from microscopics [224]. In Ref. [224], the phase shifts are bosonic and calculated from the Bethe ansatz for the Lieb-Liniger model. In Eq. (7.23) above, the expressions for the exponents refers to fermionic  $\delta_{\pm}$ , consistent with the notations of Refs. [224, 218]. The final answer for the exponents in Refs. [224, 232] are all in agreement provided the correct  $\delta_{\pm}$  are used.

By analyzing the scaling of the form factor of the creation/annihilation operator with  $n_r = n_l = 0$  we obtain

$$|\langle k, N \mp 1 | \psi^{(\dagger)} | N \rangle|^2 \approx \frac{2\pi \overline{A_{\mp}(k)}}{L} \left(\frac{2\pi}{L}\right)^{\overline{\mu_R} + \overline{\mu_L}}, \qquad (7.24)$$

with  $\overline{\mu_{R(L)}}$  specified in Eq. (7.23). The state  $|k, N \pm 1\rangle$  refers to a state with an additional particle or hole such that the total momentum is k, while  $|N\rangle$  is the ground state of N bosons.

Similarly, near  $\varepsilon_2(k)$  and  $-\varepsilon_1(k)$  we have

$$A(k,\omega) = \theta(\omega \mp \varepsilon_{2(1)}(k)) \frac{2\pi \underline{A}_{\pm}(k)(\omega \mp \varepsilon_{2(1)}(k))^{\underline{\mu}_{R}+\underline{\mu}_{L}-1}}{\Gamma(\underline{\mu}_{R}+\underline{\mu}_{L})(v+v_{d})^{\underline{\mu}_{L}}|v-v_{d}|^{\underline{\mu}_{R}}},$$
(7.25)

with exponents [232]

$$\underline{\mu_{\pm}} = 1 - \underline{\mu_R} - \underline{\mu_L}, \\ \underline{\mu_{R(L)}} = \left(\frac{3\sqrt{K}}{2} \mp \frac{1}{\sqrt{K}} - \frac{\delta_{\pm}(k)}{2\pi}\right)^2.$$
(7.26)

We note again that the phase shifts  $\delta_{\pm}$  are meant to be fermionic in line with notations of Refs. [232, 218]. Alternate expressions for the bosonic exponents with bosonic phase shifts calculated in terms of microsocopics of the Lieb-Liniger model can be found in Ref. [224]. Moreover for the prefactors we obtain

$$|\langle k, N \mp 1 | \psi^{(\dagger)} | N \rangle|^2 \approx \frac{2\pi A_{\pm}(k)}{L} \left(\frac{2\pi}{L}\right)^{\underline{\mu_R} + \underline{\mu_L}},\tag{7.27}$$

with  $\underline{\mu}_{R(L)}$  specified in Eq. (7.23). The state  $|k, N \pm 1\rangle$  refers to a state with two particles (holes) near the right quasi-Fermi point and an additional hole (particle) such that the total momentum is k, while  $|N\rangle$  is the ground state of N bosons. Let us also mention that for certain parameters  $A(k, \omega)$  can have a non-analyticity at  $-\varepsilon_1(k)$  instead of a divergence [232]. In this case  $\underline{A}_{-}(k)$  refers to the prefactor of the non-analytic part. The results for prefactors of the singularities in the spectral function for fermionic models are presented in Ref. [218] along with expressions for the relevant exponents.

### 7.4 Dynamic structure factor of CSM

We demonstrate here how the relationship between non-universal prefactors of correlation functions and form factors of excited states calculated for the corresponding operators, established in Eqs. (7.12) and (7.21) can be used to calculate prefactors in the correlation functions of the Calogero-Sutherland Model (CSM)[239, 5, 241] described by the Hamiltonian

$$\hat{H}_{\rm CSM} = -\sum_{j=1}^{N} \frac{\partial^2}{\partial z_j^2} + \sum_{1 \le j < k \le N} \frac{\lambda(\lambda - 1)\pi^2}{L^2 \sin^2 \left[\pi(z_j - z_k)/L\right]}.$$
(7.28)

Here N is the total number of particles of mass 1/2, contained in a system of length L held at density  $\rho_0 = N/L$  and  $\lambda = p/q > 1/2$  with p, q coprime controls the strength of the long range interactions between the constituent particles. The CSM admits an exact solution and consequently one obtains the energies of the ground state and the spectrum of excitations. Furthermore, the CSM ground state wavefunction has a product form [239]

$$\psi_{\rm GS} = \prod_{i < j} (z_i - z_j)^{\lambda} \prod_k z_k^{-\lambda(N-1)/2}, \text{ where } z_j = e^{\frac{2\pi i x_j}{L}},$$
(7.29)

and can be interpreted qualitatively as the wavefunction of a gas of non-interacting particles with fractional exchange statistics. The excited states can moreover be constructed from the ground state by multiplying by Jack symmetric polynomials [5] and are completely characterized by a set of N quantum numbers  $n_1, ..., n_N$ . These quantum numbers allow us to solve for the "asymptotic" quasimomenta which allow us to calculate physical observables like energy and excitation spectra, using [241]:

$$p_j = \frac{2\pi n_j}{L} + \frac{\pi(\lambda - 1)(2j - N - 1)}{L}, \quad j = 1, ..., N.$$
(7.30)

One may use the intuitive appeal of asymptotic plane wave states to interpret the quantum numbers  $n_j$  as the wave numbers of these asymptotic states. The algebraic structure of these polynomials is efficiently captured in terms of operations performed over Young tableaux [275, 276].

The CSM exhibits an additional property that leads to the existence of closed form expressions for form factors of physically relevant operators. The action of, e.g. the density operator, on the ground state can only result in particular types of states allowed under "selection rules", corresponding to states with a finite number of excitations [248]. Such a structure is a consequence of the fact that the ground state wavefunction and the operators acting on it admit symmetrized representations in terms of Jack polynomials which have to satisfy orthogonality relations. Qualitatively, creation of states with finite numbers of excitations can be thought of as a generalization of the action of the operator on the gas of free fermions where it results in a finite number of (real) particle-hole processes. Thus, the space of eigenstates of the CSM possesses a structure reminiscent of Fock space, which can equivalently be seen from the form of the ground state wavefunction. This property greatly constrains the complexity of the form factors of the CSM and allows one to obtain analytic expressions.

An expression for the density-density correlator is available for a finite sized system for the CSM due to Ref. [248]. One begins with a representation of the density fluctuation operator as

$$\rho(x) = \frac{1}{L} \sum_{j=1}^{N} \delta(x - x_j) - \frac{N}{L}$$
  
=  $\frac{1}{L} \left( \sum_{m=1}^{\infty} e^{\frac{2\pi i m}{L} x} \sum_{j=1}^{N} e^{-\frac{2\pi i m}{L} x_j} + \text{c.c.} \right),$  (7.31)

which may in turn be expanded in terms of Jack polynomials. Using the orthogonality relation for these polynomials the density-density correlator may be written as a sum over Young Tableaux[248]:

$$\langle \rho(x,t)\rho(0,0)\rangle = \frac{1}{L^2\lambda^2} \sum_{\kappa} \frac{|\kappa|^2 ([0']^{\lambda}_{\kappa})^2 [N]^{\lambda}_{\kappa}}{j^{\lambda}_{\kappa} [N-1+1/\lambda]^{\lambda}_{\kappa}} e^{i(2\pi|\kappa|/L)x - i(E_{\kappa}-\mu)t}.$$
(7.32)

where in the above expression the following notation is employed:

$$E_{\kappa} = \left(\frac{2\pi}{L}\right)^{2} \sum_{j=1}^{N} (\kappa_{j}^{2} + \lambda(N+1-2j)\kappa_{j}),$$

$$[a]_{\kappa}^{\lambda} = \prod_{(i,j)\in\kappa} (a + (j-1)/\lambda - (i-1)),$$

$$j_{\kappa}^{\lambda} = \prod_{(i,j)\in\kappa} \left(\kappa_{j}' - i + \frac{1+\kappa_{i}-j}{\lambda}\right)$$

$$\times \left(\kappa_{j}' - i + 1 + \frac{\kappa_{i}-j}{\lambda}\right),$$
(7.33)

where  $\kappa_i$  and  $\kappa'_j$  refer to the total length of the  $i^{th}$  row and the  $j^{th}$  column respectively. Moreover  $|\kappa|$ , called the "weight" of a partition is the total number of blocks appearing in a given Young diagram. The Young diagrams above are indexed by  $\kappa$  and particular "cells" or blocks contained in the diagram are indexed by (i, j), with  $i, j \ge 1$ . Note that the prime in [0'] is an instruction to skip over the cell i = 1, j = 1 which will cause all terms to evaluate to 0, see Eq. (7.33) in the product.

The expression in Eq. (7.32) is in direct correspondence to the form factor expansion of the correlation functions, see Eq. (7.6), which involves a sum over all excited eigenstates of the system; every term in the sum Eq. (7.32) explicitly contains the momentum k and energy  $\omega$  dependence of the state in the exponential term. Thus we may uniquely identify the energy and momentum of the state associated with a Young diagram in the sum. This provides a recipe for constructing Young diagrams associated with excited states created by the action of the density operator on the ground state; we start by ordering the quantum numbers of the ground state and record the shift in the  $i^{th}$  quantum number of the excited state as the length of the  $i^{th}$  row of the Young diagram ( $\kappa_i$  in the above notation). It should be noted that the selection rule mentioned earlier is encoded in the term  $[0']^{\lambda}_{\kappa}$  which appears as a coefficient when expanding the density operator in terms of Jack polynomials in Eq. (7.31). This term is zero unless the Young diagram  $\kappa$  contains a  $p \times q$  block. We may interpret this as an excitation of p quasiparticles and q quasiholes, and the mathematical structure reflects the fundamental way in which the density operator may act on the ground state.

We may directly obtain the form factor contribution from an excited state with a definite energy and momentum in terms of algebraic operations on a Young diagram. However to extract the prefactor of the correlation function in the thermodynamic Figure 7.2 : (a) Typical Young diagram which appears in the sum in the expression for the density-density correlator see Eq. (7.32). The basic block appears in all nonvanishing contributions to the density-density correlation function and is a  $q \times p$ block. Excited states correspond to states with quasiparticle (quasihole) excitations, rows (columns) of total length  $r_1, r_2, ...(c_1, c_2, ...)$  above the basic configuration, where  $\lim_{N\to\infty} c, r/N \neq 0$ ; (b) The Young diagram corresponding to an excited state of momentum k, with energy  $\varepsilon(k) = \lambda(k^2 - k_F^2)$  which defines the edge of support. For free fermions this state would correspond to a state with a particle-hole pair with momentum transfer k on top of the N particle ground state

limit from the form factor, one needs to carefully separate the non-trivial power-law of the system size L, see Eq. (7.21), from the remaining contribution. We carry out this analysis below for the prefactor of the dynamic structure factor and obtain analytic results.

We wish to identify a single diagram that captures the contribution to the dynamic structure factor when  $\omega \approx |\varepsilon(k)|$ , i.e. in the vicinity of the edge of support with  $\varepsilon(k) = \lambda(k^2 - k_F^2)$ , and evaluate the corresponding form factor in the thermodynamic limit. We know from the finite size analysis of the effective three subband model, see Refs. [218, 232], that the contribution to the prefactor S(k) comes from the form factor of the lowest energy state of momentum  $0 < k < 2k_F$ . Such a state is the CSM analog of free fermions with a particle near the right branch, and a hole of momentum  $k_F - k$ . Following our prescription for constructing Young diagrams for states with particle-hole excitations over the ground state, this corresponds to a Young diagram with a single column of length  $c_1 = \frac{L}{2\pi}k - (p-1)(q-1)$ . We note here that there are also singularities for k outside the range  $(0,2k_F)$  and the prefactors of these singularities can be obtained from form factors of the state with additional umklapp excitations (a hole on the left branch, a particle on the right) on top of the configuration described above. For simplicity we present only the result for the first prefactor. We will choose groups of terms appearing in the form factor expansion in Eq. (7.32) to evaluate together. This is necessitated by the fact that some terms may individually diverge factorially ( $\sim N^N$ ) in the thermodynamic limit, but their divergence is suppressed by other terms in the expression in such a way that the full expression will contain a non-trivial power law in L and a prefactor.

We first consider the following group of terms:

$$\mathcal{T}_1 = \frac{[N]^{\lambda}_{\kappa}}{[N + \frac{1}{\lambda} - 1]^{\lambda}_{\kappa}}.$$
(7.34)

Let us first evaluate the contribution from the basic block (see Fig. (7.2)) which should be present in all terms:

$$\mathcal{T}_{1}^{\text{b.b}} = \prod_{i=1}^{q} \prod_{j=1}^{p} \frac{\left(N + \frac{(j-1)}{\lambda} - (i-1)\right)}{\left(N + \frac{j}{\lambda} - i\right)}$$
$$= \left(1 + \frac{1}{N}\right) \prod_{j=1}^{p} \left(\frac{\lambda N + j - 1}{\lambda N - p + \lambda + j}\right)$$
$$\times \prod_{i=1}^{q} \left(\frac{N + 1 - i}{N + q - i}\right)$$
$$= 1 + O(1/N).$$
(7.35)

Additionally, the presence of particle-hole like excitations i.e. columns with length large in the thermodynamic sense, will lead to the following contribution:

$$\mathcal{T}_{1}^{\text{ex}} = \prod_{i=q+1}^{c_{1}} \frac{N-i+1}{N+\frac{1}{\lambda}-i} \\ = \frac{\Gamma(N-q+1)\Gamma(N-c_{1}+1/\lambda)}{\Gamma(N-q+1/\lambda)\Gamma(N-c_{1}+1)} = \left(1-\frac{k}{2k_{F}}\right)^{\frac{1}{\lambda}-1}.$$
 (7.36)

Next we consider the term  $\mathcal{T}_2 = \frac{([0']_{\kappa}^{\lambda})^2}{j_{\kappa}^{\lambda}}$ .

,

We again calculate separately the contribution from the first column corresponding to the particle-hole like excitation:

$$\mathcal{T}_{2}^{\text{ex}} = \prod_{i=2}^{q} \frac{(i-1)^{2}}{(c_{1}-i+q)(c_{1}-i+1+q-1/\lambda)} \\
\times \prod_{i=q+1}^{c_{1}} \frac{(i-1)^{2}}{(c_{1}-i+1/\lambda)(c_{1}-i+1)} \\
= \Gamma\left(\frac{1}{\lambda}\right) \frac{\Gamma(c_{1})^{3}}{\Gamma(c_{1}+q)\Gamma(c_{1}+q+1-1/\lambda)} \\
\times \frac{\Gamma(c_{1}+1-1/\lambda)}{\Gamma(c_{1}-q+1/\lambda)\Gamma(c_{1}-q+1)} \\
= \left(\frac{L}{2\pi}\right)^{-1-\frac{1}{\lambda}} \Gamma\left(\frac{1}{\lambda}\right) k^{-1-\frac{1}{\lambda}}.$$
(7.37)

The remaining terms evaluate to unity when properly normalized by requiring the basic block form factor evaluates to  $\rho_0$ . We may now combine the above expressions to obtain a prefactor of the dynamic structure factor using Eq. (7.21), the correspondence between the Luttinger parameter K and the interaction parameter  $\lambda$ ,  $\frac{1}{\lambda} = K$ , and the exponents  $\tilde{\mu}_R, \tilde{\mu}_L$  given by

$$\tilde{\mu}_{R(L)} = \left[\frac{\sqrt{K}}{2} + (-)\frac{1}{2\sqrt{K}} + \frac{\delta_{+(-)}(k)}{2\pi}\right]^2, \\ \delta_{\pm} = \mp \left(\frac{\sqrt{K}}{2} - \frac{1}{2\sqrt{K}}\right).$$
(7.38)

Thus we have

$$S_{\text{CSM}}(k) = \lim_{L \to \infty} 2\pi \left(\frac{L}{2\pi}\right)^{1+\frac{1}{\lambda}} |\langle k; N|\hat{\rho}|0, N\rangle|^2$$
$$= \frac{2\pi}{\lambda} \Gamma \left(1+\frac{1}{\lambda}\right) \left(\frac{2k_F k}{2k_F - k}\right)^{1-\frac{1}{\lambda}}.$$
(7.39)

We were also able to evaluate the equal-time density-density correlation prefactor  $A_1$ , see Eq. (7.1), by considering the form factor for a state with a single column of length N over the basic configuration. We obtain for the prefactor

$$A_1 = 2 \frac{\Gamma \left(1 + \frac{1}{\lambda}\right)^2}{(2\pi)^{\frac{2}{\lambda}}},\tag{7.40}$$

in agreement with the result of Ref. [215], where general expressions for the prefactors of oscillating components of the density-density correlators were obtained using the Replica Method.

## 7.5 Prefactors of the Lieb-Liniger Bose Gas

The one dimensional Bose gas with contact interactions of strength c > 0 is described by the Hamiltonian

$$H = \int dx \left[ \partial_x \psi^{\dagger}(x) \partial_x \psi(x) + c \psi^{\dagger}(x) \psi^{\dagger}(x) \psi(x) \psi(x) \right], \qquad (7.41)$$

where  $\psi^{\dagger}, \psi$  are the boson creation and annihilation operators, and where we assume the particles to have mass 1/2. The problem has an exact solution given by the Bethe Ansatz [242]. The solution of the *N*-particle interacting Bose gas is obtained in terms of well defined ground and excited states characterized by sets of *N* quasimomenta  $\{\lambda\}$  and  $\{\mu\}$ , respectively.

The quasimomenta of the ground state for the problem are given as the solutions

of the Bethe equations [203]:

$$L\lambda_j + \sum_{k=1}^N \theta(\lambda_j - \lambda_k) = 2\pi n_j = 2\pi (j - (N+1)/2), \qquad (7.42)$$
$$j = 1, 2, ..., N,$$

where  $\theta(\lambda) = i \log \left(\frac{ic+\lambda}{ic-\lambda}\right) = 2 \arctan \left(\frac{\lambda}{c}\right)$ , and where the equation carries the physical meaning of a particle traversing an entire turn of a ring and returning to its origin having picked up a total phase shift resulting from pairwise two particle scattering from the other particles in the way.

An arbitrary excited state may be created from the ground state by simply erasing some finite m < N of the  $n_j$ ,  $\{n_1^-, n_2^-, ..., n_m^-\}$ , and replacing them with new quantum numbers  $\{n_1^+, n_2^+, ..., n_m^+\}$ , that are not from the original set of  $n_j$ . If we call the new set of quantum numbers  $\{\tilde{n}_j\}$ , then  $\{\tilde{n}_j\}$  is obtained as  $\{n_j\}/\{n^-\} \cup \{n^+\}$ . The quasimomenta  $\mu_j$  characterizing this excited state are given by the solutions of the equations:

$$L\mu_j + \sum_{k=1}^N \theta(\mu_j - \mu_k) = 2\pi \tilde{n}_j, \quad j = 1, 2, ..., N.$$
(7.44)

#### 7.5.1 Form Factors

As demonstrated in the previous sections, full knowledge of matrix elements calculated from the microscopic theory is sufficient to obtain the associated prefactor of a correlation function. Thus, we wish to obtain the thermodynamic limits of various form factors between ground state and excited states specified by the field theory. The final expression for the limit of the form factors is expected to have a power law behavior as a function of the system length L, see Eqs. (7.11)-(7.12), and Eq. (7.21). Again our task is to separate the power law from the prefactor in the form factor

(7.43)

when faced with terms that are badly divergent  $(O(N^N))$ , so we proceed in a similar spirit to the calculation of the prefactor of the dynamic structure factor of the CSM.

We begin by considering the exact expressions for the form factors of the finite size Bose gas that arise from the machinery of the Algebraic Bethe Ansatz [203].

The form factor of the density operator between normalized eigenstates  $|\{\mu\}_N\rangle$ and  $|\{\lambda\}_N\rangle$  is given by the following expression [249]:

$$\mathcal{F} = \langle \{\mu\}_N | \rho(0) | \{\lambda\}_N \rangle$$
  
=  $\left| \frac{i P_{ex}}{\exp[-ix P_{ex}] - 1} \langle \{\mu\}_N | \int_0^x \mathrm{dy} \rho(y) | \{\lambda\}_N \rangle \right|$   
=  $\left| \frac{i P_{ex} \Omega}{||\{\mu\}_N ||^{1/2} ||\{\lambda\}_N ||^{1/2}} \right|,$  (7.45)

where

$$\Omega = \prod_{j} (V_{j}^{+} - V_{j}^{-}) \prod_{j,k} \left( \frac{\lambda_{jk} + ic}{\mu_{j} - \lambda_{k}} \right)$$
$$\times \frac{\text{Det}(\delta_{jk} + U_{jk})}{V_{p}^{+} - V_{p}^{-}}, \qquad (7.46)$$

$$V_j^{\pm} = \prod_k \frac{\mu_k - \lambda_j \pm ic}{\lambda_k - \lambda_j \pm ic}, \qquad (7.47)$$

$$U_{jk} = \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \left( \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j} \right) \\ \times (K(\lambda_j - \lambda_k) - K(\lambda_p - \lambda_k)),$$
(7.48)

$$K(\lambda_j, \lambda_k) = K(\lambda_j - \lambda_k) = \frac{2c}{(\lambda_j - \lambda_k)^2 + c^2}.$$
(7.49)

Note that in the above expression p is any integer and this freedom of choice is due to the rank deficient structure of  $U_{jk}$  [249], [269].

Similarly, the form factor for the boson annihilation operator is given by [249], [269]

$$\mathcal{G}^{-} = |\langle \{\mu\}_{N-1} | \psi(0) | \{\lambda\}_{N} \rangle |$$
  
=  $\left| \frac{\Xi}{||\{\mu\}_{N-1} ||^{1/2} ||\{\lambda\}_{N} ||^{1/2}} \right|,$  (7.50)

where

$$\Xi = \frac{1}{c^{1/2}} \frac{\prod_{j,k} (\lambda_{jk}^2 + c^2)^{1/2} \prod_j^{N-1} (\tilde{V}_j^+ - \tilde{V}_j^-)}{\prod_{j,k,k \neq N} (\lambda_j - \mu_k)}$$

$$\times \quad \text{Det}_{N-1} (\delta_{jk} + S_{jk}^-), \qquad (7.51)$$

$$\tilde{V}_j^{\pm} = \frac{\prod_{k=1}^{N-1} \mu_k - \lambda_j \pm ic}{\prod_{k=1}^{N} \lambda_k - \lambda_j \pm ic}, \qquad (7.52)$$

$$S_{jk}^{-} = \frac{i(\mu_j - \lambda_j)}{\tilde{V}_j^+ - \tilde{V}_j^-} \frac{\prod_{m \neq j}^{N-1} (\mu_m - \lambda_j)}{\prod_{m \neq j}^N (\lambda_m - \lambda_j)} \times (K(\lambda_j - \lambda_k) - K(\lambda_N - \lambda_k)).$$
(7.53)

Moreover, the form factor for the creation operator  $\mathcal{G}^+$  is obtained from the one for the annihilation operator  $\mathcal{G}^-$  by Hermitian conjugation.

In the above expressions the norms are given by [262], [277], [249], [203]

$$||\{\lambda\}_N|| = c^N \left\{ \prod_{j \neq k} \frac{\lambda_j - \lambda_k + ic}{\lambda_j - \lambda_k} \right\}$$
$$\times \operatorname{Det}_N \left( \delta_{jk} \left[ L + \sum_{m=1}^N K(\lambda_j - \lambda_m) \right] - K(\lambda_j - \lambda_k) \right).$$
(7.54)

Using the density operator and boson creation and annihilation operators, we may obtain expressions for the dynamic structure factor (DSF) and spectral function (SF) using the Lehmann representation [270].

#### 7.5.2 Thermodynamic Limits and Finte Size corrections

The various terms in the expressions for the form factors, Eqs. (7.45) - (7.50), depend directly on the quasimomenta of the ground and excited states. A thermodynamic description should not make reference to these discrete quasimomenta. We wish to define "thermodynamic quantities" that provide an equivalent, but sensibly defined description in the limit of large N, L. In the thermodynamic limit, the ground state of the Bose gas can be described using a continuous distribution of quasimomenta  $\lambda$ belonging to the set of real numbers (-q,q), while some excited state with n holes and m particles consists of quasimomenta in the set  $(-q,q)/(\lambda_1^-,...\lambda_n^-) \cup (\lambda_1^+,...,\lambda_m^+)$ . For this purpose we will use the density function  $\rho(\lambda)$  and the shift function  $F(\lambda|\nu)$ , that are conventionally used in thermodynamic descriptions of the Bose gas. These functions are given by [203]

$$\rho(\lambda) - \frac{1}{2\pi} \int_{-q}^{q} d\mu K(\lambda - \mu) \rho(\mu) = \frac{1}{2\pi},$$
(7.55)

$$F(\lambda|\nu) - \frac{1}{2\pi} \int_{-q}^{q} d\mu K(\lambda - \mu) F(\mu|\nu) = \frac{\theta(\lambda - \nu)}{2\pi},$$
(7.56)

where the shift function picks up an overall positive or negative sign depending on whether the excitation  $\nu$  in Eq. (7.56) is a particle or hole. Thus, the shift function for a particle-hole pair excitation can be described by  $F(\lambda|\mu^+, \lambda^-) = F(\lambda|\mu^+) - F(\lambda|\lambda^-)$ . Moreover using the linearity of Eq. (7.56), a general excited state with multiple excitations of both types can be written as a sum of shift functions taken with appropriate signs.

Furthermore, we may express the number density,  $\rho_0$ , of the Bose gas using the ground state density function

$$\int_{-q}^{q} d\lambda \rho(\lambda) = \rho_0. \tag{7.57}$$

To successfully account for all constant factors in the thermodynamic limit, we will need to consider finite size corrections (in orders of 1/L) to these functions and collect any corrections that sum to finite values in the thermodynamic limit. We begin by writing the system of N Bethe Ansatz equations that give the ground state quasimomenta of the N particle interacting Bose gas

$$L\lambda_j + \sum_{k=1}^N \theta(\lambda_j - \lambda_k) = 2\pi n_j = 2\pi (j - (N+1)/2),$$
  
$$j = 1, 2, ..., N.$$
 (7.58)

The quantum numbers  $n_j$  on the right hand side give us a natural way to index the quasimomenta as we take the above system over to the thermodynamic limit - we will want to keep the ratio of  $n_j/L$  a constant as we take  $L \to \infty$ . It is convenient to construct a generalized continuum version of the  $n'_is$  that smoothly interpolates between them in the thermodynamic limit, as described in Ref. [203].

Let us define a variable x that satisfies

$$L\lambda(x) + \sum_{k=1}^{N} \theta(\lambda(x) - \lambda_k) = 2L\pi x.$$
(7.59)

We now define a function  $\rho_L$  as

$$\rho_L(\lambda(x)) = \frac{dx}{d\lambda}.\tag{7.60}$$

This function carries the usual meaning of the density of quasiparticles in a given quasimomentum interval, but we will require it to retain finite size corrections.

To obtain finite size corrections to our thermodynamic quantities we may use the Euler-McLaurin formula [278] which quantifies the difference between a sum and an integral in terms of a series in powers of the discretization (in our case 1/L). We obtain for  $\rho_L$  [203]:

$$\rho_{L}(\lambda(x)) = \frac{1}{2\pi} + \frac{1}{2\pi L} \sum_{k=1}^{N} K(\lambda(x) - \lambda_{k}) \\
= \frac{1}{2\pi} + \frac{1}{2\pi L} \int_{-N/2L}^{N/2L} K(\lambda(x) - \mu(y)) L dy \\
- \frac{1}{2\pi L} \frac{B_{2}}{2} \left(1 - \frac{1}{2}\right) \left(\frac{dK(\lambda(x) - \mu(y))}{L dy}\right) \Big|_{y=-N/2L}^{y=-N/2L} \\
= \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-q}^{q} K(\lambda - \mu) \rho_{L}(\mu) d\mu - \frac{1}{2\pi L^{2}} \frac{1}{24} \left(\frac{K'(\lambda - \mu)}{\rho_{L}(\mu)}\right) \Big|_{\mu=-q}^{\mu=-q} \\
= \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-q}^{q} K(\lambda - \mu) \rho_{L}(\mu) d\mu \\
- \frac{1}{48\pi L^{2} \rho_{L}(q)} \left(K'(\lambda - q) - K'(\lambda + q)\right) + O(1/L^{3}).$$
(7.61)

Let us note two things about the above calculation. Firstly, in the above expression the discrepancy between the boundary value of  $x_{b.c.} = N/2L$  and  $n_N/L$ , the quantum number associated with the edge of the distribution q can be resolved by modifying the definition of q to absorb the linear term from the Euler-McLaurin expansion [203], i.e. we redefine q as,  $q \to \lambda_N + \frac{1}{2L\rho(\lambda_N)}$ . Secondly, we will only need to keep track of corrections to O(1/L) in the subsequent calculations since this captures all finite results in the thermodynamic limit.

We would like to characterize the excited state with the same precision as the ground state. Excited states are obtained from the ground state by replacing a finite number of ground state quantum numbers  $n_j$  with new quantum numbers  $\tilde{n}_j$  that are not from the set of ground state  $n_j$ . For a choice of finite N, L these excitations are well defined in that we will have two finite sets of quasimomenta  $\{\mu^+\}, \{\lambda^-\}$  corresponding to the particles and holes respectively. The notation is intended to be suggestive of the fact that  $\mu^+$  are "actual" quasimomenta in the excited state, while  $\lambda^-$  will occur only as a subset of the set of ground state quasimomenta and are absent

in the excited state.

It will be more convenient for our purposes to also consider "artificial" hole quasimomenta  $\{\mu^{-}\}\$  and attribute them to the excited state. This is meant in the following sense - all the quasimomenta of the excited state are shifted with respect to the ground state quasimomenta. We expect this shift to be of O(1/L). Had the hole quasimomenta been present in the excited state, they too would have been shifted with respect to their ground state counterparts,  $\{\lambda^{-}\}$ , on the order of 1/L. Consequently we may realize  $\mu_i^-$  as  $\lambda_i^- + O(1/L)$ .

We would now like to obtain thermodynamic versions of  $\{\mu^{\pm}\}, \{\lambda^{-}\}$  and retain O(1/L) corrections to them.

Let us start by considering the simplest case of a single particle-hole pair and some finite N, L. Furthermore let us denote the quantum number corresponding to the particle,  $n^+$ , and the quasimomentum,  $\mu^+$ , with the corresponding hole and its counterpart in the excited state defined as  $\lambda^-, \mu^-$  respectively.

For convenience, let us define the following notation. A single prime accompanying a sum,  $\Sigma'$ , means we are leaving out terms corresponding to  $\mu^+$ ,  $\lambda^-$  in the sum. A double prime accompanying the sum,  $\Sigma''$ , means we are adding in  $\mu^-$  in place of  $\mu^+$ . To go from  $\Sigma$  to  $\Sigma'$ , we explicitly treat the finite number of excitation terms. To go from  $\Sigma'$  to  $\Sigma''$  we compensate the extra terms with terms outside the sum of the opposite sign.

Starting from the Bethe equation for the particle excitation we proceed as follows:

$$L\mu^{+} = 2\pi n^{+} - \sum_{k=1}^{N} \theta(\mu^{+} - \mu_{k})$$

$$L\mu^{+} = 2\pi n^{+} - \sum_{k=1}^{N} (\theta(\mu^{+} - \mu_{k}) - \theta(\mu^{+} - \mu^{-}) + \theta(\mu^{+} - \mu^{-}))$$

$$L\mu^{+} = 2\pi n^{+} - \sum_{k=1}^{N} (\theta(\mu^{+} - \lambda_{k}) - K(\mu^{+} - \lambda_{k})(\mu_{k} - \lambda_{k})) + \theta(\mu^{+} - \lambda^{-})$$

$$-K(\mu^{+} - \lambda^{-})(\mu^{-} - \lambda^{-}) + O(1/L^{2})$$

$$\mu^{+} = 2\pi \frac{n^{+}}{L} - \sum_{k=1}^{N} \left( \frac{\theta(\mu^{+} - \lambda_{k}) + K(\mu^{+} - \lambda_{k}) \frac{F(\lambda_{k})}{L\rho_{L}(\lambda)}}{L} \right) + \frac{\theta(\mu^{+} - \lambda^{-})}{L} + O(1/L^{2})$$

$$\mu^{+} = 2\pi \frac{n^{+}}{L} - \int_{-q}^{q} d\lambda \theta(\mu^{+} - \lambda) \rho_{L}(\lambda) + \frac{1}{L} \left( -\int_{-q}^{q} d\lambda K(\mu^{+} - \lambda) F(\lambda) + \theta(\mu^{+} - \lambda^{-}) \right)$$

$$+O(1/L^{2}).$$
(7.62)

Note that in the above derivation we have used the fact that we expect  $\mu_k - \lambda_k, \mu^- - \lambda^-$  to be O(1/L), and the relation,  $(\lambda_j - \mu_j) = \frac{F(\lambda_j)}{L\rho(\lambda_j)} + O(1/L^2)$ . Using the last step of the above as our starting point, we may now take the thermodynamic limit. The prescription we use is to keep  $n^+/L$  constant as we send  $N, L \to \infty$ . Furthermore let us separate the O(1) and O(1/L) contributions to  $\mu^+$  for the sake of clarity, i.e.  $\mu^+ = \mu_0^+ + \mu_{1/L}^+ + O(1/L^2)$ . We obtain

$$\mu_{0}^{+} + \mu_{1/L}^{+} = 2\pi \frac{n^{+}}{L} - \int_{-q}^{q} d\lambda \theta(\mu_{0}^{+} - \lambda)\rho(\lambda) - \mu_{1/L}^{+} \int_{-q}^{q} d\lambda K(\mu_{0}^{+} - \lambda)\rho(\lambda) + \frac{1}{L} \left( -\int_{-q}^{q} d\lambda K(\mu_{0}^{+} - \lambda)F(\lambda) + \theta(\mu_{0}^{+} - \lambda^{-}) \right) + O(1/L^{2}),$$
(7.63)

where on the right hand side we have substituted  $\rho$  for  $\rho_L$ , etc. because the lowest order difference between such terms is higher order in 1/L than we are keeping.

Thus we obtain as the thermodynamic limit and the first order correction

$$\mu_{0}^{+} = 2\pi \frac{n^{+}}{L} - \int_{-q}^{q} d\lambda \theta(\mu_{0}^{+} - \lambda)\rho(\lambda),$$
  

$$\mu_{1/L}^{+} = \frac{1}{L} \left( -\frac{\int_{-q}^{q} d\lambda K(\mu^{+} - \lambda)F(\lambda) - \theta(\mu^{+} - \lambda^{-})}{1 + \int_{-q}^{q} d\lambda K(\mu_{0}^{+} - \lambda)\rho(\lambda)} \right)$$
  

$$= -\frac{F(\mu_{0}^{+})}{L\rho(\mu_{0}^{+})}.$$
(7.64)

In the last step above, we have used Eqs. (7.55), (7.56).

Similarly, let us consider the Bethe equation for the ground state quasimomentum,  $\lambda^{-}$ ,

$$L\lambda^{-} = 2\pi n^{-} - \sum_{k=1}^{N} \theta(\lambda^{-} - \lambda_{k})$$
$$\lambda^{-} = 2\pi \frac{n^{-}}{L} - \int_{-q}^{q} d\lambda \theta(\lambda^{-} - \lambda)\rho(\lambda) + O(1/L^{2}).$$
(7.65)

We wish to now obtain  $\mu^-$ . Since we expect  $\mu^- = \lambda^- + O(1/L)$ , and the lowest order correction comes from the usual shift in the excited state quasimomenta, we can quantify this exactly as

$$\mu_{0}^{-} = 2\pi \frac{n^{-}}{L} - \int_{-q}^{q} d\lambda \theta (\mu_{0}^{-} - \lambda) \rho(\lambda),$$
  
$$\mu_{1/L}^{-} = -\frac{F(\mu_{0}^{-})}{L\rho(\mu_{0}^{-})}.$$
 (7.66)

We are now ready to obtain the lowest order finite size corrections to the shift function. Let us start with a definition for the finite sized shift function. For an excited state with some set of particles and holes,  $\{\mu_1^+, \mu_2^+, ..., \mu_n^+\}, \{\mu_1^-, \mu_2^-, ..., \mu_n^-\},$ where  $\mu^-$  is used in the sense described above, we have

$$F_L(\lambda_j | \{\mu_1^+, \mu_2^+, ..., \mu_n^+\} \{\mu_1^-, \mu_2^-, ..., \mu_n^-\}) = (\lambda_j - \mu_j) L \rho_L(\lambda_j),$$
(7.67)

where  $\lambda_j, \mu_j$  are the ground and excited state quasimomenta respectively.

We may obtain an equation for  $F_L$  by subtracting the Bethe equations for  $\mu_j$  and  $\lambda_j$  for  $\mu_j$  not in  $\{\mu^+, \mu^-\}$ :

$$\begin{split} L(\lambda_{j} - \mu_{j}) + \sum_{k=1}^{N} (\theta(\lambda_{j} - \lambda_{k}) - \theta(\mu_{j} - \mu_{k})) &= 0 \\ L(\lambda_{j} - \mu_{j}) + \sum^{''} (\theta(\lambda_{j} - \lambda_{k}) - \theta(\mu_{j} - \mu_{k})) + \theta(\mu_{j} - \mu^{-}) - \theta(\mu_{j} - \mu^{-}) - \theta(\mu_{j} - \mu^{+}) &= 0 \\ L(\lambda_{j} - \mu_{j}) + \sum^{''} (\theta(\lambda_{j} - \lambda_{k}) - \theta(\lambda_{j} - \lambda_{k}) - K(\lambda_{j}, \lambda_{k})(\mu_{j} - \mu_{k} - \lambda_{j} + \lambda_{k}) \\ - \frac{1}{2}K'(\lambda_{j} - \lambda_{k})(\mu_{j} - \mu_{k} - \lambda_{j} + \lambda_{k})^{2} &= \theta(\mu_{j} - \mu^{+}) - \theta(\mu_{j} - \mu^{-}) \\ L(\lambda_{j} - \mu_{j}) \left(1 + \frac{1}{L} \sum^{''} K(\lambda_{j}, \lambda_{k})\right) &= \sum^{''} K(\lambda_{j}, \lambda_{k})(\lambda_{k} - \mu_{k}) + \theta(\lambda_{j} - \mu_{0}^{+}) - \theta(\lambda_{j} - \mu_{0}^{-}) \\ + \sum^{''} \frac{1}{2}K'(\lambda_{j} - \lambda_{k})(\mu_{j} - \mu_{k} - \lambda_{j} + \lambda_{k})^{2} + K(\lambda_{j}, \mu_{0}^{+})(\mu_{j} - \lambda_{j} - \mu_{1/L}^{+}) \\ - K(\lambda_{j}, \mu_{0}^{-})(\mu_{j} - \lambda_{j} - \mu_{1/L}^{-}), \\ 2\pi L(\lambda_{j} - \mu_{j})\rho_{L}(\lambda_{j}) &= \sum^{''} K(\lambda_{j}, \lambda_{k}) \frac{\lambda_{k} - \mu_{k}}{L\rho_{L}(\lambda_{k})} L\rho_{L}(\lambda_{k}) + \theta(\lambda_{j} - \mu_{0}^{+}) - \theta(\lambda_{j} - \mu_{0}^{-}) \\ + \sum^{''} \frac{1}{2}K'(\lambda_{j} - \lambda_{k})(\mu_{j} - \mu_{k} - \lambda_{j} + \lambda_{k})^{2} + K(\lambda_{j}, \mu_{0}^{+})(\mu_{j} - \lambda_{j} - \mu_{1/L}^{+}) \\ - K(\lambda_{j}, \mu_{0}^{-})(\mu_{j} - \lambda_{j} - \mu_{1/L}^{-}) \\ 2\pi F_{L}(\lambda) &= \theta(\lambda - \mu_{0}^{+}) - \theta(\lambda - \mu_{0}^{-}) + \int_{-N/2L}^{N/2L} Ldy K(\lambda, \mu(y)) \frac{F_{L}(\mu(y))}{L\rho_{L}(\mu(y))} \\ - \frac{1}{L} \left[ K(\lambda, \mu_{0}^{+}) \left( \frac{F(\lambda)}{\rho_{L}(\lambda)} - \frac{F(\mu_{0}^{+})}{\rho_{L}(\mu_{0}^{+})} \right) - K(\lambda, \mu_{0}^{-}) \left( \frac{F(\lambda)}{\rho_{L}(\lambda)} - \frac{F(\mu_{0}^{-})}{\rho_{L}(\mu_{0}^{-})} \right)^{2} + O(1/L^{2}). \end{split}$$
(7.68)

This makes the final equation for  $F_L(\lambda)$  up to  $O(1/L^2)$ 

$$F_{L}(\lambda) = \frac{\theta(\lambda - \mu_{0}^{+}) - \theta(\lambda - \mu_{0}^{-})}{2\pi} + \frac{1}{2\pi} \int_{-q}^{q} d\mu K(\lambda, \mu) F_{L}(\mu)$$
$$-\frac{1}{2\pi L} \left[ K(\lambda, \mu_{0}^{+}) \left( \frac{F_{L}(\lambda)}{\rho_{L}(\lambda)} - \frac{F_{L}(\mu_{0}^{+})}{\rho_{L}(\mu_{0}^{+})} \right) - K(\lambda, \mu_{0}^{-}) \left( \frac{F_{L}(\lambda)}{\rho_{L}(\lambda)} - \frac{F_{L}(\mu_{0}^{-})}{\rho_{L}(\mu_{0}^{-})} \right) \right]$$
$$+ \frac{1}{4\pi L} \int_{-q}^{q} d\mu \rho_{L}(\mu) K'(\lambda - \mu) \left( \frac{F_{L}(\lambda)}{\rho_{L}(\lambda)} - \frac{F_{L}(\mu)}{\rho_{L}(\mu)} \right)^{2} + O(1/L^{2}). \quad (7.69)$$

Note that in the above derivation,  $F_L(\lambda)$  is a condensed notation for  $F_L(\lambda|\mu^+, \mu^-)$ , and moreover this  $F_L$  is related to the more general one defined in Eq. (7.67) as

$$F_L(\lambda | \{\mu_1^+, \mu_2^+, ..., \mu_n^+\}; \{\mu_1^-, \mu_2^-, ..., \mu_n^-\})$$
  
=  $F_L(\lambda | \mu_1^+, \mu_1^-) + ... + F_L(\lambda | \mu_n^+, \mu_n^-).$  (7.70)

Furthermore, we expect that in the thermodynamic limit  $F_L(\lambda | \mu_i^+, \mu_i^-) = F(\lambda | \mu_i^+) - F(\lambda | \mu_i^-) + O(1/L)$ , where  $F(\lambda | \mu_i^\pm)$  is given by Eq. (7.56).

It is also convenient to define an analog of the ground state momentum density function for the excited state. This will help in calculating the normalization of the excited state that appears in Eq. (7.45) and Eq. (7.50). Before proceeding, let us write down the integral equations for the derivatives of  $\rho_L$ ,  $F_L$  as these will be used in the simplifications to follow.

$$2\pi F'_{L}(\lambda) = \int_{-q}^{q} d\mu K'(\lambda - \mu) F_{L}(\mu) + K(\lambda_{j} - \mu_{0}^{+}) - K(\lambda_{j} - \mu_{0}^{-}) + O(1/L),$$
$$2\pi \rho'_{L}(\lambda) = \int_{-q}^{q} d\mu K'(\lambda - \mu) \rho_{L}(\mu) + O(1/L^{2}).$$
(7.71)

To obtain the density function for the excited state, we start with the Bethe equation for a generic quasimomentum from the excited state, Eq. (7.44), and differentiate once with respect to  $\mu_j$ :

$$L = 2\pi L\rho_{ex,L}(\mu_{j}) - \sum_{k} 'K(\mu_{j} - \mu_{k}) - K(\mu_{j} - \mu^{-}) + K(\mu_{j} - \mu^{-}) - K(\mu_{j} - \mu^{+})$$

$$L = 2\pi L\rho_{ex,L}(\mu_{j}) - \sum_{k} ''K(\mu_{j} - \mu_{k}) - K(\mu_{j} - \mu^{+}) + K(\mu_{j} - \mu^{-})$$

$$L = 2\pi L\rho_{ex,L}(\lambda_{j}) - \sum_{k=1}^{N} \left[ K(\lambda_{j} - \lambda_{k}) - K'(\lambda_{j} - \lambda_{k}) \left( \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})} - \frac{F_{L}(\lambda_{k})}{L\rho_{L}(\lambda_{k})} \right) \right]$$

$$-2\pi \rho_{L}'(\lambda_{j}) \frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})} - K(\lambda_{j} - \mu_{0}^{+}) + K(\lambda_{j} - \mu_{0}^{-}) + O(1/L)$$

$$2\pi \rho_{ex}(\lambda) - 2\pi \rho_{L}'(\lambda) \frac{F_{L}(\lambda)}{L\rho_{L}(\lambda)} = 1 - \frac{K(\lambda - \mu_{0}^{+}) - K(\lambda - \mu_{0}^{-})}{L}$$

$$+ \int_{-q}^{q} d\nu \left[ K(\lambda - \nu)\rho_{L}(\nu) - K'(\lambda - \nu) \left( \rho_{L}(\nu) \frac{F_{L}(\lambda)}{L\rho_{L}(\lambda)} - \frac{F_{L}(\nu)}{L} \right) \right] + O(1/L^{2})$$

$$2\pi \rho_{L}(\lambda) + 2\pi \delta \rho(\lambda) - 2\pi \rho_{L}'(\lambda) \frac{F_{L}(\lambda)}{L\rho_{L}(\lambda)} = 1 + \int_{-q}^{q} d\nu K(\lambda - \nu)\rho_{L}(\nu)$$

$$-2\pi \rho_{L}'(\lambda) \frac{F_{L}(\lambda)}{L\rho_{L}(\lambda)} + 2\pi \frac{F_{L}'(\lambda)}{L}.$$
(7.72)

The first two steps of the above set of equations is exact. From the third step on we retain only terms up to O(1/L). In going to the third step we have expanded all terms dependent on  $\mu_j$  in terms of  $\lambda_j$  as this is what is useful for us in our final expression (see the following sections). In going to the last step we have used the relations given by Eq. (7.71).

From Eq. (7.72) we have

$$\rho_{ex,L}(\mu_j) - \rho_L(\lambda_j)$$

$$= \frac{1}{L} \left( F'_L(\lambda_j) - \frac{F_L(\lambda_j)\rho'_L(\lambda_j)}{\rho_L(\lambda_j)} \right) + O(1/L^2).$$
(7.73)

It is useful to consider the notion of a "partial thermodynamic limit". For instance the algebraic expression for the norm of the eigenstate appearing in Eq. (7.54) can be expressed in terms of a partial limit as established in Refs. [203], [262], [249]

$$\lim_{\text{partial}} ||\{\lambda\}||^2 = \prod_{j>k} \frac{\lambda_{jk}^2 + c^2}{\lambda_{jk}^2} \prod_j (2\pi Lc\rho(\lambda_j))$$
$$\times \text{Det}\left(1 - \frac{1}{2\pi}K\right), \qquad (7.74)$$

where the determinant is intended to be a Fredholm Determinant (see Ref. [279], Appendix D for more details). The above expression is a "partial" limit in the sense that it contains both the quasimomenta of the ground state which should be absent when the "full" thermodynamic limit is taken, as well as the Fredholm Determinant which is well defined in the TDL.

Similarly, we may write down the norm for the excited state as

$$\lim_{\text{partial}} ||\{\mu\}||^2 = \prod_{j>k} \frac{\mu_{jk}^2 + c^2}{\mu_{jk}^2} \prod_j (2\pi Lc\rho_{ex}(\mu_j)) \times \text{Det}\left(1 - \frac{1}{2\pi}K\right).$$
(7.75)

We will frequently use the notion of such partial limits because individual terms in the algebraic expressions for the form factors may not have good thermodynamic limits - they may often diverge in a non polynomial way. However, they can be regrouped to obtain expressions that have good (finite or power law divergent) limits. Thus we want the final expression for the form factor to be well defined in the limit, however the intermediate steps leading up to this will be a mixture of thermodynamically well defined quantities and the aforementioned partial thermodynamic limits. We will take partial limits of simple groupings occurring in the form factors in the following sections and later collect them and express the final answer for the form factors.

Let us consider the term  $V_j^+/V_j^-$  with  $V_j^{\pm}$  as defined in Eq. (7.47)

$$\begin{split} &\log\left(\frac{V_{j}^{+}}{V_{j}^{-}}\right) = \sum_{i=1}^{n} \log\left(\frac{\mu_{i}^{+} - \lambda_{j} + ic}{\mu_{i}^{+} - \lambda_{j} - ic}\right) - \sum_{i=1}^{n} \log\left(\frac{\lambda_{i}^{-} - \lambda_{j} + ic}{\lambda_{i}^{-} - \lambda_{j} - ic}\right) \\ &+ \sum_{m=1}^{N} \log\left(1 - \frac{F_{L}(\lambda_{m})}{L\rho_{L}(\lambda_{m})(\lambda_{m} - \lambda_{j} + ic)}\right) - \sum_{i=1}^{n} \log\left(\frac{\mu_{i}^{-} - \lambda_{j} + ic}{\lambda_{i}^{-} - \lambda_{j} + ic}\right) + \sum_{i=1}^{n} \log\left(\frac{\mu_{i}^{-} - \lambda_{j} - ic}{\lambda_{i}^{-} - \lambda_{j} - ic}\right) \\ &= \sum_{i=1}^{n} \log\left(\frac{\mu_{i}^{+} - \lambda_{j} + ic}{\mu_{i}^{+} - \lambda_{j} - ic}\right) - \sum_{i=1}^{n} \log\left(\frac{\mu_{i}^{-} - \lambda_{j} + ic}{\mu_{i}^{-} - \lambda_{j} - ic}\right) \\ &+ \sum_{m=1}^{N} i \frac{2cF_{L}(\lambda_{m})}{L\rho_{L}(\lambda_{m})((\lambda_{m} - \lambda_{j})^{2} + c^{2})} + \sum_{m=1}^{N} \frac{i}{2} \frac{4c(\lambda_{m} - \lambda_{j})F_{L}^{2}(\lambda_{m})}{L^{2}\rho_{L}^{2}(\lambda_{m})((\lambda_{m} - \lambda_{j})^{2} + c^{2})^{2}} + O(1/L^{2}) \\ &= \sum_{i=1}^{n} i \left[\theta(\lambda_{j} - \mu_{i,0}^{+}) - K(\lambda_{j} - \mu_{i,0}^{+})\mu_{i,1/L}^{+} - \theta(\lambda_{j} - \mu_{i,0}^{-}) + K(\lambda_{j} - \mu_{i,0}^{-})\mu_{i,1/L}^{-}\right] \right] \\ &+ \sum_{m=1}^{N} i \frac{F_{L}(\lambda_{m})K(\lambda_{m} - \lambda_{j})}{L\rho_{L}(\lambda_{m})} - \sum_{m=1}^{N} \frac{i}{2} \frac{K'(\lambda_{m} - \lambda_{j})F_{L}^{2}(\lambda_{m})}{L^{2}\rho_{L}^{2}(\lambda_{m})} + O(1/L^{2}) \\ &= 2\pi iF_{L}(\lambda_{j}) + \frac{i}{L} \left(K(\lambda_{j} - \mu_{0}^{+})\frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})} - K(\lambda_{j} - \mu_{0}^{-})\frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})}\right) \\ &- \frac{i}{L} \int_{-q}^{q} d\mu \frac{F_{L}^{2}(\mu)}{\rho_{L}(\mu)}K'(\lambda_{j} - \mu) + O(1/L^{2}) \\ &= 2\pi iF_{L}(\lambda_{j}) + \frac{i}{L} \left(K(\lambda_{j} - \mu_{0}^{+})\frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})} - K(\lambda_{j} - \mu_{0}^{-})\frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})}\right) \\ &+ \frac{i}{L} \int_{-q}^{q} d\mu K'(\lambda_{j} - \mu)\frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})} \left(F_{L}(\mu) - \frac{F_{L}(\lambda_{j})\rho_{L}(\mu)}{2\rho_{L}(\lambda_{j})}\right) + O(1/L^{2}). \end{split}$$

Now using the relations given by Eq. (7.71) we have

$$\left(K(\lambda_j - \mu_0^+) - K(\lambda_j - \mu_0^-) + \int_{-q}^{q} d\mu K'(\lambda_j - \mu) \left(F_L(\mu) - \frac{F_L(\lambda_j)\rho_L(\mu)}{2\rho_L(\lambda_j)}\right)\right) \\
= 2\pi \left(F'_L(\lambda_j) - \frac{F_L(\lambda_j)\rho'_L(\lambda_j)}{2\rho_L(\lambda_j)}\right). (7.77)$$

170
Substituting in Eq. (7.76) we obtain

$$\log\left(\frac{V_j^+}{V_j^-}\right) = 2\pi i F_L(\lambda_j) \left[1 + \frac{1}{L\rho_L(\lambda_j)} \left(F_L'(\lambda_j) - \frac{F_L(\lambda_j)\rho_L'(\lambda_j)}{2\rho_L(\lambda_j)}\right)\right] + O(1/L^2)(7.78)$$

Thus we may handle the following term appearing in  $\Omega$ , Eq. (7.46), as follows:

$$\prod_{j}^{N} (V_{j}^{+} - V_{j}^{-}) = \prod_{j}^{N} V_{j}^{+} \left( 1 - \exp\left[ -2\pi i F_{L}(\lambda_{j}) \left( 1 + \frac{1}{L\rho_{L}(\lambda_{j})} \left( F_{L}'(\lambda_{j}) - \frac{F_{L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{2\rho_{L}(\lambda_{j})} \right) \right) \right] \right) \\
= \prod_{j}^{N} V_{j}^{+} e^{i\phi(j)} 2 \sin\left[ \pi F_{L}(\lambda_{j}) \left( 1 + \frac{1}{L\rho_{L}(\lambda_{j})} \left( F_{L}'(\lambda_{j}) - \frac{F_{L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{2\rho_{L}(\lambda_{j})} \right) \right) \right],$$
(7.79)

where in the above expression the term  $\phi(j)$  is purely a phase. Such terms will drop out in the final answer because we only need the absolute square of the form factor. The product of sine terms can be expanded in the following way

$$V = \prod_{j}^{N} \sin \left[ \pi F_{L}(\lambda_{j}) \left( 1 + \frac{1}{L\rho_{L}(\lambda_{j})} \left( F_{L}'(\lambda_{j}) - \frac{F_{L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{2\rho_{L}(\lambda_{j})} \right) \right) \right]$$
  
$$= \left( \prod_{j}^{N} \sin[\pi F_{L}(\lambda_{j})] \right) \exp \left[ \sum_{j}^{N} \frac{\pi F_{L}(\lambda_{j}) \cos(\pi F_{L}(\lambda_{j}))}{L\rho_{L}(\lambda_{j}) \sin(\pi F_{L}(\lambda_{j}))} \left( F_{L}'(\lambda_{j}) - \frac{F_{L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{2\rho_{L}(\lambda_{j})} \right) \right]$$
  
$$= \left( \prod_{j}^{N} \sin[\pi F_{L}(\lambda_{j})] \right) \exp \left[ \pi \int_{-q}^{q} \frac{\cos(\pi F_{L}(\lambda))}{\sin(\pi F_{L}(\lambda))} F_{L}(\lambda) \left( F_{L}'(\lambda) - \frac{F_{L}(\lambda)\rho_{L}'(\lambda)}{2\rho_{L}(\lambda)} \right) \right]$$
(80)

The other terms in  $\Omega$  may also be regrouped

$$\Omega = \Theta \times V \prod_{j} 2ie^{i\phi(j)}V_{j}^{+} \prod_{j,k} \left(\frac{\lambda_{jk} + ic}{\mu_{j} - \lambda_{k}}\right)$$

$$= \Theta \times V \prod_{j} e^{i\phi(j) + 3i\pi/2}V_{j}^{+} \frac{2}{\lambda_{j} - \mu_{j}} \prod_{j,k} (\lambda_{jk} + ic) \prod_{j \neq k} \frac{1}{\mu_{j} - \lambda_{k}}$$

$$= \Theta \times V \prod_{j} e^{i\phi'(j)}V_{j}^{+} \frac{2L\rho_{L}(\lambda_{j})}{F_{L}(\lambda_{j})} \prod_{j,k} (\lambda_{jk} + ic) \prod_{j \neq k} \frac{1}{\mu_{j} - \lambda_{k}} \prod_{i=1}^{n} \left(\frac{F_{L}(\lambda_{i}^{-})}{L\rho_{L}(\lambda_{i}^{-})(\lambda_{i}^{-} - \mu_{i}^{+})}\right).$$
(7.81)

where we use  $\Theta$  to denote  $\frac{\text{Det}(\delta_{jk}+U_{jk})}{V_p^+-V_p^-}$ .

With this form for  $\Omega$  we may combine it with the norm terms :

$$\begin{aligned} |\mathcal{F}| &= \left| iP_{ex}\Theta \times V \prod_{j} e^{i\phi'(j)} V_{j}^{+} \frac{2L\rho_{L}(\lambda_{j})}{F_{L}(\lambda_{j})} \prod_{j,k} (\lambda_{jk} + ic) \prod_{j\neq k} \frac{1}{\mu_{j} - \lambda_{k}} \prod_{i=1}^{n} \left( \frac{F_{L}(\lambda_{i}^{-})}{L\rho_{L}(\lambda_{i}^{-})(\lambda_{i}^{-} - \mu_{i}^{+})} \right) \right. \\ &\times \prod_{j\neq k} \frac{\lambda_{jk}^{1/2} \mu_{jk}^{1/2}}{(\lambda_{jk} + ic)^{1/4} (\lambda_{jk} - ic)^{1/4} (\mu_{jk} + ic)^{1/4} (\mu_{jk} - ic)^{1/4}} \times \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j} \frac{1}{(2\pi L c \rho_{L}(\lambda_{j}))} \left( 1 + \frac{\rho_{ex}(\mu_{j}) - \rho_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})} \right)^{-1/2} \right| \\ &= \left| iP_{ex}\Theta \times V \prod_{j} V_{j}^{+} \frac{1}{\pi F_{L}(\lambda_{j})} \prod_{j,k} (\lambda_{jk} + ic) \prod_{j\neq k} \frac{1}{\mu_{j} - \lambda_{k}} \\ &\times \prod_{j\neq k} \frac{\lambda_{jk}^{1/2} \mu_{jk}^{1/2}}{(\lambda_{jk} + ic)^{1/4} (\lambda_{jk} - ic)^{1/4} (\mu_{jk} - ic)^{1/4}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{i=1}^{n} \left( \frac{F_{L}(\lambda_{i}^{-})}{L(\rho_{L}(\lambda_{i}^{-})\rho_{ex}(\mu_{i}^{+}))^{1/2} (\lambda_{i}^{-} - \mu_{i}^{+})} \right) \times \prod_{j} \left( 1 + \frac{F_{L}'(\lambda_{j}) - \frac{F_{L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{L\rho_{L}(\lambda_{j})}} \right)^{-1/2} \right| \\ &= \left| iP_{ex}\Theta \times V \prod_{j} \frac{1}{\pi F_{L}(\lambda_{j})} \prod_{j\neq k} \frac{\lambda_{jk}^{1/2} \mu_{jk}^{1/2}}{\mu_{j} - \lambda_{k}} \prod_{i=1}^{n} \left( \frac{F_{L}(\lambda_{i}^{-})}{L(\rho_{L}(\lambda_{i}^{-})\rho_{ex}(\mu_{i}^{+}))^{1/2} (\lambda_{i}^{-} - \mu_{i}^{+})} \right) \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \times \prod_{j,k} \frac{(\lambda_{jk} + ic)^{1/4} (\mu_{jk} + ic)^{1/4}}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \times \prod_{j,k} \frac{(\lambda_{jk} + ic)^{1/4} (\mu_{jk} + ic)^{1/4}}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1}{2\pi} K \right)^{-1} \\ &\times \prod_{j,k} \frac{(\mu_{k} - \lambda_{j} + ic)}{(\lambda_{jk} + ic)^{1/2} (\mu_{jk} + ic)^{1/2}} \operatorname{Det} \left( 1 - \frac{1$$

In going to the last line we have collected a purely phase term in the last product. After substituting the expression for V and regrouping terms we obtain the final form

$$|\mathcal{F}| = \left| \left[ \prod_{j,k} \left( \frac{(\lambda_j - \mu_k + ic)(\lambda_j - \mu_k + ic)}{(\lambda_{jk} + ic)(\mu_{jk} + ic)} \right)^{1/2} \right] \times \left\{ \prod_j \frac{\sin(\pi F_L(\lambda_j))}{\pi F_L(\lambda_j)} \prod_{j \neq k} \left( \frac{\lambda_{jk}\mu_{jk}}{(\mu_j - \lambda_k)^2} \right)^{1/2} \right\} \right. \\ \left. \times \prod_{i=1}^n \left( \frac{F_L(\lambda_i^-)}{L(\rho_L(\lambda_i^-)\rho_{ex}(\mu_i^+))^{1/2}(\lambda_i^- - \mu_i^+)} \right) \frac{iP_{ex} \text{Det}(\delta_{jk} + U_{jk})}{(V_p^+ - V_p^-)\text{Det}\left(1 - \frac{\hat{K}}{2\pi}\right)} \right] \right] \\ \exp \left[ \int_{-q}^q \left\{ \frac{\pi F_L(\lambda)\cos(\pi F_L(\lambda))}{\sin(\pi F_L(\lambda))} \left( F_L'(\lambda) - \frac{F_L(\lambda)\rho_L'(\lambda)}{2\rho_L(\lambda)} \right) - \frac{1}{2} \left( F_L'(\lambda) - \frac{F_L(\lambda)\rho_L'(\lambda)}{\rho_L(\lambda)} \right) \right\} \right] \right|.$$
(7.83)

Similar manipulations can be performed to obtain the partial thermodynamic limit of the form factors associated with the boson creation/annihilation operators. For the creation/annihilation operators we consider a matrix element between states with different numbers of particles (see Eq. (7.50)). For the creation operator form factor, the ground state has N particles while the excited state has N + 1 particles, while for the annihilation operator form factor the ground state has N particles while the excited state has N - 1 particles. This means that in the construction of the excited state, there is either a missing or extra quantum number, relative to the ground state. This difference should manifest as an extra hole (for annihilation operator) or particle (for creation operator) in the excited state. To account for this key difference from the calculation of the density operator matrix element, we will introduce modified shift functions to express terms in the form factors of the creation and annihilation operators. We define these modified shift functions as

$$F_{+}(\lambda) = F(\lambda | \{\mu_{1}^{+}, ..., \mu_{n+1}^{+}\}; \{\mu_{1}^{-}, ..., \mu_{n}^{-}\}) + \pi \rho(\lambda),$$
(7.84)

$$F_{-}(\lambda) = F(\lambda | \{\mu_{1}^{+}, ..., \mu_{n}^{+}\}; \{\mu_{1}^{-}, ..., \mu_{n+1}^{-}\}) - \pi \rho(\lambda),$$
(7.85)

for  $n \ge 0$  and with  $F_+$  appearing in the creation operator form factor and  $F_-$  appearing in the annihilation operator. The terms in Eqs. (7.84), (7.85) can be justified as follows.

The first term in Eqs. (7.84), (7.85) corresponds to the particle/hole excitations of the state  $|\mu\rangle$ , including the extra particle or hole excitation due to the difference in number of particles in  $|\mu\rangle$  versus  $|\lambda\rangle$ . This term is analogous to the shift function used for the density operator in Eq. (7.70),  $F(\lambda|\{\mu_1^+,...,\mu_n^+\};\{\mu_1^-,...,\mu_n^-\}) =$  $F(\lambda|\mu_1^+) - F(\lambda|\mu_1^-) + \dots + F(\lambda|\mu_n^+) - F(\lambda|\mu_n^-)$  where  $\mu_i^+$  and  $\mu_i^-$  are particle and hole quasimomenta with respect to the N particle ground state. The second term, an additional factor of  $\pm \pi \rho(\lambda)$  has a more subtle origin - the derivation of the equation for the shift function, Eq. (7.56) from [203], assumes a change of periodic boundary conditions to antiperiodic ones with the change of particle number. Phase shifts calculated from this shift function correspond to the fermionic Cheon-Shigehara model [280] dual to the bosonic Lieb-Liniger model. To obtain the desired phase shifts, one may "correct" the shift function by adding  $\pi \rho(\lambda)$  to the unpaired shift function in Eq. (7.84) and Eq. (7.85) [224]. The sign before this correction is picked up according to whether the unpaired shift comes from an extra particle or hole. The reason these two terms are simply summed to give the correct total shift functions comes from the fact that we can sum the integral equation for the shift function for two different particle-hole configurations and obtain the integral equation for the composite shift function, i.e. the shift when all the individual particle hole configurations occur together.

Furthermore, there are a few modified terms in the form factor of the creation/annihilation operators that need to be carefully accounted for. To do so we will use the following procedure, focusing on the annihilation operator for concreteness. Let us choose one of the n holes in the excited state and consider its quantum number. There should be a ground state quasimomentum corresponding to this quantum number, with some index which we will call  $n^-$ . We are assured of at least one such hole since there is always one less quasiparticle in the excited state used for obtaining the creation operator form factor. We will seemingly treat this hole specially, but this is just a convenience as we could have picked any of the potentially n available holes - but we will commit to one to simplify calculations. The final answers for the prefactors will be independent of the particular choice of  $n^-$ .

Now we reindex the excited state quasimomenta as follows. For  $i < n^-, \mu_i \to \tilde{\mu}_i$ , for  $i \ge n^-, \mu_i \to \tilde{\mu}_{i+1}$ . Thus, in all subsequent steps there is a "gap" in the indices for  $\mu$  at  $\mu_{n-}$ . We will artificially define  $\mu_{n+1}^- = \lambda_{n-} - \frac{F_-(\lambda_{n-})}{L_{\rho}(\lambda_{n-})}$ . Thus we have n+1holes and n particles in the excited state with quasimomenta,  $\mu_i^{\pm}$  for  $n \ge 0$  and we will "remember" the index of one of the holes,  $n^-$ . Note that  $\tilde{\mu}_i$  is simply a reindexing of the original set of  $\mu_i$  with no change in numerical values implied. Under this reordering it becomes possible to define  $F_-(\lambda_i) = (\lambda_i - \tilde{\mu}_i)L_{\rho}(\lambda_i), i \ne n^-$  and  $F_-(\lambda_{n-}) = (\lambda_{n-} - \mu_{n+1}^-)L_{\rho}(\lambda_{n-})$ , as in Eq. (7.67), where the  $F_-(\lambda)$  is the one defined in Eq. (7.85).

Let us consider the combination  $\tilde{V}_j^+/\tilde{V}_j^-$  appearing in the form factors in Eq. (7.52)

$$\frac{\tilde{V}_{j}^{+}}{\tilde{V}_{j}^{-}} = \left(\prod_{i=1}^{n} \frac{\mu_{i}^{+} - \lambda_{j} + ic}{\mu_{i}^{+} - \lambda_{j} - ic}\right) \left(\prod_{i=1}^{n+1} \frac{\mu_{i}^{-} - \lambda_{j} + ic}{\mu_{i}^{-} - \lambda_{j} - ic}\right)^{-1} \left(\prod_{k=1}^{N} \frac{\tilde{\mu}_{k} - \lambda_{j} + ic}{\lambda_{k} - \lambda_{j} + ic}\right) \\
\times \left(\prod_{k=1}^{n} \frac{\mu_{i}^{+} - \lambda_{j} + ic}{\lambda_{k} - \lambda_{j} - ic}\right)^{-1} \\
= \left(\prod_{i=1}^{n} \frac{\mu_{i}^{+} - \lambda_{j} + ic}{\mu_{i}^{+} - \lambda_{j} - ic}\right) \left(\prod_{i=1}^{n+1} \frac{\mu_{i}^{-} - \lambda_{j} + ic}{\mu_{i}^{-} - \lambda_{j} - ic}\right)^{-1} \left(\prod_{k=1}^{N} \frac{\tilde{\mu}_{k} - \lambda_{j} + ic}{\lambda_{k} - \lambda_{j} + ic}\right) \\
\times \left(\prod_{k=1}^{N} \frac{\tilde{\mu}_{k} - \lambda_{j} - ic}{\lambda_{k} - \lambda_{j} - ic}\right)^{-1} \\
= \exp\left\{2\pi i F_{-,L}(\lambda_{j})\left[1 + \frac{1}{L\rho_{L}(\lambda_{j})}\left(F_{-,L}'(\lambda_{j}) - \frac{F_{-,L}(\lambda_{j})\rho_{L}'(\lambda_{j})}{2\rho_{L}(\lambda_{j})}\right)\right]\right\} \\
+ O(1/L^{2}).$$
(7.86)

We use the double prime notation as described in earlier sections (see the text

prior to Eq. (7.62)) and collect the hole created by having one less particle in  $|\mu\rangle$  with the other *n* holes of the excited state and raise the index for such terms to n + 1. To obtain the last line we have used the same steps as in Eq. (7.76).

We will now consider the following grouping of terms appearing in Eq. (7.50)

$$= \left| \frac{\prod_{j,k} (\lambda_{jk}^{2} + c^{2})^{1/2} \prod_{j\neq n^{-}}^{N} \tilde{V}_{j}^{+}}{\prod_{j,k\neq n^{-}}^{N} (\lambda_{jk}^{2} + c^{2})^{1/4} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk}^{2} + c^{2})^{1/4}} \right|$$

$$= \left| \frac{\prod_{j,k}^{N} (\lambda_{jk}^{2} + c^{2})^{1/2} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{k} - \lambda_{j} + ic)}{\prod_{j,k}^{N} \prod_{j,k\neq n^{-}}^{N} (\lambda_{kj} + ic) \prod_{j,k\neq n^{-}}^{N} (\lambda_{jk}^{2} + c^{2})^{1/4} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk}^{2} + c^{2})^{1/4}} \right|$$

$$= \left| \frac{\prod_{j,k\neq n^{-}}^{N} (\lambda_{jk}^{2} + c^{2})^{1/4} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{k} - \lambda_{j} + ic)}{\prod_{j,k\neq n^{-}}^{N} \prod_{j,k\neq n^{-}}^{N} (\lambda_{kj}^{2} + c^{2})^{1/4} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk}^{2} + c^{2})^{1/4}} \right|$$

$$= \left| \frac{\prod_{j,k\neq n^{-}}^{N} (\lambda_{kj}^{2} + c^{2})^{1/4} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{k}^{2} - \lambda_{j} + ic)}{\prod_{j,k\neq n^{-}}^{N} (\lambda_{kj} + ic) \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk}^{2} + c^{2})^{1/4}} \times \frac{c^{1/2} \prod_{j\neq n^{-}}^{N} (\lambda_{jn^{-}}^{2} + c^{2})^{1/2}}{\prod_{j\neq n^{-}}^{N} (\lambda_{kj} + ic) \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk}^{2} + c^{2})^{1/4}} \times \frac{c^{1/2} \prod_{j\neq n^{-}}^{N} (\lambda_{jn^{-}}^{2} + c^{2})^{1/2}}{\prod_{j\neq n^{-}}^{N} (\lambda_{kj} + ic) \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk} - \lambda_{j} + ic)}}{\prod_{j\neq n^{-}}^{N} (\lambda_{kj} + ic)^{1/2} \prod_{j,k\neq n^{-}}^{N} (\tilde{\mu}_{jk} + ic)^{1/2}} \right|.$$

$$(7.87)$$

Moreover, the following terms from Eq. (7.50) give

$$\left(\frac{\prod_{j\neq k}^{N}\lambda_{jk}\prod_{j\neq k\neq n^{-}}^{N}\tilde{\mu}_{jk}}{\prod_{j=1}^{N}\prod_{k\neq n^{-}}^{N}(\lambda_{j}-\tilde{\mu}_{k})^{2}}\right)^{1/2} = \prod_{j\neq n^{-}}^{N}\frac{L\rho_{L}(\lambda_{j})}{F_{-,L}(\lambda_{j})}\left(\prod_{j\neq k\neq n^{-}}^{N}\frac{\lambda_{jk}\tilde{\mu}_{jk}}{(\lambda_{j}-\tilde{\mu}_{k})^{2}}\right)^{1/2}\prod_{j\neq n^{-}}^{N}\frac{\lambda_{n^{-}}-\lambda_{j}}{\lambda_{n^{-}}-\tilde{\mu}_{j}}.$$
(7.88)

On combining these results with the rest of the annihilation form factor we obtain as the partial limit of Eq. (7.50)

$$\mathcal{G}^{-} = \left| \prod_{j,k\neq n^{-}}^{N} \left( \frac{(\lambda_{j} - \tilde{\mu}_{k} + ic)(\lambda_{j} - \tilde{\mu}_{k} - ic)}{(\lambda_{jk} + ic)(\tilde{\mu}_{jk} + ic)} \right)^{1/2} \times \left\{ \prod_{j\neq n^{-}}^{N} \frac{\sin(F_{-,L}(\lambda_{j}))}{\pi F_{-,L}(\lambda_{j})} \left( \prod_{j\neq k\neq n^{-}}^{N} \frac{\lambda_{jk}\tilde{\mu}_{jk}}{(\lambda_{j} - \tilde{\mu}_{k})^{2}} \right)^{1/2} \right\} \\ \left( \prod_{j\neq n^{-}}^{N} \frac{\lambda_{n^{-}} - \lambda_{j}}{\lambda_{n^{-}} - \tilde{\mu}_{j}} \right) \prod_{i=1}^{n} \left( \frac{F_{-,L}(\mu_{i}^{-})}{L(\rho_{L}(\mu_{i}^{-})\rho_{L}(\mu_{i}^{+}))^{1/2}(\mu_{i}^{-} - \mu_{i}^{+})} \right) \frac{\operatorname{Det}(\delta_{jk} + S_{jk}^{-})}{(2\pi L\rho_{L}(\mu_{n+1}^{-}))^{1/2}\operatorname{Det}\left(1 - \frac{\hat{K}}{2\pi}\right)} \\ \exp\left[ \int_{-q}^{q} d\lambda \left\{ \frac{\pi F_{-,L}(\lambda)\cos(\pi F_{-,L}(\lambda))}{\sin(\pi F_{-,L}(\lambda))} \left( F_{-,L}'(\lambda) - \frac{F_{-,L}(\lambda)\rho_{L}'(\lambda)}{2\rho_{L}(\lambda)} \right) \right\} \right] \\ \exp\left[ -\frac{1}{2} \int_{-q}^{q} d\lambda \left\{ F_{-,L}'(\lambda) - \frac{F_{-,L}(\lambda)\rho_{L}'(\lambda)}{\rho_{L}(\lambda)} \right\} \right] \right|. \tag{7.89}$$

The derivation of the result for  $\mathcal{G}^+$  is almost the same as the one for  $\mathcal{G}^-$ , hence we present only the answer:

$$\mathcal{G}^{+} = \left| \left[ \prod_{j,k}^{N} \left( \frac{(\lambda_{j} - \tilde{\mu}_{k} + ic)(\lambda_{j} - \tilde{\mu}_{k} + ic)}{(\lambda_{jk} + ic)(\tilde{\mu}_{jk} + ic)} \right)^{1/2} \right] \times \left\{ \prod_{j=1}^{N} \frac{\sin(F_{+,L}(\lambda_{j}))}{\pi F_{+,L}(\lambda_{j})} \left( \prod_{j\neq k}^{N} \frac{\lambda_{jk}\tilde{\mu}_{jk}}{(\lambda_{j} - \tilde{\mu}_{k})^{2}} \right)^{1/2} \right\}$$

$$\prod_{j=1}^{N} \left( \frac{\tilde{\mu}_{j} - \mu_{n+1}^{+}}{\lambda_{j} - \mu_{n+1}^{+}} \right) \times \prod_{i=1}^{n} \left( \frac{F_{+,L}(\mu_{i}^{-})}{L(\rho_{L}(\mu_{i}^{-})\rho_{L}(\mu_{i}^{+}))^{1/2}(\mu_{i}^{-} - \mu_{i}^{+})} \right) \frac{\operatorname{Det}(\delta_{jk} + S_{jk}^{+})}{(2\pi L\rho_{ex}(\mu_{N+1}))^{1/2}\operatorname{Det}\left(1 - \frac{\hat{K}}{2\pi}\right)}$$

$$\exp\left[ \int_{-q}^{q} d\lambda \left\{ \frac{\pi F_{+,L}(\lambda) \cos(\pi F_{+,L}(\lambda))}{\sin(\pi F_{+,L}(\lambda))} \left( F_{+,L}'(\lambda) - \frac{F_{+,L}(\lambda)\rho_{L}'(\lambda)}{2\rho_{L}(\lambda)} \right) \right\} \right]$$

$$\exp\left[ -\frac{1}{2} \int_{-q}^{q} d\lambda \left\{ F_{+,L}'(\lambda) - \frac{F_{+,L}(\lambda)\rho_{L}'(\lambda)}{\rho_{L}(\lambda)} \right\} \right] \left| .$$

$$(7.90)$$

Note that in Eq. (7.89) and Eq. (7.90) the notation  $S_{jk}^{\pm}$  is used to differentiate between the matrices appearing in Eq. (7.50) when the excited state has  $N \pm 1$ quasimomenta. The matrices are given by

$$S_{jk}^{-} = \frac{i(\tilde{\mu}_{j} - \lambda_{j})}{\tilde{V}_{j}^{+} - \tilde{V}_{j}^{-}} \frac{\prod_{m \neq j}^{N-1} (\tilde{\mu}_{m} - \lambda_{j})}{\prod_{m \neq j}^{N} (\lambda_{m} - \lambda_{j})} (K(\lambda_{j} - \lambda_{k}) - K(\mu_{n+1}^{-} - \lambda_{k})),$$
  

$$S_{jk}^{+} = \frac{i(\tilde{\mu}_{j} - \lambda_{j})}{\tilde{V}_{j}^{+} - \tilde{V}_{j}^{-}} \frac{\prod_{m \neq j}^{N+1} (\tilde{\mu}_{m} - \lambda_{j})}{\prod_{m \neq j}^{N} (\lambda_{m} - \lambda_{j})} (K(\lambda_{j} - \lambda_{k}) - K(\lambda_{j} - \mu_{n+1}^{+})).$$
(7.91)

It is more convenient to separately evaluate the thermodynamic limits of specific groups of terms appearing in the expressions Eqs. (7.83), (7.89), (7.90). We begin with the terms in the square brackets.

# 7.5.3 Evaluation of $M_1$

We will denote by  $M_1$  the first group of terms appearing in square brackets in Eqs. (7.83), (7.89), (7.90). These terms have common origins and the evaluation of their limits is essentially the same. The only difference lies in the fact that the shift function, F, for the creation/annihilation operators, accounts for an extra particle or hole, as described earlier.

Let us start with the density form factor case

$$M_{1} = \left| \prod_{j,k=1}^{N} \left( \frac{(\lambda_{j} - \mu_{k} + ic)(\lambda_{j} - \mu_{k} + ic)}{(\lambda_{jk} + ic)(\mu_{jk} + ic)} \right)^{1/2} \right|.$$
(7.92)

We expect the first group of terms to be finite in the TDL because there are no obvious singularities in the individual terms. We start by breaking the term into four parts as follows

$$M_{1} = p_{1} \times p_{2} \times p_{3} \times p_{4},$$

$$p_{1}^{2} = \left| \prod_{j,k} \frac{\lambda_{j} - \mu_{k} + ic}{\lambda_{jk} + ic} \right|,$$

$$p_{2}^{2} = \left| \prod_{j,k} \frac{\lambda_{j} - \mu_{k} - ic}{\mu_{jk} - ic} \right|,$$
(7.93)

$$p_{3} = \left| \prod_{h=1}^{n} \prod_{j} \left( \frac{(\lambda_{j} - \mu_{h}^{+} + ic)(\lambda_{j} - \mu_{h}^{+} + ic)}{(\lambda_{j} - \lambda_{h}^{-} + ic)(\mu_{j} - \mu_{h}^{+} + ic)} \right) \right|,$$

$$p_{4} = \left| \prod_{h_{1},h_{2}}^{n} \left( \frac{(\lambda_{h_{1}}^{-} - \mu_{h_{2}}^{+} + ic)(\lambda_{h_{1}}^{-} - \mu_{h_{2}}^{+} + ic)}{(\lambda_{h_{1}}^{-} - \lambda_{h_{2}}^{-} + ic)(\mu_{h_{1}}^{+} - \mu_{h_{2}}^{+} + ic)} \right)^{1/2} \right|,$$
(7.94)

where the prime notation is the same as used in the earlier sections, see definitions before Eq. (21). Note that because we are only interested in the absolute value when evaluating the term  $M_1$ , we can freely replace terms by their complex conjugate in order to avoid generating unbounded imaginary parts in the various terms, see e.g.  $p_2^2$ . The *n* quasimomenta corresponding to excitations are treated separately and are indexed by *h*.

We start with the first two pairs of numerator and denominator terms

$$p_{1}^{2} = \left| \prod_{j,k} \frac{\lambda_{j} - \mu_{k} + ic}{\lambda_{jk} + ic} \right|$$

$$= \left| \prod_{j,k} \frac{\lambda_{jk} + \frac{F_{L}(\lambda_{k})}{L\rho_{L}(\lambda_{k})} + ic}{\lambda_{jk} + ic} \right|$$

$$= \left| \prod_{j,k} \frac{1}{L\rho_{L}(\lambda_{k})(\lambda_{jk} + ic)}{L\rho_{L}(\lambda_{k})(\lambda_{jk} + ic)} \right|.$$
(7.95)

Similarly,

$$p_{2}^{2} = \left| \prod_{j,k} \frac{\lambda_{j} - \mu_{k} - ic}{\mu_{jk} - ic} \right|$$

$$= \left| \prod_{j,k} \frac{1}{L\rho(\lambda_{j})(\lambda_{jk} - ic + \frac{F_{L}(\lambda_{k})}{L\rho(\lambda_{k})})} \right|^{-1} \right|$$

$$= \left| \prod_{j,k} \frac{1}{L\rho(\lambda_{k})(\lambda_{jk} + ic - \frac{F_{L}(\lambda_{j})}{L\rho(\lambda_{j})})} \right|^{-1} \right|$$

$$= \left| \prod_{j,k} \frac{F_{L}(\lambda_{k})}{L\rho(\lambda_{k})(\lambda_{jk} + ic)} + \frac{F_{L}(\lambda_{j})F_{L}(\lambda_{k})}{L^{2}\rho(\lambda_{j})\rho(\lambda_{k})(\lambda_{jk} + ic)^{2}} \right|^{-1} \right|.$$
(7.96)

To evaluate the products above we do a logarithmic expansion:

$$\log(p_1 p_2) = \sum_{j,k} \log(p_1) + \log(p_2) = -\frac{1}{2} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \frac{F(\lambda)F(\mu)}{(\lambda - \mu + ic)^2} + O(1/L).$$
(7.97)

Similarly, the term  $p_{3}\ \mathrm{can}\ \mathrm{be}\ \mathrm{reduced}\ \mathrm{to}\ \mathrm{the}\ \mathrm{following}\ \mathrm{form}$ 

$$p_{3} = \left| \prod_{j} \prod_{h=1}^{n} \left( \frac{\mu_{j} - \lambda_{h}^{-} + ic}{\lambda_{j} - \lambda_{h}^{-} + ic} \right) \left( \frac{\mu_{j} - \mu_{h}^{+} + ic}{\lambda_{j} - \mu_{h}^{+} + ic} \right)^{-1} \right| \\ = \left| \prod_{j} \prod_{h=1}^{n} \left( 1 + \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})} \frac{\mu_{h}^{+} - \lambda_{h}^{-}}{(\lambda_{j} - \lambda_{h}^{-} + ic)(\lambda_{j} - \mu_{h}^{+} + ic)} + O\left(\frac{1}{L^{2}}\right) \right) \right| \\ = \exp\left[ \sum_{h=1}^{n} \int_{-q}^{q} d\lambda F(\lambda) \frac{\mu_{h}^{+} - \lambda_{h}^{-}}{(\lambda - \lambda_{h}^{-} + ic)(\lambda - \mu_{h}^{+} + ic)} \right] + O\left(\frac{1}{L}\right).$$
(7.98)

Thus, the overall factor  $M_1$  takes the following form

$$M_{1} = \exp\left[-\frac{1}{2}\int_{-q}^{q}d\mu\int_{-q}^{q}d\lambda\frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}}\right]\prod_{h_{1},h_{2}}^{n}\left[\frac{(\mu_{h_{1}}^{-}-\mu_{h_{2}}^{+}+ic)^{2}}{(\mu_{h_{1},h_{2}}^{-}+ic)(\mu_{h_{1},h_{2}}^{+}+ic)}\right]^{1/2}$$

$$\times \exp\left[\sum_{h=1}^{n}\int_{-q}^{q}d\lambda\frac{F(\lambda)(\mu_{h}^{+}-\mu_{h}^{-})}{(\lambda-\mu_{h}^{-}+ic)(\lambda-\mu_{h}^{+}+ic)}\right].$$
(7.99)

To obtain the analogous term for boson creation/annihilation form factor, we use the same expression as above in Eq. (7.99), but substitute the shift function  $F(\lambda)$ , with  $F_{\pm}(\lambda)$ .

## 7.5.4 Obtaining term $M_2$

Here we will focus on the term

$$M_2 = \left\{ \prod_j \frac{\sin(\pi F_L(\lambda_j))}{\pi F_L(\lambda_j)} \prod_{j \neq k} \left( \frac{\lambda_{jk} \mu_{kj}}{(\mu_k - \lambda_j)^2} \right)^{1/2} \right\}.$$
 (7.100)

This term is expected to contain a power law divergence and a prefactor, and appears in all form factors. We require a consistent and physically clear method of extracting the divergence and all contributions to the prefactor which are finite in the thermodynamic limit. The intuition we will use to do this comes from the fact that we know the final answer is expected to scale as a power law of L. In the thermodynamic limit, the information about L contained in the quantization of  $\lambda, \mu$ . Consequently it is reasonable to expect that terms which collect to give this power law divergence must appear as a difference in  $\lambda_j - \lambda_k$  when  $\lambda_j$  and  $\lambda_k$  are near one another. Therefore it is important to isolate such terms on the basis of the nearness of the  $\lambda's$ . Thus we propose to use a cutoff in order to control the nearness of these parameters and perform controlled expansions to extract the divergence and the prefactor. The cutoff will drop out of the final answer. This is made more precise below. The term  $M_2$  appears in the form factors associated with the density operator and with the creation/annihilation operators, with a slight modification accounting for the difference. We will explicitly calculate the density form factor and point out how to modify the result for the creation/annihilation form factors. Furthermore we will consider first a single particle-hole pair, with quasimomenta,  $\mu^-$ ,  $\mu^+$  and indices,  $i^-$ ,  $i^+$ , and lastly generalize the calculation to include multiple excitations.

It is easier to calculate the thermodynamic limit of  $M_2$  after regrouping terms in a convenient way. Our procedure will be the following.

First we rewrite the terms in round brackets in Eq. (7.100) as T' as shown below

$$T' = \prod_{j \neq k} \left( \frac{\lambda_{jk} \mu_{kj}}{(\mu_k - \lambda_j)^2} \right)^{1/2}$$

$$= \left[ \prod_{j \neq k} \left( \frac{\lambda_j - \mu_k}{\lambda_j - \lambda_k} \right)^{-2} \left( \frac{\mu_j - \mu_k}{\lambda_j - \lambda_k} \right) \right]^{1/2}$$

$$= \prod_{j \neq k} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)(\lambda_j - \lambda_k)} \right)^{-1/2} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)(\lambda_j - \lambda_k)} - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda_k)} \right)^{1/2}$$

$$\times \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda_k)} \right)^{-1/2}.$$
(7.101)

The prime notation is the same as used earlier - i.e. we leave off the quasimomenta corresponding to particles and holes.

It is more convenient to evaluate a "temporarily incorrect" term, which we will call T'', where we include  $\mu^-$  instead of  $\mu^+$  and then correct the mistake with a separate term. Thus to obtain the correct T', we will calculate a correction term  $T_{hole}$  that must be multiplied to T'' in order to remove the extra terms:

$$T' = T'' \times T_{hole} \tag{7.102}$$

The terms that we need to remove are exactly those in which the difference,  $\mu_k^- - \lambda_k^-$  appears. Consequently, we obtain  $T_{hole}$  in the following way:

$$T_{hole} = \prod_{j \neq i^{-}} \left( 1 + \frac{F_L(\lambda^{-})}{L\rho_L(\lambda^{-})(\lambda_j - \lambda^{-})} \right) \prod_{j \neq i^{-}} \left( 1 + \frac{F_L(\mu^{-})}{L\rho_L(\lambda^{-})(\lambda_j - \lambda^{-})} - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda^{-})} \right)^{-1/2}$$

$$\prod_{k \neq i^{-}} \left( 1 + \frac{F_L(\lambda_k)}{L\rho(\lambda_k)(\lambda^{-} - \lambda_k)} - \frac{F_L(\lambda^{-})}{L\rho_L(\lambda^{-})(\lambda^{-} - \lambda_k)} \right)^{-1/2}$$

$$= \prod_{j \neq i^{-}} \left( 1 + \frac{F_L(\lambda^{-})}{L\rho_L(\lambda^{-})(\lambda_j - \lambda^{-})} \right) \prod_{j \neq i^{-}} \left( 1 + \frac{F_L(\lambda^{-})}{L\rho_L(\lambda^{-})(\lambda_j - \lambda^{-})} - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda^{-})} \right)^{-1}$$

$$= \prod_{j \neq i^{-}} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda^{-})} \left( 1 + \frac{F_L(\lambda^{-})}{L\rho_L(\lambda^{-})(\lambda_j - \lambda^{-})} \right) \right)^{-1}$$

$$= \prod_{j \neq i^{-}} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda^{-})} + \frac{F_L(\lambda^{-})\rho_L(\lambda_j)}{\rho_L(\lambda^{-})} \right)^{-1}.$$
(7.103)

In the second line, we have relabeled index k as j to obtain line 3 in Eq. (7.103).

Finally, the terms that were removed must be replaced by the correct terms. Let us call the product of these correct terms  $T_{particle}$ . The way to obtain this term is similar to the process used to remove the incorrect terms as in Eq. (7.103). We get

$$T_{particle} = \prod_{j \neq i^{-}} \left( 1 + \frac{\lambda^{-} - \mu^{+}}{\lambda_{j} - \lambda^{-}} \right)^{-1} \prod_{j \neq i^{-}} \left( 1 + \frac{\lambda^{-} - \mu^{+}}{\lambda_{j} - \lambda^{-}} - \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda^{-})} \right)^{1/2}$$

$$\prod_{k \neq i^{-}} \left( 1 + \frac{F_{L}(\lambda_{k})}{L\rho(\lambda_{k})(\lambda^{-} - \lambda_{k})} - \frac{\lambda^{-} - \mu^{+}}{\lambda^{-} - \lambda_{k}} \right)^{1/2}$$

$$(7.104)$$

$$= \prod_{j \neq i^{-}} \left( 1 - \frac{F_{L}(\lambda_{j})}{\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda^{-})\left(1 + \frac{\lambda^{-} - \mu^{+}}{\lambda_{j} - \lambda^{-}}\right)} \right)$$

$$(7.105)$$

$$= \prod_{j \neq i^{-}} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \mu^+)} \right).$$
(7.106)

Thus, the final answer will be given by

$$M_2 = T'' \times T_{hole} \times T_{particle}.$$
(7.107)

We start with the expression

$$T'' = \prod_{j \neq k} \left( \frac{\lambda_{jk} \mu_{kj}}{(\mu_k - \lambda_j)^2} \right)^{1/2}$$

$$= \left[ \prod_{j \neq k} \left( \frac{\lambda_j - \mu_k}{\lambda_j - \lambda_k} \right)^{-2} \left( \frac{\mu_j - \mu_k}{\lambda_j - \lambda_k} \right) \right]^{1/2}$$

$$= \prod_{j \neq k} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)(\lambda_j - \lambda_k)} \right)^{-1/2} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)(\lambda_j - \lambda_k)} - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda_k)} \right)^{1/2}$$

$$\times \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda_k)} \right)^{-1/2}.$$
(7.108)

At this stage there are two levels of approximations that can be made. One, we can express differences in  $\lambda$  using

$$j - k = L\left(x(\lambda_j) - x(\lambda_k)\right),$$

$$j - k = L\left(x(\lambda_j) - x(\lambda_j) - x'(\lambda_j)(\lambda_k - \lambda_j) - x''(\lambda_j)(\lambda_k - \lambda_j)^2/2\right) + O(\lambda_{jk}^3),$$

$$j - k = L\rho_L(\lambda_j)(\lambda_j - \lambda_k) - L\rho'_L(\lambda_j)(\lambda_j - \lambda_k)^2/2 + O(\lambda_{jk}^3),$$

$$L\rho_L(\lambda_j - \lambda_k) = (j - k) + \frac{\rho'_L(\lambda_j)}{2L\rho_L(\lambda_j)^2}(j - k)^2 + O(1/L^2)(7.109)$$

Two, the products in Eq. (7.108) above can be exponentiated, and the resulting logarithms expanded order by order in 1/L.

Both these procedures have a region of validity. For instance, it is incorrect to perform the logarithmic expansion when j and k are near one another. However, when j and k are far away, the approximation in Eq. (7.109) breaks down. We calculate T'' by combining these two approximations. The idea behind this is to distinguish

two regions of the range of  $\lambda_j$ ,  $\lambda_k$  using a cutoff - a region when they are near one another, and a region when they are far away. Then the two approximations outlined above can be used in the region in which they are valid.

This is illustrated in Fig. 7.3. The blue region I, corresponds to the case when j and k are far enough from each other for the logarithmic expansion to become valid. The red region II corresponds to when j and k are near enough for Eq. (7.109) to become valid. The third, yellow region III will be treated more carefully since Eq. (7.109) is valid here, but proximity to the quasi-Fermi points plays a role in how terms are treated in this region. Moreover, the denotations a and b are used to differentiate the region where j > k and j < k, respectively, to make the calculation more convenient.

The separation of the regions described above is not arbitrary. To do this we introduce a cutoff in the following way - in region I, we only allow the index k to get within  $n^* \gg 1$  of the index j for all products/sums. In the figure this corresponds to the lines at the interface of the red and blue regions. Since we will be working in the continuum limit in region I, we would like to know what this condition about indices means for the quasi momenta. Since  $n^*$  is at the crossover where the approximation (7.109) just starts to break down, we will use this approximation to define the  $\nu^*$  corresponding to  $n^*$ 

$$\nu^*(\lambda) = |\lambda_j - \lambda_k| \approx \left| \frac{j - j \pm n^*}{L\rho_L(\lambda_j = \lambda)} \right| = \frac{n^*}{L\rho_L(\lambda)}.$$
(7.110)

Note that we have a choice of either keeping  $n^*$  or  $\nu^*$  constant - fixing one parameter endows the other with a dependence on its position in the range [-q,q] or [1,N] respectively. Our particular choice keeps  $n^*$  fixed, and makes  $\nu^*(\lambda)$  dependent on  $\lambda$ .

Using the two approximations in the relevant regions should produce, first, a (principal value) integral which captures the contribution to the prefactor from the

"far-away" region (I a,b in Fig.7.3). Second, a constant from the entire region where  $\lambda_j$  is near  $\lambda_k$ , but when they are not both at the same quasi-Fermi point (II a,b in Fig. 7.3). Lastly, a constant and a power law divergence from the region where both  $\lambda$  are near the same quasi-Fermi point (III a,b in Fig. 7.3). While the intermediate steps may produce cutoff dependent terms, these terms should mutually cancel. The final answer will be shown to be independent of the cutoff parameter,  $n^* \gg 1$ .

Figure 7.3 : Schematic of range of  $\lambda$ 's. Cutoff parameter  $n^*$  is used to separate regions I, II and III. In region I the indices j, k are far enough to perform logarithmic expansions as in, for example, Eq. (7.111). In region II and III, the approximation given by Eq. (7.109) is valid, but the logarithmic expansion fails. Consequently products must be carefully and explicitly evaluated discretely. In region III proximity to the quasi-Fermi point demands greater care in evaluating products as demonstrated in Eq. (7.125), for example.

Let us denote the value of T'' in region I as  $T_I$ . To treat the product in region I

we may expand the products in T'' logarithmically in orders of 1/L. Only terms of order  $1/L^2$  and higher survive after the double products are evaluated. Without any additional approximation, we obtain the following term

$$T_{I} = \prod_{j \neq k} \left( 1 + \frac{F_{L}(\lambda_{k})}{L\rho_{L}(\lambda_{k})(\lambda_{j} - \lambda_{k})} \right)^{-1/2} \left( 1 + \frac{F_{L}(\lambda_{k})}{L\rho_{L}(\lambda_{k})(\lambda_{j} - \lambda_{k})} - \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda_{k})} \right)^{1/2} \times \left( 1 - \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda_{k})} \right)^{-1/2} \approx \exp \left[ \frac{1}{2} \sum_{j \neq k} \frac{F_{L}(\lambda_{j})F_{L}(\lambda_{k})}{L^{2}\rho_{L}(\lambda_{j})\rho_{L}(\lambda_{k})(\lambda_{j} - \lambda_{k})^{2}} \right]. \quad (7.111)$$

With the definition of the cutoff in  $\lambda$ , Eq. (7.110), we may write

$$\log(T_{I}) = \frac{1}{2} \sum_{j \neq k} \frac{F_{L}(\lambda_{j})F_{L}(\lambda_{k})}{L^{2}\rho_{L}(\lambda_{j})\rho_{L}(\lambda_{k})(\lambda_{j}-\lambda_{k})^{2}}$$

$$= \frac{1}{2} \left( \int_{-q+\nu^{*}(-q)}^{q} d\lambda \int_{-q}^{\lambda-\nu^{*}(\lambda)} d\mu \frac{F_{L}(\lambda)F_{L}(\mu)}{(\lambda-\mu)^{2}} + \int_{-q}^{q-\nu^{*}(q)} d\lambda \int_{\lambda+\nu^{*}(\lambda)}^{q} d\mu \frac{F_{L}(\lambda)F_{L}(\mu)}{(\lambda-\mu)^{2}} \right)$$

$$= \frac{1}{2} \int_{-q+\nu^{*}(-q)}^{q} F_{L}^{2}(\lambda)d\lambda \int_{-q}^{\lambda-\nu^{*}(\lambda)} d\mu \left(\frac{1}{\lambda-\mu}\right)^{2}$$

$$+ \frac{1}{2} \int_{-q}^{q-\nu^{*}(q)} F_{L}^{2}(\lambda)d\lambda \int_{\lambda+\nu^{*}(\lambda)}^{\lambda-\nu^{*}(\lambda)} d\mu \left(\frac{F_{L}(\lambda)-F_{L}(\mu)}{\lambda-\mu}\right)^{2}$$

$$- \frac{1}{4} \int_{-q}^{q-\nu^{*}(q)} d\lambda \int_{\lambda+\nu^{*}(\lambda)}^{q} d\mu \left(\frac{F_{L}(\lambda)-F_{L}(\mu)}{\lambda-\mu}\right)^{2}.$$
(7.112)

In the last step we have isolated a straightforwardly integrable (lines 3 and 4) and a cutoff dependent part (lines 1 and 2).

Let us first analyze the term

$$\frac{1}{2} \int_{-q+\nu^{*}(-q)}^{q} F_{L}^{2}(\lambda) d\lambda \int_{-q}^{\lambda-\nu^{*}(\lambda)} d\mu \frac{1}{(\lambda-\mu)^{2}} = \frac{1}{2} \int_{-1+\nu^{*}(-q)/q}^{1} dx F_{L}^{2}(qx) \left(\frac{1}{\nu^{*}(qx)/q} - \frac{1}{x+1}\right) \\
= -\frac{1}{2} F_{L}^{2}(-q) \log(qL) - \frac{1}{2} \left[ F_{L}^{2}(-q) \log\left(\frac{\rho_{L}(q)}{n^{*}}\right) - \int_{-q+\nu^{*}(q)}^{q} d\lambda \frac{F_{L}^{2}(\lambda)}{\nu^{*}(\lambda)} \right] - \frac{1}{2} P_{-} \int_{-1}^{1} dx \frac{F_{L}^{2}(qx)}{x+1}, \tag{7.113}$$

where we introduced the generalized principal value integrals denoted by  $P_-$ ,  $P_+$ ,  $P_{\pm}$ , defined in Appendix B. Note that such integrals can only be well defined when the integrand is made dimensionless. This is achieved by mapping the range of integration from  $(-q, q) \rightarrow (-1, 1)$ .

Similarly we may obtain the second cutoff dependent term of Eq. (7.112). The combined answer in region I becomes

$$T_{I} = \left(\frac{\nu^{*}(q)}{q}\right)^{\frac{1}{2}(F_{L}^{2}(q)+F_{L}^{2}(-q))} \exp\left\{P_{\pm}\int_{-1}^{1} dx \frac{F_{L}^{2}(qx)}{x^{2}-1^{2}} - \frac{1}{4}\int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{L}(\lambda) - F_{L}(\mu)}{\lambda - \mu}\right)^{2}\right\} \times \exp\left\{\frac{L}{n^{*}}\int_{-q}^{q-\nu^{*}(q)} d\lambda \rho_{L}(\lambda)F_{L}^{2}(\lambda) + \frac{L}{n^{*}}\int_{-q+\nu^{*}(-q)}^{q} d\lambda \rho_{L}(\lambda)F_{L}^{2}(\lambda)\right\}.$$
(7.114)

In Region II we know that we can no longer expand the log of the products like in the previous section because here all terms are O(1) or bigger. We will consider the two sets of products in this region, products in IIa, and, IIb, separately. In both these products we can approximate  $\lambda_j - \lambda_k$  as in Eq. (7.109). The second thing is to treat terms like  $F_L(\lambda_j) - F_L(\lambda_k)$  with the same precision with which we treat differences in  $\lambda$  in this region. Thus we need to evaluate the difference in  $F_L$  to O(1/L) as follows

$$\frac{F_L(\lambda_j)}{\rho_L(\lambda_j)} - \frac{F_L(\lambda_k)}{\rho_L(\lambda_k)} = \frac{d}{d\lambda} \left(\frac{F_L(\lambda)}{\rho_L(\lambda)}\right)|_{\lambda = \lambda_j} (\lambda_j - \lambda_k).$$
(7.115)

Let us define the following notation,  $F_j = F_L(\lambda_j)$ ,  $C_j^a = \left(\frac{F_L(\lambda_j)}{\rho_L(\lambda_j)}\right)'$ , where the prime denotes that the derivative has been taken with respect to  $\lambda$  and evaluated at  $\lambda = \lambda_j$ . Similarly, define  $C_j^b = -\frac{\rho'_L(\lambda_j)}{2\rho_L(\lambda_j)^2}$ .

Thus we have from Eq. (7.108)

$$T_{IIa} = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)} \right)^{-1/2} \left( 1 + \frac{F_L(\lambda_k)}{L\rho_L(\lambda_k)} - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)} \right)^{1/2} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)} \right)^{-1/2} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(L\rho_L(\lambda_j)\lambda_{jk})^{1/2}(L\rho_L(\lambda_j)\lambda_{jk}(1 - C_j^a/L))^{1/2}}{(I\rho_L(\lambda_j)\lambda_{jk} - F_j)^{1/2}(L\rho_L(\lambda_j)\lambda_{jk}(1 - C_j^a/L) + F_j)^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}C_j^b(j-k))(1 + \frac{1}{L}C_j^b(j-k))^{-1}(1 - C_j^a/L)^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}(1 - C_j^a/L)^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}C_j^b(j-k))(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}(1 - C_j^a/L)^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}F_j^b(j-k))^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}F_j^b(j-k))^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}F_j^b(j-k))^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}F_j^b(j-k))^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}F_j^b(j-k))(1 - C_j^a/L)})^{1/2}}{(j-k - \frac{F_j}{1 + \frac{1}{L}C_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{(1 + \frac{1}{L}C_j^b(j-k))(1 - C_j^a/L)})^{1/2}} \\ = \prod_{j=n^*+1}^{N} \prod_{k=j-n^*}^{j-1} \frac{(j-k)(1 + \frac{1}{L}F_j^b(j-k)}{(j-k - \frac{F_j}{1 + \frac{1}{L}F_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{1 + \frac{F_j}{L}F_j^b(j-k)})^{1/2}}}{(j-k - \frac{F_j}{1 + \frac{1}{L}F_j^b(j-k)})^{1/2}(j-k + \frac{F_j}{1 + \frac{F_j}{L}F_j^b(j-k)})^{1/2}}}{(j-k - \frac{F$$

In the above expressions, only O(1/L) terms will survive and consequently terms of higher order in 1/L have been dropped in the intermediate steps. Similarly for the region IIb

$$T_{IIb} = \prod_{j=1}^{N-n^*} \prod_{k=j+1}^{j+n^*} \frac{(j-k)(1+\frac{1}{L}F_jC_j^b)^{-1/2}(1-\frac{1}{L}F_jC_j^b)^{-1/2}}{(j-k-\frac{F_j}{1+\frac{1}{L}F_jC_j^b})^{1/2}(j-k+\frac{F_j}{1-\frac{1}{L}C_j^a-\frac{1}{L}F_jC_j^b})^{1/2}}$$
  
$$= \prod_{j=1}^{N-n^*} \frac{\Gamma(n^*+1)\Gamma(1+F_j-\frac{1}{L}F_j^2C_j^b)^{1/2}\Gamma(1-F_j-\frac{1}{L}(F_j^2C_j^b+F_jC_j^a))^{1/2}}{\Gamma(n^*+1+F_j-\frac{1}{L}F_j^2C_j^b)^{1/2}\Gamma(n^*+1-F_j-\frac{1}{L}(F_j^2C_j^b+F_jC_j^a))^{1/2}}$$
(17)

We may expand the log of the cutoff dependent terms in the  $n^* \gg 1$  limit. This

leaves the following terms

$$log(T_{cutoff}) = -\sum_{j=1}^{N-n^*} \frac{F_j^2}{2n^*} - \sum_{j=n^*}^{N} \frac{F_j^2}{2n^*} + O\left(\frac{1}{n^*}\right)$$
$$= -\frac{L \int_{-q}^{q-\nu^*(q)} d\lambda F_L^2(\lambda) \rho_L(\lambda)}{n^*} - \frac{L \int_{-q+\nu^*(-q)}^{q} d\lambda F_L^2(\lambda) \rho_L(\lambda)}{n^*} + O\left(\frac{1}{n^*}\right).$$
(7.118)

The first two terms exactly cancel the cutoff dependent term from region I in Eq. (7.114). The last term can be ignored with the precision to which we are considering expansions in the parameter  $n^*$ .

Now we focus on the terms that are not cutoff dependent. First we note that all the  $C_j^b$  terms drop out to O(1/L). We would like to treat the  $C_j^a$  terms. Using the notation,  $\psi(x) = \frac{d}{dx} \log(\Gamma(x))$ , we expand the terms to precision O(1/L) as follows

$$\Gamma(1 \pm \frac{F_j}{1 - C_j/L}) = \exp\left[\log(\Gamma(1 \pm \frac{F_j}{1 - C_j/L}))\right]$$
  

$$\approx \exp\left[\log(\Gamma(1 \pm F_j \pm F_jC_j/L))\right]$$
  

$$\approx \exp\left[\log(\Gamma(1 \pm F_j)) \pm \psi(1 \pm F_j)F_jC_j/L\right]$$
  

$$= \Gamma(1 \pm F_L(\lambda_j))$$
  

$$\times \exp\left[\pm \psi(1 \pm F_L(\lambda_j))\frac{1}{L}F_L(\lambda_j)\left(\frac{F_L(\lambda_j)}{\rho_L(\lambda_j)}\right)'\right].$$
(7.119)

We will need to evaluate the product over j for such terms. This can be done by first noting as a consequence of the chain rule

$$\frac{\partial}{\partial x}\log(\Gamma(x)) = \frac{\partial}{\partial \lambda}\log(\Gamma(x(\lambda))) \times \frac{1}{\frac{\partial x(\lambda)}{\partial \lambda}}.$$
(7.120)

We will evaluate the product of such terms as follows

$$\begin{split} &\prod_{j=n^*}^{N-n^*} \exp\left[\frac{C_j F_j}{L} \left(\frac{\partial}{\partial x} \log(\Gamma(x))|_{x=1+F_L(\lambda_j)} - \frac{\partial}{\partial x} \log(\Gamma(x))|_{x=1-F_L(\lambda_j)}\right)\right] \\ &= \exp\left[\sum_j \frac{C_j F_j}{L F'_L(\lambda_j)} \frac{\partial}{\partial \lambda} \left(\log(\Gamma(1-F_L(\lambda_j))\Gamma(1+F_L(\lambda_j)))\right)\right] \\ &= \exp\left[\sum_j \frac{C_j F_j}{L F'_L(\lambda_j)} \frac{\partial}{\partial \lambda} \left(\log\left(\frac{\pi F_L(\lambda_j)}{\sin(\pi F_L(\lambda_j))}\right)\right)\right] \\ &= \exp\left[\int_{-q+\nu^*}^{q-\nu^*} d\lambda \rho_L(\lambda) \frac{F_L(\lambda)}{F'_L(\lambda)} \frac{\partial}{\partial \lambda} \left(\frac{F_L(\lambda)}{\rho_L(\lambda)}\right) \frac{\partial}{\partial \lambda} \left(\log\left(\frac{\pi F_L(\lambda)}{\sin(\pi F_L(\lambda))}\right)\right)\right] \\ &= \exp\left[\int_{-q}^{q} d\lambda \rho_L(\lambda) \frac{F_L(\lambda)}{F'_L(\lambda)} \frac{\partial}{\partial \lambda} \left(\frac{F_L(\lambda)}{\rho_L(\lambda)}\right) \frac{\partial}{\partial \lambda} \left(\log\left(\frac{\pi F_L(\lambda)}{\sin(\pi F_L(\lambda))}\right)\right)\right]. \end{split}$$
(7.121)

Note that we have let  $\nu^*$  go to zero. In so doing, we have added in some terms that occur at the edges, i.e. form 1 to  $n^*$  and from  $N - n^*$  to N. However, these terms only make an order 1/L contribution and can be safely treated. Moreover, we treat the  $\Gamma(1+F_j)\Gamma(1-F_j)$  terms by extending the product from 1 to N and dividing by the "extra terms"

$$\prod_{j=1}^{N-n^{*}} (\Gamma(1+F_{j})\Gamma(1-F_{j}))^{1/2} \prod_{j=n^{*}+1}^{N} (\Gamma(1+F_{j})\Gamma(1-F_{j}))^{1/2}$$
$$= \prod_{j=1}^{N} \left(\frac{\pi F_{L}(\lambda_{j})}{\sin(\pi F_{L}(\lambda_{j}))}\right) \left(\frac{\sin(\pi F_{L}(q))\sin(\pi F_{L}(-q))}{\pi^{2}F_{L}(-q)F_{L}(q)}\right)^{n^{*}/2},$$
(7.122)

where, in the last step we have set all the  $F_j$  within  $n^*$  of the edges to be  $F_L(\pm q)$ since this only generates a 1/L error that can be ignored. We have to carry out the above procedure since terms involving  $\Gamma(1 \pm F_j)$  are O(1) and any terms added or removed may result in a finite constant in the final answer. We combine all the terms obtained in region II as follows

$$T_{II} = \prod_{j} \left( \frac{\pi F_{L}(\lambda_{j})}{\sin(\pi F_{L}(\lambda_{j}))} \right) \exp\left[ \frac{1}{2} \int_{-q}^{q} d\lambda \rho_{L}(\lambda) \frac{F_{L}(\lambda)}{F_{L}'(\lambda)} \frac{\partial}{\partial \lambda} \left( \frac{F_{L}(\lambda)}{\rho_{L}(\lambda)} \right) \frac{\partial}{\partial \lambda} \left( \log\left( \frac{\pi F_{L}(\lambda)}{\sin(\pi F_{L}(\lambda))} \right) \right) \right]$$

$$\times \exp\left[ -\frac{L}{n^{*}} \int_{-q}^{q-\nu^{*}(q)} d\lambda \rho_{L}(\lambda) F_{L}^{2}(\lambda) - \frac{L}{n^{*}} \int_{-q+\nu^{*}(-q)}^{q} d\lambda \rho_{L}(\lambda) F_{L}^{2}(\lambda) \right]$$

$$\times \left( \frac{1}{\Gamma(1 - F_{L}(q))\Gamma(1 + F_{L}(q))\Gamma(1 + F_{L}(-q))\Gamma(1 - F_{L}(-q))} \right)^{n^{*}/2}.$$
(7.123)

In this region both  $\lambda_j$ ,  $\lambda_k$  are near the same quasi-Fermi point. Moreover, because there are only at most  $n^*$  terms to consider in this region, we do not require the precision we used in the rest of region II. This is because  $n^*/L$  can be neglected in the thermodynamic limit. Thus, by ignoring 1/L terms in the near edge region, and, simply sending  $\nu^*$  to zero in the integral in Eq. (7.123), we will only be making O(1/L) errors in the final answer.

This simplifies the analysis considerably, since we will be setting  $F_j = F_k = F_L(\pm q)$  in this region. We obtain two sets of products

$$T_{IIIa} = \prod_{j=1}^{n^*} \prod_{k=1}^{j-1} \frac{(j-k)}{(j-k+F_L(-q))^{1/2}(j-k-F_L(-q))^{1/2}},$$
  
$$T_{IIIb} = \prod_{j=N-n^*+1}^N \prod_{k=j+1}^N \frac{(j-k)}{(j-k+F_L(q))^{1/2}(j-k-F_L(q))^{1/2}}.$$
 (7.124)

Starting with the first expression and expanding the answer for  $n^* \gg 1$ , we obtain

$$T_{IIIa} = \prod_{j=1}^{n^*} \frac{\Gamma(j)\Gamma(1+F_L(-q))^{1/2}\Gamma(1-F_L(-q))^{1/2}}{\Gamma(j+F_L(-q))^{1/2}\Gamma(j-F_L(-q))^{1/2}}$$
$$= \frac{G(n^*+1)G(1+F_L(-q))^{1/2}G(1-F_L(-q))^{1/2}\Gamma(1+F_L(-q))^{n^*/2}\Gamma(1-F_L(-q))^{n^*/2}}{G(n^*+F_L(-q)+1)^{1/2}G(n^*-F_L(-q)+1)^{1/2}}$$
$$\approx \Gamma(1+F_L(-q))^{n^*/2}\Gamma(1-F_L(-q))^{n^*/2}G(1-F_L(-q))^{1/2}G(1+F_L(-q))^{1/2}(n^*)^{-\frac{F_L^2(-q)}{2}},$$
(7.125)

where G(x) denotes the Barnes G function, (see Eqs.(A1) - (A4)).

Similarly, for the other product

$$T_{IIIb} = \Gamma (1 + F_L(q))^{n^*/2} \Gamma (1 - F_L(q))^{n^*/2} G (1 - F_L(q))^{1/2} G (1 + F_L(q))^{1/2} (n^*)^{-\frac{F_L^2(q)}{2}}.$$
(7.126)

The final result for T'' is given by

$$T'' = (qL\rho_L(q))^{-\frac{1}{2}(F_L^2(q) + F_L^2(-q))} (G(1 + F_L(q))G(1 + F_L(-q))G(1 - F_L(q))G(1 - F_L(-q)))^{1/2} \\ \times \left(\prod_{j=1}^N \frac{\pi F_L(\lambda_j)}{\sin(\pi F_L(\lambda_j))}\right) \exp\left\{P_{\pm} \int_{-1}^1 dx \frac{F_L^2(qx)}{x^2 - 1} - \frac{1}{4} \int_{-q}^q d\lambda \int_{-q}^q d\mu \left(\frac{F_L(\lambda) - F_L(\mu)}{\lambda - \mu}\right)^2\right\} \\ \times \exp\left[\frac{1}{2} \int_{-q}^q d\lambda \{1 - \pi F_L(\lambda) \cot(\pi F_L(\lambda))\} \left(F_L'(\lambda) - \frac{F_L(\lambda)\rho_L'(\lambda)}{\rho_L(\lambda)}\right)\right].$$
(7.127)

Having obtained the expression for T'', we need to remove the "incorrect" hole terms, Eq. (7.103), to obtain T' as in Eq. (7.102). The treatment of this term depends on the distance of the hole from the quasi-Fermi points. To quantify the notion of the distance from the nearest quasi-Fermi point, we define a quantity  $q_k$  in the following way

$$q_k^+ = n_k^- - n_N - 1. (7.128)$$

Thus if the  $k^{th}$  hole is at the right quasi-Fermi point,  $q_k = -1$ , if it is in the middle of distribution then  $q_k \approx -N/2$  etc. Moreover, we say that a hole is near the right quasi-Fermi point, if  $q_k/L$  is 0 in the thermodynamic limit, and conversely we say it is "deep", or far from the right quasi-Fermi point, if  $q_k/L$  is a constant in the thermodynamic limit.

Similarly for holes near the left quasi-Fermi point, we define  $q_k^-$  to be

$$q_k^- = n_k^- - n_1 + 1. (7.129)$$

Now we wish to evaluate

$$T_{hole} = \prod_{j \neq i^-} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \lambda^-) + \frac{F_L(\lambda^-)\rho_L(\lambda_j)}{\rho_L(\lambda^-)}} \right)^{-1}.$$
(7.130)

We would again like to use the cutoff procedure used to obtain T''. In the region where  $|j - i^-| \ge n^*$ , we expand  $T_{hole}$  logarithmically as follows

$$T_{hole}^{I} = \exp\left[-\sum_{|j-i^{-}|\geq n^{*}} \log\left(1 - \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda^{-}) + \frac{F_{L}(\lambda^{-})\rho_{L}(\lambda_{j})}{\rho_{L}(\lambda^{-})}}\right)\right]$$
$$= \exp\left[\sum_{|j-i^{-}|\geq n^{*}} \frac{F_{L}(\lambda_{j})}{L\rho_{L}(\lambda_{j})(\lambda_{j} - \lambda^{-})}\right] + O\left(\frac{1}{L}\right).$$
(7.131)

Meanwhile, in the region where  $|j - i^-| < n^*$ , we use the approximation in Eq. (7.109), to evalute discrete products as follows

$$T_{hole}^{II} = \prod_{|j-i^-| < n^*} \frac{j - i^- + F(\lambda^-)}{j - i^-}.$$
(7.132)

# Case I : Hole is deep inside the distribution

When the hole is deep inside the distribution, we obtain from Eqs. (7.131), (7.132)

$$\log(T_{hole}^{k,deep}) = \int_{-q}^{\lambda_k^- - \nu^*(\lambda_k^-)} d\lambda \frac{F_L(\lambda)}{\lambda - \lambda_k^-} + \int_{\lambda_k^- + \nu^*(\lambda_k^-)}^{q} d\lambda \frac{F_L(\lambda)}{\lambda - \lambda_k^-} - \log\left(\frac{\Gamma(1 + F_L(\lambda_k^-))\Gamma(1 - F_L(\lambda_k^-))\Gamma(n^*)^2)}{\Gamma(n^* + F_L(\lambda_k^-))\Gamma(n^* - F_L(\lambda_k^-))}\right).$$
(7.133)

We get cancellation between divergent and cutoff dependent terms from the integrals due to the symmetric cutoff. Thus in the thermodynamic limit we have

$$T_{hole}^{k,deep} = \frac{\sin[\pi F(\mu_k^{-})]}{\pi F(\mu_k^{-})} \exp\left(P \int_{-1}^{1} dx \frac{F(qx)}{x - \frac{\mu_k^{-}}{q}}\right).$$
 (7.134)

#### Case II: Hole near the quasi-Fermi point

Meanwhile when the hole is near either  $\pm q$ , we obtain from Eqs. (7.131), (7.132), the following expression

$$T_{hole}^{k,edge} = (qL\rho(q))^{\mp F(\pm q)} \frac{\sin[\pi F(\pm q)]}{\pi F(\pm q)} \frac{\Gamma(\mp q_k^{\pm} \pm F(\pm q))}{\Gamma(\mp q_k^{\pm})}$$
$$\times \exp\left(P_{\pm} \int_{-1}^1 dx \frac{F(qx)}{x \mp 1}\right), \qquad (7.135)$$

where we use  $q_k^{\pm}$  to refer to the location of holes near a quasi-Fermi point as defined in Eqs. (7.128), (7.129).

In order to replace the "correct" term in the evaluation of  $M_2$ , we require the following term:

$$T_{particle} = \prod_{j \neq i^{-}} \left( 1 - \frac{F_L(\lambda_j)}{L\rho_L(\lambda_j)(\lambda_j - \mu_0^+) + \frac{F(\mu_0^+)\rho(\lambda_j)}{\rho(\mu_0^+)}} \right).$$
(7.136)

Again, we distinguish the case where the particle excitation is far from either edge and the case where it is near the edge. For this purpose we define a means of quantifying nearness to a quasi-Fermi point. Let us define,  $p_k^+ = n_k^+ - n_N - 1$ , for a particle near the right quasi-Fermi point, and  $p_k^- = n_k^+ - n_1 + 1$ , for a particle near the left quasi-Fermi point. We treat two distinct cases,

#### Case I: Particle far from edge

If we find  $p_k/L$  is finite in the thermodynamic limit, then we have the following convergent term

$$T_{particle}^{k,far} = \exp\left(-\int_{-1}^{1} dx \frac{F(qx)}{x - \frac{\mu_{k}^{+}}{q}}\right).$$
 (7.137)

Case II: Particle near quasi-Fermi Point

If  $p_k^{\pm}/L$  vanishes in the thermodynamic limit, we need to use our cutoff procedure to separately evaluate the contribution to  $T_{particle}$  from the region where  $\lambda_j$  is near  $\mu^+$ , and where they are far. We let the *j* product extend as near as  $\nu^*(\pm q)$  to the relevant quasi-Fermi point, and treat the terms within  $\nu^*$  of the quasi-Fermi point separately

$$T_{particle}^{k,near} = \left(\frac{qL\rho(q)}{n^{*}}\right)^{\pm F(\pm q)} \frac{\Gamma(n^{*})\Gamma(\pm p_{k}^{\pm} + 1 \mp F(\pm q))}{\Gamma(\pm p_{k}^{\pm} + 1)\Gamma(n^{*} \mp F(\pm q))} \\ = (qL\rho(q))^{\pm F(\pm q)} \frac{\Gamma(\pm p_{k}^{\pm} + 1 \mp F(\pm q))}{\Gamma(\pm p_{k}^{\pm} + 1)} \\ \times \exp\left(-P_{\pm} \int_{-1}^{1} dx \frac{F(qx)}{x \mp 1}\right).$$
(7.138)

Now we consider how the term  $M_2$  needs to be modified when there are *n* particlehole pairs. Most obviously, the shift function used,  $F(\lambda)$ , becomes the sum of the shift functions with the different particle-hole contributions. The term T'' is unaltered since it is evaluated with  $\mu_i^-$  substituted for  $\mu_i^+$ , making the definition of  $F(\lambda)$  in Eq. (7.67) valid for all  $\lambda_j$ . In order to "correct" for this convenient substitution, we include the terms  $T_{hole}$  associated with each of the holes, and terms  $T_{particle}$  associated with each of the particles as described in the previous subsections. However, when there are multiple particle-hole pairs, this is no longer sufficient to correctly evaluate  $M_2$ . There will be another group of terms which we shall call  $T_{cross}$  whose origin can be understood in the following way. Let us start by writing down an expression for  $M_2$  and show how to arrive at the correct final answer

$$M_{2} = T'' \times \prod_{k=1}^{n} T_{particle}^{(k)} \times T_{hole}^{(k)}$$

$$= \prod_{j \neq k}^{N} \cdots \left( \frac{\lambda_{jk} \mu_{kj}}{(\mu_{k} - \lambda_{j})^{2}} \right)^{1/2} \times \prod_{k=1}^{n} \prod_{j < n_{k}^{-}} \left( \frac{\mu_{j} - \mu_{k}^{-}}{\lambda_{j} - \mu_{k}^{-}} \right)^{-1} \left( \frac{\mu_{j} - \mu_{k}^{+}}{\lambda_{j} - \mu_{k}^{+}} \right)$$

$$= \prod_{j \neq k}^{N} \cdots \left( \frac{\lambda_{jk} \mu_{kj}}{(\mu_{k} - \lambda_{j})^{2}} \right)^{1/2} \times \prod_{k=1}^{n} \prod_{j}^{N} \cdots \left( \frac{\mu_{j} - \mu_{k}^{-}}{\lambda_{j} - \mu_{k}^{-}} \right)^{-1} \left( \frac{\mu_{j} - \mu_{k}^{+}}{\lambda_{j} - \mu_{k}^{+}} \right)$$

$$\times \prod_{k_{1} \neq k_{2}}^{n} \left( \frac{(\mu_{k_{1}}^{-} - \mu_{k_{2}}^{-})(\mu_{k_{1}}^{+} - \mu_{k_{2}}^{+})}{(\mu_{k_{1}}^{-} - \mu_{k}^{+})^{2}} \right)^{1/2}$$

$$= T'' \times \left( \prod_{k=1}^{n} T_{pChapter}^{(k)} \times T_{hole}^{(k)} \right) \times T_{cross}, \qquad (7.139)$$

where the notation  $T_{hole}^{(k)}(T_{particle}^{(k)})$  means the contribution from the hole (particle) term specific to the details of the excitation,  $\mu_k^-(\mu_k^+)$ , and  $n_k^-$  refers to the index corresponding to the excitation pair  $\mu_k^+, \mu_k^-$ .

Thus we obtain the expression

$$T_{cross} = \prod_{k_1 \neq k_2}^{n} \left( \frac{(\mu_{k_1}^- - \mu_{k_2}^-)(\mu_{k_1}^+ - \mu_{k_2}^+)}{(\mu_{k_1}^- - \mu_{k_2}^+)^2} \right)^{1/2}.$$
 (7.140)

We expect that the contributions to  $T_{particle}$ ,  $T_{hole}$  from the excitations  $\{\mu_1^+, ..., \mu_n^+ | \mu_1^-, ..., \mu_n^-\}$  fall into one of the cases discussed in previous subsections. Thus, the form of these terms is always known in principle.

The term  $T_{cross}$  is sensitive to the details of the excitations - for instance it will contain divergences when some number of the particles, or holes, are clustered near each other. For our purposes, this is only relevant to form factors of states containing high order Umklapp excitations, i.e. several particles and holes near the left (right) quasi-Fermi points. We will discuss the term  $T_{cross}$  in more detail in the section devoted to Umklapp form factors. The discussion above can be made applicable to  $M_2$  in the creation/annihilation operators with two modifications. First we need to replace  $F_L(\lambda)$  by  $F_{\pm,L}(\lambda)$  defined in Eqs. (7.84), (7.85), as discussed in the section following these definitions.

Secondly, if we wish to retain the calculation performed in the previous subsection then we need to extend/reduce the upper bounds of the indices of the products in  $M_2$  (see Eq. (7.100)) from N-1 to N by using the relation,  $\mu_{n+1}^- = \lambda_{n-1} - \frac{F_-(\lambda_{n-1})}{L\rho_L(\lambda_{n-1})} + O(1/L^2)$  to define the "missing" ground state or excited state quasi momentum (see Section IV.3), and for concreteness we again concentrate on the case of the annihilation operator. This will introduce some error to be corrected to obtain the final answer for  $M_2^{\psi}$  and  $M_2^{\psi^{\dagger}}$  - for the creation and annihilation operator respectively.

We will follow the consequences of such a replacement and correction for the annihilation operator and just present the final answer for the creation operator since the derivation is essentially the same.

Consider the product

$$M_2^{\psi} = \left(\prod_{j \neq k \neq n^-}^N \frac{\lambda_{jk} \tilde{\mu}_{jk}}{(\lambda_j - \tilde{\mu}_k)^2}\right)^{1/2}.$$
(7.141)

Now extending the upper limit of indices to N introduces the following extra terms

$$\prod_{j \neq n^{-}}^{N} \frac{(\lambda_{n^{-}} - \lambda_{j})(\mu_{n+1}^{-} - \tilde{\mu}_{j})}{(\lambda_{n^{-}} - \tilde{\mu}_{j})(\lambda_{j} - \mu_{n+1}^{-})}.$$
(7.142)

Notice, however that one group of terms in the above expression is present in the final answer for the annihilation operator,  $\mathcal{G}^-$ , which can be seen explicitly in Eq. (7.88). Thus we may write

$$M_{2}^{\psi} \times \prod_{\substack{j \neq n^{-} \\ j \neq n^{-}}}^{N} \frac{\lambda_{n^{-}} - \lambda_{j}}{\lambda_{n^{-}} - \mu_{j}} = \left(\prod_{\substack{j \neq k}}^{N} \frac{\lambda_{jk} \tilde{\mu}_{jk}}{(\lambda_{j} - \tilde{\mu}_{k})^{2}}\right)^{1/2}$$
$$\times \prod_{\substack{j \neq n^{-} \\ \mu_{n+1}^{-} - \mu_{j}}}^{N} \frac{\mu_{n+1}^{-} - \lambda_{j}}{\mu_{n+1}^{-} - \mu_{j}}, \qquad (7.143)$$

where the last product serves to cancel the unwanted terms in the parentheses. For notational convenience let us call the product multiplying  $M_2^{\psi}$  on the left hand side of the above equation,  $T_{extra}^{\psi}$ . However, as before it is more convenient to evaluate our double primed products where we substitute  $\mu_i^-$  in place of  $\mu_i^+$  and correct this mistake separately as in Eq. (7.102). Consequently we obtain from Eq. (7.143) and Eq. (7.139)

$$M_2^{\psi} \times \prod_{j \neq n^-}^N \frac{\lambda_{n^-} - \lambda_j}{\lambda_{n^-} - \tilde{\mu}_j} = \left[ T'' \times \left( \prod_{k=1}^n T_{particle}^{(k)} \times \prod_{k=1}^{n+1} T_{hole}^{(k)} \right) \times T_{cross}^{\psi} \right], \quad (7.144)$$

with

$$T_{cross}^{\psi} = \left[\frac{\prod_{k_1 \neq k_2}^{n+1} (\mu_{k_1}^- - \mu_{k_2}^-) \prod_{k_1 \neq k_2}^{n} (\mu_{k_1}^+ - \mu_{k_2}^+)}{\prod_{k_1 \neq k_2}^{n+1} \prod_{k_2=1}^{n} (\mu_{k_1}^- - \mu_{k_2}^+)}\right]^{1/2}.$$
(7.145)

The corresponding term for the creation operator form factor can be obtained by switching particle and hole quasimomenta in the above expression.

We obtain a similar expression for the creation operator and the answers are summarized in the next section.

The most general result for  $M_2$  in the case of the density form factor is given by

$$M_{2} = (qL\rho_{L}(q))^{-\frac{1}{2}(F_{L}^{2}(q)+F_{L}^{2}(-q))} (G(1+F_{L}(q))G(1+F_{L}(-q))G(1-F_{L}(q))G(1-F_{L}(-q)))^{1/2} \\ \times \left(\prod_{j=1}^{N} \frac{\pi F_{L}(\lambda_{j})}{\sin(\pi F_{L}(\lambda_{j}))}\right) \exp\left\{P_{\pm} \int_{-1}^{1} dx \frac{F_{L}^{2}(qx)}{x^{2}-1} - \frac{1}{4} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{L}(\lambda) - F_{L}(\mu)}{\lambda - \mu}\right)^{2}\right\} \\ \times \exp\left[\frac{1}{2} \int_{-q}^{q} d\lambda \{1 - \pi F_{L}(\lambda) \cot(\pi F_{L}(\lambda))\} \left(F_{L}'(\lambda) - \frac{F_{L}(\lambda)\rho_{L}'(\lambda)}{\rho_{L}(\lambda)}\right)\right] \\ \times \left[\prod_{k=1}^{n} T_{hole}^{(k)} \times T_{particle}^{(k)}\right] \times T_{cross}.$$
(7.146)

Similarly, for the creation/annihilation operators it is given by

$$M_{2}^{\psi/\psi^{\dagger}} = (qL\rho_{L}(q))^{-\frac{1}{2}(F_{\pm,L}^{2}(q)+F_{\pm,L}^{2}(-q))} \\ \times (G(1+F_{\pm,L}(q))G(1+F_{\pm,L}(-q))G(1-F_{\pm,L}(q))G(1-F_{\pm,L}(-q)))^{1/2} \\ \times \left[\prod_{k=1}^{n(+1)} T_{hole}^{(k)} \times \prod_{k=1}^{n+1(-1)} T_{particle}^{(k)}\right] \times T_{cross}^{\psi/\psi^{\dagger}} \left(\prod_{j=1}^{N} \frac{\pi F_{\pm,L}(\lambda_{j})}{\sin(\pi F_{\pm,L}(\lambda_{j}))}\right) \\ \times \exp\left\{P_{\pm} \int_{-1}^{1} dx \frac{F_{\pm,L}^{2}(qx)}{x^{2}-1} - \frac{1}{4} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{\pm,L}(\lambda) - F_{\pm,L}(\mu)}{\lambda - \mu}\right)^{2}\right\} \\ \times \exp\left[\frac{1}{2} \int_{-q}^{q} d\lambda \{1 - \pi F_{\pm,L}(\lambda) \cot(\pi F_{\pm,L}(\lambda))\} \left(F_{\pm,L}'(\lambda) - \frac{F_{\pm,L}(\lambda)\rho_{L}'(\lambda)}{\rho_{L}(\lambda)}\right)\right].$$
(7.147)

# 7.5.5 Fredholm Determinants

The last terms left to express in the thermodynamic limit are the determinant terms appearing in the form factors, such as  $\Theta$  in Eq. (7.81). We would like to write such terms as Fredholm determinants (see Appendix D and Ref. [279] for details on Fredholm determinants). The determinants are slightly different for the density and creation/annihilation operators. We will first do the calculation for the determinant in the density form factor, and then use some of these results to express the determinant for the creation/annihilation form factors.

We need to evaluate

$$\Theta = \frac{\operatorname{Det}\left(\delta_{jk} + \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j} (K(\lambda_j, \lambda_k) - K(\lambda_p, \lambda_k))\right)}{V_p^+ - V_p^-}.$$
(7.148)

Due to properties of the matrices involved in the determinant, the choice of  $\lambda_p$  is entirely arbitrary [249] and it need not be from the set  $\{\lambda_i\}$ . We can use this fact by taking  $\lambda_p$  to be much larger than all other parameters of the problem. Under these circumstances,  $K(\lambda_p, \lambda_k) \to \frac{2c}{\lambda_p^2}$ . Meanwhile the denominator lends itself to the following expansion

$$V_{p}^{\pm} = \prod_{h=1}^{n} \left( 1 - \frac{\mu_{h}^{+} - \lambda_{h}^{-}}{\lambda_{p}} - \frac{(\lambda_{h}^{-} - \mu_{h}^{+})(\lambda_{h}^{-} \pm ic)}{\lambda_{p}^{2}} \right) \\ \times \prod_{m} '' \left( 1 + \frac{F(\lambda_{m})}{L\rho(\lambda_{m})\lambda_{p}} + \frac{F(\lambda_{m})(\lambda_{m} \pm ic)}{L\rho(\lambda_{m})\lambda_{p}} \right) \\ + O\left(\frac{1}{\lambda_{p}^{3}}\right).$$
(7.149)

Using this, one can evaluate the denominator in this limit as

$$V_p^+ - V_p^- = \frac{2ic}{\lambda_p^2} \left( \sum_h \lambda_h^- - \mu_h^+ + \int_{-q}^q F(\lambda) d\lambda \right)$$
$$= \frac{-2icP_{ex}}{\lambda_p^2}, \tag{7.150}$$

where we have used the relation between momentum and quasimomenta as in Ref. [203].

The numerator also lends itself to a convenient re-expression. Essentially the numerator has the form  $Det(A + \alpha \frac{B}{c})$ , where

$$A = \delta_{jk} + \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j} K(\lambda_j, \lambda_k),$$
  

$$B = -\frac{i(\mu_j - \lambda_j)}{c(V_j^+ - V_j^-)} \prod_{m \neq j} \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j},$$
  

$$\alpha = \frac{2c^2}{\lambda_p^2}.$$
(7.151)

Using the fact that B is a matrix of rank one, we can expand the determinant using rows and minors alternately from A and B. Using the expression for the determinant of a sum of matrices [203], we find that because of B's rank, only terms with one row from B will survive. Moreover the determinant of A also vanishes permitting further simplification. Thus the determinant can be written

$$Det(A + \alpha B) = Det(A) + \alpha \sum B_{ij}a_{ij} + \alpha \sum A_{ij}a_{ij} - \alpha \sum A_{ij}a_{ij}$$
$$= Det(A) - \alpha Det(A) + \alpha Det(A + B)$$
$$= \alpha Det(A + B).$$
(7.152)

Taken together with the previous statements we get

$$\Theta = \frac{ic}{P_{ex}} \operatorname{Det} \left( \delta_{jk} + \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j} \left( \frac{2c}{(\lambda_j - \lambda_k)^2 + c^2} - \frac{1}{c} \right) \right). \quad (7.153)$$

To express the above as a Fredholm determinant, we consider the following term

$$a_j = \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j}.$$
(7.154)

The terms  $V_j^{\pm}$  admit the following partial limit

$$V_j^{\pm} = \prod_{h=1}^n \frac{\mu_h^+ - \lambda_j \pm ic}{\lambda_h^- - \lambda_j \pm ic} \exp\left[\int_{-q}^q \frac{F_L(\lambda)}{\lambda - \lambda_j \pm ic} + O(1/L)\right].$$
(7.155)

The infinite product in Eq. (7.153) is not as easy to treat. We cannot make the same kind of continuum approximation as above because of the bad behavior of such an integral around  $\lambda_j$ . This can be treated by temporarily introducing a cutoff into the continuum version of the product (an integral) and extracting any constant (cutoff independent) error committed in so doing to finally obtain an answer that is cutoff independent. We obtain

$$\prod_{m\neq j}^{N} \left( \frac{\mu_m - \lambda_j}{\lambda_m - \lambda_j} \right) = \prod_{m\neq j}^{N-1} \left( 1 - \frac{F_L(\lambda_m)}{L\rho_L(\lambda_m)(\lambda_m - \lambda_j)} \right) \times \left( \frac{\mu^+ - \lambda_j}{\lambda^- - \lambda_j} \right)$$

$$= \exp\left\{ - \int_{-q}^{\lambda_L} \frac{F_L(\lambda)}{\lambda - \lambda_j} - \int_{\lambda_R}^{q} \frac{F_L(\lambda)}{\lambda - \lambda_j} \right\}$$

$$\times \frac{\Gamma(n^* + 1 + F_j)\Gamma(n^* + 1)\Gamma(n^* + 1)\Gamma(1 - F_j)}{\Gamma(1 + F_j)\Gamma(n^* - \lambda_j)}$$

$$\times \prod_{h=1}^{n} \left( \frac{\mu_h^+ - \lambda_j}{\lambda_h^- - \lambda_j} \right).$$
(7.156)

Here  $\lambda_L$  and  $\lambda_R$  correspond to the spectral parameters corresponding to the quantum number  $j \pm n^*$ . Under the assumption that  $n^* \gg 1$ , we can use the Stirling approximation on the gamma functions:

$$\frac{\Gamma(n^* + 1 + F_j)\Gamma(n^* + 1 - F_j)}{\Gamma(1 + F_j)\Gamma(n^* + 1)\Gamma(n^* + 1)\Gamma(1 - F_j)} = \exp\left\{(n^* + 1 + F_j)\log(n^* + 1 + F_j) - n - 1 - F_j + (n^* + 1 - F_j)\log(n^* + 1 - F_j)\right\} \times \exp\left\{-n - 1 + F_j - 2(n^* + 1)\log(n^* + 1) + 2(n^* + 1)\right\} \frac{1}{\Gamma(1 + F_L(\lambda_j))\Gamma(1 - F_L(\lambda_j))} = \frac{1}{\Gamma(1 + F(\lambda_j))\Gamma(1 - F(\lambda_j))} + O(1/L).$$
(7.157)

Where the exponential terms exactly cancel out. Furthermore the integrals contribute terms at the boundaries that also mutually cancel, leaving no constant terms up to O(1/L)

$$I_{boundaries} = -F(\lambda_j) log(\lambda_L - \lambda_j) + F(\lambda_j) log(\lambda_R - \lambda_j)$$
  
$$= F(\lambda_j) \left[ log\left(\frac{n^*}{L\rho(\lambda_j)}\right) - log\left(\frac{n^*}{L\rho(\lambda_j)}\right) \right]$$
  
$$= 0.$$
(7.158)

This allows us to express  $a_j$  as

$$a_{j} = \frac{i(\mu_{j} - \lambda_{j})}{\prod_{h=1}^{n} \frac{\mu_{h}^{+} - \lambda_{j} + ic}{\lambda_{h}^{-} - \lambda_{j} + ic}} \exp\left[\int_{-q}^{q} d\lambda \frac{F(\lambda)}{\lambda - \lambda_{j} + ic}\right] - c.c} \prod_{h=1}^{n} \frac{\mu_{h}^{+} - \lambda_{j}}{\lambda_{h}^{-} - \lambda_{j}} \frac{\exp\left[P\int_{-1}^{1} dx \frac{F(qx)}{x - \lambda_{j}/q}\right]}{\Gamma(1 + F(\lambda_{j}))\Gamma(1 - F(\lambda_{j}))}$$
$$= \frac{1}{2\pi L\rho(\lambda_{j})} \prod_{h=1}^{n} \frac{\lambda_{h}^{-} - \lambda_{j} + ic}{\mu_{h}^{+} - \lambda_{j} + ic} \times \frac{\mu_{h}^{+} - \lambda_{j}}{\lambda_{h}^{-} - \lambda_{j}}$$
$$\times \exp\left[-P\int_{-1}^{1} dx \frac{F(qx)}{x - \lambda_{j}/q} + i\pi F(\lambda_{j}) + \int_{-q}^{q} d\lambda \frac{F(\lambda)}{\lambda - \lambda_{j} + ic}\right].$$
(7.159)

Let us define an operator,  $\hat{G}$  that acts on  $[-q,q]\times [-q,q]$  and is given by

$$G(\mu,\nu) = a(\mu) \left( K(\mu-\nu) - \frac{1}{c} \right),$$
(7.160)

where the function  $a(\mu)$  appearing above is

$$a(\mu) = \frac{1}{2\pi} \prod_{h=1}^{n} \frac{\lambda_{h}^{-} - \mu + ic}{\mu_{h}^{+} - \mu + ic} \times \frac{\mu_{h}^{+} - \mu}{\lambda_{h}^{-} - \mu} \\ \exp\left[-P \int_{-1}^{1} dx \frac{F(qx)}{x - \mu/q} + i\pi F(\mu) + \int_{-q}^{q} d\lambda \frac{F(\lambda)}{\lambda - \mu + ic}\right].$$
(7.161)

Using Eqs. (7.153), (7.160), we obtain

$$\Theta = \frac{ic}{P_{ex}} \operatorname{Det} \left( I + \hat{G} \right).$$
(7.162)

The determinant terms appearing in the creation/annihilation form factors are a slightly modified version of the one for the density form factor, and are given by

$$\zeta^{-} = \operatorname{Det}\left(\delta_{jk} + \frac{i(\tilde{\mu}_{j} - \lambda_{j})}{\tilde{V}_{j}^{+} - \tilde{V}_{j}^{-}} \frac{\prod_{m \neq j \neq n^{-}}^{N} (\tilde{\mu}_{m} - \lambda_{j})}{\prod_{m \neq j}^{N} (\lambda_{m} - \lambda_{j})} (K(\lambda_{j} - \lambda_{k}) - K(\mu_{n+1}^{-} - \lambda_{k}))\right),$$
  
$$\zeta^{+} = \operatorname{Det}\left(\delta_{jk} + \frac{i(\tilde{\mu}_{j} - \lambda_{j})}{\tilde{V}_{j}^{+} - \tilde{V}_{j}^{-}} \frac{\prod_{m \neq j}^{N+1} (\tilde{\mu}_{m} - \lambda_{j})}{\prod_{m \neq j}^{N} (\lambda_{m} - \lambda_{j})} (K(\lambda_{j} - \lambda_{k}) - K(\lambda_{j} - \mu_{n+1}^{+}))\right),$$
  
(7.163)

where the +/- in the subscript correspond to the determinant for the creation/annihilation operators respectively. Note that by  $\tilde{\tilde{V}}_{j}^{\pm}$  we mean the term occurring in the creation operator form factor defined analogously to Eq. (7.52).

The procedure we use to express  $\zeta^{\pm}$  as a Fredholm determinant is similar to what we used for the case of the density form factor. Let us define functions  $b_j^{\pm}$  similar to  $a_j$ :

$$b_j^- = \frac{i(\tilde{\mu}_j - \lambda_j)}{\tilde{V}_j^+ - \tilde{V}_j^-} \frac{\prod_{m \neq j}^{N-1} (\tilde{\mu}_m - \lambda_j)}{\prod_{m \neq j}^N (\lambda_m - \lambda_j)},$$
  

$$b_j^+ = \frac{i(\tilde{\mu}_j - \lambda_j)}{\tilde{\tilde{V}}_j^+ - \tilde{\tilde{V}}_j^-} \frac{\prod_{m \neq j}^{N-1} (\tilde{\mu}_m - \lambda_j)}{\prod_{m \neq j}^N (\lambda_m - \lambda_j)}.$$
(7.164)

In the thermodynamic limit, and to the same accuracy with which we calculated  $a(\mu)$  we find

$$b^{-}(\mu) = \frac{1}{2\pi} \prod_{i=1}^{n+1} \frac{\lambda_{i}^{-} - \mu + ic}{\lambda_{i}^{-} - \mu} \prod_{j=1}^{n} \frac{\mu_{j}^{+} - \mu}{\mu_{j}^{+} - \mu + ic}$$

$$\exp\left[-P \int_{-1}^{1} dx \frac{F_{-}(qx)}{x - \mu/q} + i\pi F_{-}(\mu) + \int_{-q}^{q} d\lambda \frac{F_{-}(\lambda)}{\lambda - \mu + ic}\right],$$

$$b^{+}(\mu) = \frac{1}{2\pi} \prod_{i=1}^{n} \frac{\lambda_{i}^{-} - \mu + ic}{\lambda_{i}^{-} - \mu} \prod_{j=1}^{n+1} \frac{\mu_{j}^{+} - \mu}{\mu_{j}^{+} - \mu + ic}$$

$$\exp\left[-P \int_{-1}^{1} dx \frac{F_{+}(qx)}{x - \mu/q} + i\pi F_{+}(\mu) + \int_{-q}^{q} d\lambda \frac{F_{+}(\lambda)}{\lambda - \mu + ic}\right].$$
(7.165)

Now we may evaluate  $\zeta^{\pm}$  as Fredholm determinants of  $(I + \hat{H}^{\pm}(\mu, \nu))$ , where  $\hat{H}^{\pm}$ act on (-q, q) and are given by

$$H^{-}(\mu,\nu) = b^{-}(\mu)(K(\mu-\nu) - K(\mu_{n+1}^{-}-\nu)),$$
  

$$H^{+}(\mu,\nu) = b^{+}(\mu)(K(\mu-\nu) - K(\mu-\mu_{n+1}^{+})).$$
(7.166)

## 7.5.6 Thermodynamic Limit of Form Factors

We now present form factors for a few excited states that we would like to relate to the correlation prefactors of the Lieb-Liniger model. We first present a general expression for the density form factor and then obtain specific form factors from it, and then repeat the procedure with the creation/annihilation form factors.

By combining the results from Eqs. (7.83), (7.99), (7.146), (7.162), and the simplification, (C.5), described in Appendix C, we obtain a general expression for the density form factor:

In the above expressions, L is the length of the system, q the quasi momentum at the edge of the distribution,  $\mu^-, \mu^+$  are the quasi momenta corresponding to excitations, and,  $\rho(\lambda)$  is the ground state distribution function defined in Eq. (7.55). Moreover,  $F(\lambda)$  is the composite shift function defined in Eqs. (7.56), (7.70), G(x) is the Barnes function (Appendix A), while  $\hat{G}^{\pm}$  is obtained from Sec. 4.5,  $K(\lambda) = \frac{2c}{c^2 + \lambda^2}$ and the terms  $T_{particle}, T_{hole}, T_{cross}$  are described in Sec. 4.4 and cannot be written down in a general form.
Let us first calculate the density form factor for the Umklapp state. This state contains m adjacent holes starting at the left quasi-Fermi point, and m particles starting at the first available spot after the right quasi-Fermi point. Consequently we obtain m contributions from  $T_{particle}$ , as in Eq. (7.138), of the following form:

$$\prod_{k=1}^{m} T_{particle}^{(k)} = (qL\rho(q))^{mF(q)} \prod_{k=1}^{m} \frac{\Gamma(k - F(q))}{\Gamma(k)}$$
$$\exp\left(-P_{+} \int_{-1}^{1} dx \frac{mF(qx)}{x - 1}\right),$$
(7.170)

and similar contribution from the product of the  $T_{hole}$  terms, given by Eq. (7.135),

$$\prod_{k=1}^{m} T_{hole}^{(k)} = (qL\rho(q))^{mF(-q)}$$

$$\times \prod_{k=1}^{m} \frac{\Gamma(k - F(-q))}{F(-q)\Gamma(k)\Gamma(F(-q))\Gamma(1 - F(-q))}$$

$$\times \exp\left(P_{-} \int_{-1}^{1} \frac{mF(qx)}{x+1}\right).$$
(7.171)

Next from the cross terms given by Eq. (7.140),  $T_{cross}$ , and using the approximation Eq. (7.109) combined with the fact that the holes and particles occupy m adjacent spots near the two quasi-Fermi points, we obtain up to O(1/L) terms of the following form:

$$\begin{split} &\prod_{j \neq k}^{m} (\mu_{jk}^{-})^{1/2} = (L\rho(q))^{-1/2(m^2 - m)} \prod_{i=1}^{m} \Gamma(i), \\ &\prod_{j \neq k}^{m} (\mu_{jk}^{+})^{1/2} = (L\rho(q))^{-1/2(m^2 - m)} \prod_{i=1}^{m} \Gamma(i), \\ &\prod_{j \neq k}^{m} (\mu_{j}^{+} - \mu_{k}^{-}) = (2q)^{m^2 - m}, \\ &T_{cross} = (2Lq\rho(q))^{-m^2 + m} G^2(m + 1). \end{split}$$
(7.172)

Lastly, there is a term coming from the product (for instance appearing in Eq. (7.167)),

$$\prod_{i=1}^{m} \left( \frac{F(\mu^{-})}{(\mu^{+} - \mu^{-})L(\rho(\mu^{-})\rho(\mu^{+}))^{1/2}} \right) = \left( \frac{L\rho(q)2q}{F(-q)} \right)^{-m},$$
(7.173)

where, we have only retained terms bigger than O(1/L) by assuming all the holes and particles occur at approximately the quasi-Fermi points. Furthermore we have used the symmetry of  $\rho(\lambda)$ .

Combining Eqs. (7.170-7.172) and using the symmetry of the shift function for the Umklapp, and, the relation (A1) we obtain

$$T_{\text{Umklapp}} = (qL\rho(q))^{2mF(q)-m^2} \frac{G(m+1-F(q))^2}{(2)^{m^2}G(1-F(q))^2\Gamma(F(q))^m\Gamma(1-F(q))^m} \times \exp\left(P_-\int_{-1}^1 dx \frac{mF(qx)}{x+1} - P_+\int_{-1}^1 dx \frac{mF(qx)}{x-1}\right).$$
(7.174)

Furthermore we may also relate the shift function  $F(\lambda)$  to the ground state density function  $\rho(\lambda)$  for the Umklapp [249]. Let us start from the equation for the shift due to a first order Umklapp,  $F(\lambda|-q) - F(\lambda|q)$ , i.e. the shift for a particle hole pair at  $\{q; -q\}$ 

$$F(\lambda) - \frac{1}{2\pi} \int_{-q}^{q} d\nu K(\lambda - \nu) F(\nu) = \frac{\theta(\lambda - q)}{2\pi} - \frac{\theta(\lambda + q)}{2\pi},$$
  

$$F(\lambda) - \frac{1}{2\pi} \int_{-q}^{q} d\nu K(\lambda - \nu) F(\nu) = -\frac{1}{2\pi} \int_{-q}^{q} d\nu K(\lambda - \nu),$$
  

$$F(\lambda) - \frac{1}{2\pi} \int_{-q}^{q} d\nu K(\lambda - \nu) (F(\nu) - 1) = 0.$$
  
(7.175)

But this last equation is solved by  $F(\lambda) = -(2\pi\rho(\lambda) - 1)$ , since

$$2\pi\rho(\lambda) - \frac{1}{2\pi} \int_{-q}^{q} d\nu K(\lambda - \nu) 2\pi\rho(\nu) - 1 = 0.$$
 (7.176)

Moreover, since an order m Umklapp can be constructed by repeatedly performing m order one Umklapps, we may use the linearity of  $F(\lambda)$  to conclude

$$F_m(\lambda|\text{Umklapp}) = m(F(\lambda|-q) - F(\lambda|q)) = -m(2\pi\rho(\lambda) - 1).$$
(7.177)

This makes the exponent of L

$$-F^{2}(q) + 2mF(q) - m^{2} = -(m\sqrt{K} - m)^{2} - 2m(m\sqrt{K} - m) - m^{2}$$
$$= -m^{2}K, \qquad (7.178)$$

where we have used the relation

$$2\pi\rho(q) = \sqrt{K},\tag{7.179}$$

from Ref. [203], where K is the Luttinger parameter [208].

We may now obtain  $A_m$  the coefficients in the equal time density-density correlator Eq. (7.1) using Eq. (7.12). We substitute the various expressions obtained above into Eq. (7.167) to obtain

$$A_{m} = 2\gamma^{2} \left(\frac{q\sqrt{K}}{\rho_{0}}\right)^{-2m^{2}K} \left(\frac{4q^{2}+c^{2}}{4c^{2}}\right)^{m^{2}} \left(\frac{G(1+m\sqrt{K})^{2}G(m+1-m\sqrt{K})}{\Gamma(m-m\sqrt{K})^{m}\Gamma(1-m+m\sqrt{K})^{m}G(1-m+m\sqrt{K})}\right)^{2} \exp\left[4mq \int_{-q}^{q} d\lambda \frac{F(\lambda)}{((\lambda+ic)^{2}-q^{2})} - \int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}}\right] \exp\left[2P_{\pm} \int_{-1}^{1} dx \frac{F^{2}(qx)-2mF(qx)}{x^{2}-1} - \frac{1}{2} \int_{-q}^{q} \int_{-q}^{q} d\lambda d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right] \frac{\operatorname{Det}^{2}(1+\hat{G})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.180)

To determine the prefactors of the singularities of the dynamic structure factor (DSF)  $S(k,\omega)$  at Lieb's colective modes  $\varepsilon_{1,2}(k)$  [242, 203] using Eq. (7.21) we need to find corresponding form factors of the density operator from Eq. (7.167).

By considering the form factor for a Bose gas with one hole at the right edge and a high momentum particle, we may determine the prefactors of the DSF singularity at  $\varepsilon_1(k)$ . To do this we need to relate the quasi momentum of the particle  $\mu^+$  to the momentum k of the excited bosonic state as follows [203, 224]:

$$k = \mu^+ - \pi \rho_0 - \int_{-q}^{q} d\lambda \theta(\mu^+ - \lambda) \rho(\lambda), \qquad (7.181)$$

where,  $\theta(\lambda) = i \ln(\frac{ic+\lambda}{ic-\lambda})$ , and q is the quasimomentum at the edge of the distribution.

For the excited state with the particle hole pair  $(\mu^+, q)$ , we substitute  $F(\lambda | \mu^+, q)$ from Eq. (7.56) and substitute this function in the relevant places in Eq. (7.167). For such a particle-hole pair, we obtain a form for  $T_{hole}$  as in Eq. (7.135), and for  $T_{particle}$  as in Eq. (7.136). Since there is only a single particle-hole pair there is no contribution like  $T_{cross}$  we obtain

$$S_{1}(k) = c^{2}\sqrt{K} \left(q\sqrt{K}\right)^{-(F^{2}(q)+F^{2}(-q)-2F(q)+2)} (2\pi)^{F(q)-F(-q)} \left(\frac{G(1+F(-q))G(1-F(q))}{\Gamma(1-F(q))}\right)^{2} \\ \exp\left\{P_{\pm}\int_{-1}^{1} dx \frac{2F^{2}(qx)}{x^{2}-1} + P_{\pm}\int_{-1}^{1} dx \frac{2F(qx)}{x-1} - \frac{1}{2}\int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right\} \\ \exp\left[\int_{-q}^{q} d\lambda \frac{2F(\lambda)(\mu^{+}-q)}{(\lambda-q+ic)(\lambda-\mu^{+}+ic)}\right] \frac{(q-\mu^{+})^{2}+c^{2}}{c^{2}} \left(\frac{F^{2}(q)}{\rho(\mu^{+})(\mu^{+}/q-1)^{2}}\right) \\ \exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}} - \int_{-q}^{q} d\lambda \frac{2F(\lambda)}{\lambda-\mu^{+}}\right] \frac{\operatorname{Det}^{2}(1+\hat{G})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.182)

Note that the momentum dependence in the above expression is contained in the shift function,  $F(\lambda) = F(\lambda|\mu^+) - F(\lambda|q)$ , as well as the terms directly involving  $\mu^+$ . Furthermore we have used the relation in Eq. (7.179) to express the answer in terms of the Luttinger parameter, K [208].

Similarly, we may use Eq. (7.167), to obtain the DSF at the Lieb mode  $\varepsilon_2(k)$ , by considering the density form factor of a system with a single high momentum hole and a low momentum particle (at the right quasi-Fermi point). This time we relate the quasi momentum of the hole,  $\mu^-$ , to the momentum, k using

$$-k = \mu^{-} - \pi \rho_{0} - \int_{-q}^{q} d\lambda \theta (\mu^{-} - \lambda) \rho(\lambda), \qquad (7.183)$$

and, use the unique solution of the above to determine a shift function,  $F(\lambda|q, \mu^{-})$ , using Eq. (7.56). We may then use this  $F(\lambda)$  in Eq. (7.167) in conjunction with the expression for  $T_{particle}$  given by Eq. (7.138), and  $T_{hole}$  given by Eq. (7.133) to get the following expression for  $S_2(k)$ :

$$S_{2}(k) = c^{2}\sqrt{K} \left(q\sqrt{K}\right)^{-(F^{2}(q)+F^{2}(-q)+2F(q)+2)} (2\pi)^{F(q)-F(-q)} \left(\frac{G(1+F(-q))G(1-F(q))\Gamma(1-F(q))}{\Gamma(1+F(\mu^{-}))\Gamma(1-F(\mu^{-}))}\right)^{2} \\ \exp\left[\int_{-q}^{q} d\lambda \frac{2F(\lambda)(q-\mu^{-})}{(\lambda-\mu^{-}+ic)(\lambda-q+ic)}\right] \frac{(q-\mu^{-})^{2}+c^{2}}{c^{2}} \left(\frac{F^{2}(\mu^{-})}{\rho(\mu^{-})(\mu^{-}/q-1)^{2}}\right) \\ \exp\left\{-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}} + P_{\pm} \int_{-1}^{1} dx \frac{2F^{2}(qx)}{x^{2}-1} - P_{\pm} \int_{-1}^{1} dx \frac{2F(qx)}{x-1}\right\} \\ \exp\left[P\int_{-1}^{1} dx \frac{2F(qx)}{x-\mu^{-}/q} - \frac{1}{2}\int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right] \times \frac{\operatorname{Det}^{2}(1+\hat{G})}{\operatorname{Det}^{2}(1-\frac{\hat{K}}{2\pi})}.$$
(7.184)

Here too the dependence on momentum, k, is carried by  $F(\lambda) = F(\lambda|q) - F(\lambda|\mu^{-})$ and  $\mu^{-}$ . Furthermore we have used the relation in Eq. (7.179) to express the answer in terms of the Luttinger parameter, K [208].

Using the results from Eqs. (7.89), (7.90), (7.99), (7.147) as well as the simplification (C.5) outlined in Appendix C, we obtain the following analytic expressions for the form factors of the creation and annihilation operators.

The most general expression for the annihilation operator form factor is given by

$$\mathcal{G}^{-} = \frac{(qL\rho(q))^{-\frac{1}{2}(F_{-}^{2}(q)+F_{-}^{2}(-q))}}{L^{1/2}\rho(\mu^{-})^{1/2}} (2\pi)^{\frac{1}{2}(F_{-}(q)-F_{-}(-q)-1)} \frac{\pi F_{-}(\mu^{-})}{\sin(\pi F_{-}(\mu^{-}))} G(1+F_{-}(-q)) G(1-F_{-}(q)) 
\prod_{i=1}^{n} \left(\frac{F_{-}(\mu_{i}^{-})}{L(\rho(\mu_{i}^{-})\rho(\mu_{i}^{+}))^{1/2}(\mu_{i}^{-}-\mu_{i}^{+})}\right) \left[\prod_{k=1}^{n} T_{particle}^{(k)} \prod_{k=1}^{n+1} \times T_{hole}^{(k)}\right] \times T_{cross} 
\exp\left\{P_{\pm} \int_{-1}^{1} dx \frac{F_{-}^{2}(qx)}{x^{2}-1} - \frac{1}{4} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{-}(\lambda)-F_{-}(\mu)}{\lambda-\mu}\right)^{2}\right\} 
\exp\left[\sum_{i=1}^{n} \int_{-q}^{q} d\lambda \frac{F_{-}(\lambda)(\mu_{i}^{+}-\mu_{i}^{-})}{(\lambda-\mu_{i}^{-}+ic)(\lambda-\mu_{i}^{+}+ic)}\right] \prod_{i,j}^{n} \left[\frac{(\mu_{i}^{-}-\mu_{j}^{+}+ic)^{2}}{(\mu_{i,j}^{-}+ic)(\mu_{i,j}^{+}+ic)}\right]^{1/2} 
\exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \left(\frac{F_{-}(\lambda)F_{-}(\mu)}{2(\lambda-\mu+ic)^{2}}\right)\right] \frac{\operatorname{Det}(1+\hat{H}^{-})}{\operatorname{Det}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.185)

The creation operator form factor is given by

$$\mathcal{G}^{+} = \frac{(qL\rho(q))^{-\frac{1}{2}(F_{+}^{2}(q)+F_{+}^{2}(-q))}}{L^{1/2}\rho(\mu^{+})^{1/2}} (2\pi)^{\frac{1}{2}(F_{+}(q)-F_{+}(-q)-1)} G(1+F_{+}(-q)) G(1-F_{+}(q))$$

$$\prod_{i=1}^{n} \left(\frac{F_{+}(\mu_{i}^{-})}{L(\rho(\mu_{h}^{-})\rho(\mu_{h}^{+}))^{1/2}(\mu_{i}^{-}-\mu_{i}^{+})}\right) \left[\prod_{k=1}^{n+1} T_{particle}^{(k)} \times \prod_{k=1}^{n} T_{hole}^{(k)}\right] \times T_{cross}$$

$$\exp\left\{P_{\pm} \int_{-1}^{1} dx \frac{F_{+}^{2}(qx)}{x^{2}-1} - \frac{1}{4} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{+}(\lambda)-F_{+}(\mu)}{\lambda-\mu}\right)^{2}\right\}$$

$$\exp\left[\sum_{i=1}^{n} \int_{-q}^{q} d\lambda \frac{F_{+}(\lambda)(\mu_{i}^{+}-\mu_{i}^{-})}{(\lambda-\mu_{i}^{-}+ic)(\lambda-\mu_{i}^{+}+ic)}\right] \prod_{i,j}^{n} \left[\frac{(\mu_{i}^{-}-\mu_{j}^{+}+ic)^{2}}{(\mu_{i,j}^{-}+ic)(\mu_{i,j}^{+}+ic)}\right]^{1/2}$$

$$\exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \left(\frac{F_{+}(\lambda)F_{+}(\mu)}{2(\lambda-\mu+ic)^{2}}\right)\right] \frac{\operatorname{Det}(1+\hat{H}^{+})}{\operatorname{Det}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.186)

In the above expressions, L is the length of the system, q the quasi momentum at the edge of the distribution,  $\mu^-$ ,  $\mu^+$  are the quasi momenta corresponding to excitations, and  $\rho(\lambda)$  is the ground state distribution function defined in Eq. (7.55). Moreover,  $F_{\pm}(\lambda)$  are the modified shift functions defined in Eqs. (7.84), (7.85), G(x)is the Barnes function (Appendix A),  $\hat{H}^{\pm}$  is obtained from Sec. 4.6,  $K(\lambda) = \frac{2c}{c^2 + \lambda^2}$ and the terms  $T_{particle}, T_{hole}, T_{cross}$  are described in Sec. 4.4 and cannot be written down in a general form.

In order to obtain from Eq. (7.185) the annihilation operator form factor for an order m Umklapp state, we first collect terms from Eqs. (7.170) - (7.172) with the appropriate modified shift function and the extra hole to obtain

$$T_{Umklapp} = (L\rho(q))^{(m-1)F_{-}(q)+mF_{-}(-q)-m(m-1)} \\ \times \frac{1}{(2q)^{m^{2}-m}} \exp\left[-(m-1)P_{+}\int_{-1}^{1} dx \frac{F_{-}(qx)}{x-1} + mP_{-}\int_{-1}^{1} dx \frac{F_{-}(qx)}{x+1}\right] \\ \times \frac{G(m+1-F_{-}(-q))G(m+1-F_{-}(q))}{G(1-F_{-}(-q))\Gamma(F_{-}(-q))^{m-1}\Gamma(1-F_{-}(-q))^{m-1}\Gamma(1-F_{-}(q))\Gamma(1+F_{-}(q))}.$$
(7.187)

For this excitation we may determine the shift function at the quasi-Fermi points,

 $F_{-}(\pm q)$ , using Eq. (7.85):

$$F_{-}(\pm q) = F_{m}(\pm q | \text{Umklapp}) - F(\pm q | q).$$
(7.188)

We can substitute  $F_m(\pm q | \text{Umklapp}) = -m(\sqrt{K}-1)$ , from Eq. (7.177) and Eq. (7.179), and substitue  $F(\pm q | q) + \pi \rho(\pm q) = 1/2 \pm (1/2 - 1/(2\sqrt{K}))$  from Ref. [224], to determine the exponent of L in the Umklapp annihilation form factor,

$$-\frac{1}{2}(F_{-}^{2}(q) + F_{-}^{2}(-q) - 2(m-1)F_{-}(q) - 2mF_{-}(-q) + 2m^{2} - 2m + 1) = -m^{2}K - \frac{1}{4K}.$$
(7.189)

where, K is the Luttinger parameter [208].

We may then use Eq. (7.10) to relate the absolute square of the annihilation operator form factor  $\mathcal{G}^-$  for the Umklapp state to determine the coefficients  $B_m$  of the Green's function of the Bose gas in Eq. (7.2) to obtain

$$B_{m>0} = q \frac{(q^2 K)^{-m^2 K - 1/4K}}{2^{2m^2 - 2m - 1}} (2\pi)^{-2 + 1/\sqrt{K}} \left(\frac{4q^2 + c^2}{c^2}\right)^{(m-1)^2} \frac{\text{Det}^2(1 + \hat{H}^-)}{\text{Det}^2\left(1 - \frac{\hat{K}}{2\pi}\right)} \\ \times \left(\frac{G(m - F_-(q))G(m + 1 - F_-(-q)))G(1 + F_-(-q))}{\Gamma(F_-(-q))^{m-1}\Gamma(1 - F_-(-q))}\right)^2 \\ \exp\left[4(m - 1)q \int_{-q}^{q} d\lambda \frac{F_-(\lambda)}{((\lambda + ic)^2 - q^2)} - \int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F_-(\lambda)F_-(\mu)}{(\lambda - \mu + ic)^2}\right] \\ \exp\left[2P_{\pm} \int_{-1}^{1} dx \frac{F_-^2(qx) - 2(m - 1/2)F_-(qx) + xF_-(qx)}{x^2 - 1} - \frac{1}{2} \int_{-q}^{q} \int_{-q}^{q} d\lambda d\mu \left(\frac{F_-(\lambda) - F_-(\mu)}{\lambda - \mu}\right)^2\right].$$
(7.190)

Note that we have used the relation in Eq. (7.179) to express the answer in terms of the Luttinger parameter, K [208].

To determine the prefactors of the singularities of the spectral function  $A(k, \omega)$ near Lieb's colective modes  $\pm \epsilon_{1,2}(k)$  [242, 203] we need to find corresponding form factors of the creation/annihilation operators from Eqs. (7.185), (7.186).

We obtain  $A_+(k)$  from the creation operator form factor for a Bose gas with a high energy particle, and obtain  $\overline{A_-(k)}$  from the annihilation operator form factor for a Bose gas with one high energy hole. These functions give the prefactors for the spectral function singularities at  $\epsilon_1(k)$  and  $-\epsilon_2(k)$  respectively. We must first relate the quasi momentum of the particle to the momentum k of the excited bosonic state as follows [203, 224]:

$$k = \mu^+ - \pi \rho_0 - \int_{-q}^{q} d\lambda \theta(\mu^+ - \lambda) \rho(\lambda), \qquad (7.191)$$

and for the quasi momentum of the hole

$$-k = \mu^{-} - \pi \rho_{0} - \int_{-q}^{q} d\lambda \theta (\mu^{-} - \lambda) \rho(\lambda), \qquad (7.192)$$

where  $\theta(\lambda) = i \ln(\frac{ic+\lambda}{ic-\lambda})$ , and q is the quasimomentum at the edge of the distribution.

Particle-hole pairs in Eqs. (7.84),(7.85) are defined with respect to ground states of  $N \pm 1$  particles, so to obtain a state with a single high energy particle (hole), a particle-hole pair needs to contain a hole (particle) at q. Such a procedure results in the following expressions for shift functions  $\overline{F_{\pm}(\lambda)}$ 

$$\overline{F_{+}(\lambda)} = F(\lambda|\mu^{+}) + \pi\rho(\lambda),$$
  
$$\overline{F_{-}(\lambda)} = -F(\lambda|\mu^{-}) - \pi\rho(\lambda).$$
 (7.193)

We may then substitute these functions in the relevant places in Eq. (7.186) and Eq. (7.185), combine terms from  $T_{hole}$  given by Eq. (7.135), and  $T_{particle}$  given by Eq. (7.136), to obtain

$$\overline{A_{\pm}(k)} = \frac{1}{\rho(\mu^{-})} \left( q\sqrt{K} \right)^{-(\overline{F_{\pm}^{2}(q)} + \overline{F_{\pm}^{2}(-q)})} (2\pi)^{\overline{F_{\pm}(q)} - \overline{F_{\pm}(-q)} - 1} (G(1 + \overline{F_{\pm}(-q)})G(1 - \overline{F_{\pm}(q)}))^{2} \\
\exp\left\{ P_{\pm} \int_{-1}^{1} dx \frac{2\overline{F_{\pm}^{2}(qx)}}{x^{2} - 1} \mp (P) \int_{-1}^{1} dx \frac{2\overline{F_{\pm}(qx)}}{x - \mu^{\pm}/q} - \frac{1}{2} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left( \frac{\overline{F_{\pm}(\lambda)} - \overline{F_{\pm}(\mu)}}{\lambda - \mu} \right)^{2} \right\} \\
\exp\left[ - \int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{\overline{F_{\pm}(\lambda)} \overline{F_{\pm}(\mu)}}{(\lambda - \mu + ic)^{2}} \right] \times \frac{\operatorname{Det}^{2}(1 + \hat{H}^{-})}{\operatorname{Det}^{2}\left(1 - \frac{\hat{K}}{2\pi}\right)} \frac{((q - \mu^{\pm})^{2} + c^{2})}{c^{2}} \\
\exp\left[ \pm 2 \int_{-q}^{q} d\lambda \frac{\overline{F_{\pm}(\lambda)}(\mu^{\pm} - q)}{(\lambda - \mu^{\pm} + ic)(\lambda - q + ic)} \right].$$
(7.194)

Note that the momentum dependence in the above expressions is contained in the shift function,  $\overline{F_{\pm}(\lambda)}$  defined above, as well as the terms directly involving  $\mu^{\pm}$ . Furthermore we have used the relation in Eq. (7.179) to express the answer in terms of the Luttinger parameter, K [208].

We obtain the prefactors of the spectral function singularities,  $\underline{A_{+}(k)}$  and  $\underline{A_{-}(k)}$ , near the Lieb modes  $\epsilon_2(k)$  and  $-\epsilon_1(k)$  from the form factors of the creation and annihilation operator respectively. We can obtain the prefactor  $\underline{A_{+}(k)}$  from the creation operator form factor of a system with a high momentum hole and two particles at the right quasi-Fermi point. From the annihilation operator form factor of a system with a high momentum particle and two holes at the right quasi-Fermi point, we obtain the prefactor  $\underline{A_{-}(k)}$ . We again relate the quasimomenta of the particle and hole to the momentum k using, Eq. (7.191) and Eq. (7.192) and determine  $F_{\pm}(\lambda)$  using Eqs. (7.84), (7.85).

Particle-hole pairs in Eqs. (7.84),(7.85) are defined with respect to ground states of  $N \pm 1$  particles, so to obtain a state with a single high energy particle (hole), a particle-hole pair needs to contain a hole (particle) at q. Such a procedure results in the following expressions for shift functions  $\underline{F}_{\pm}(\lambda)$ :

$$\frac{F_{+}(\lambda)}{F_{-}(\lambda)} = 2F(\lambda|q) - F(\lambda|\mu^{-}) + \pi\rho(\lambda),$$

$$\frac{F_{-}(\lambda)}{F_{-}(\lambda)} = F(\lambda|\mu^{+}) - 2F(\lambda|q) - \pi\rho(\lambda).$$
(7.195)

Substituting these results in Eq. (7.186) and Eq. (7.185) in conjunction with the expression for  $T_{particle}$  given by Eq. (7.138), and  $T_{hole}$  given by Eq. (7.133) we get the following expressions:

$$\underline{A_{+}(k)} = \frac{1}{\rho(\mu^{-})(\mu^{-}/q-1)^{4}} \left(q\sqrt{K}\right)^{-\left(\frac{F_{+}^{2}(q)}{F_{+}^{2}(q)} + \frac{F_{+}^{2}(-q)}{F_{+}^{2}(q)} + 4\right)} (2\pi) \frac{F_{+}(q)}{F_{+}(q)} - \frac{F_{+}(-q)}{F_{+}(-q)} - 2\frac{((q-\mu^{-})^{2}+c^{2})}{c^{2}} \\
\times \left(\frac{G(1+F_{+}(-q))G(1-F_{+}(q))\Gamma(1-F_{+}(q))\Gamma(2-F_{+}(q))}{\Gamma(1-F_{+}(\mu^{-}))}\right)^{2} \times \frac{\text{Det}^{2}(1+\hat{H}^{+})}{\text{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)} \\
\exp\left\{P_{\pm}\int_{-1}^{1} dx \frac{2F_{+}^{2}(qx)}{x^{2}-1} - P_{+}\int_{-1}^{1} dx \frac{4F_{+}(qx)}{x-1} + 2\int_{-q}^{q} d\lambda \frac{F_{+}(\lambda)(q-\mu^{-})}{(\lambda-\mu^{-}+ic)(\lambda-q+ic)}\right\} \\
\exp\left[P\int_{-1}^{1} d\lambda \frac{2F_{+}(qx)}{x-\mu^{-}/q} - \frac{1}{2}\int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F_{+}(\lambda)-F_{+}(\mu)}{\lambda-\mu}\right)^{2}\right] \\
\exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F_{+}(\lambda)}{(\lambda-\mu+ic)^{2}}\right].$$
(7.196)

$$\underline{A_{-}(k)} = \frac{1}{\rho(\mu^{+})(\mu^{+}/q-1)^{4}} \left(q\sqrt{K}\right)^{-(\underline{F_{-}^{2}(q)} + \underline{F_{-}^{2}(-q)} + 4\underline{F_{-}(q)} + 4)} (2\pi)^{\underline{F_{-}(q)} - \underline{F_{-}(-q)} - 2} \\
\frac{\text{Det}^{2}(1+\hat{H}^{-})}{\text{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)} \frac{((q-\mu^{+})^{2} + c^{2})}{c^{2}} \left(\frac{G(1+\underline{F_{-}(-q)})G(1-\underline{F_{-}(q)})\Gamma(1+\underline{F_{-}(q)})\Gamma(2+\underline{F_{-}(q)})}{\Gamma(\underline{F_{-}(q)})\Gamma(1-\underline{F_{-}(q)})}\right)^{2} \\
\exp\left\{P_{\pm}\int_{-1}^{1} dx \frac{2\underline{F_{-}^{2}(qx)}}{x^{2}-1} + P_{+}\int_{-1}^{1} dx \frac{4\underline{F_{-}(qx)}}{x-1} - \frac{1}{2}\int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{\underline{F_{-}(\lambda)}-\underline{F_{-}(\mu)}}{\lambda-\mu}\right)^{2}\right\} \\
\exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{\underline{F_{-}(\lambda)}}{(\lambda-\mu+ic)^{2}} - \int_{-q}^{q} d\lambda \frac{2\underline{F_{-}(\lambda)}}{\lambda-\mu+ic}\right] \\
\exp\left[2\int_{-q}^{q} d\lambda \frac{\underline{F_{-}(\lambda)}(\mu^{+}-q)}{(\lambda-\mu+ic)(\lambda-\mu^{+}+ic)}\right].$$
(7.197)

Here too the dependence on momentum, k, is carried by  $\underline{F_{\pm}(\lambda)}$  defined above and  $\mu^{\pm}$ . Furthermore we have used the relation in Eq. (7.179) to express the answer in terms of the Luttinger parameter, K [208].

#### 7.5.7 Numerical Results

Let us plot here some prefactors which are obtained using above analytical results.

A few prefactors of equal time correlators  $A_m, B_m$ , see Eqs. (7.1) and (7.2) are plotted in Fig. 7.4

 $S_1(k)$ (blue),  $S_2(k)$  (orange, dashed) are plotted in Fig. 7.5 for  $\gamma = 4.52, \rho_0 = 1, K = 1.81$  as functions of  $k/k_F$ . We can analyze the limiting behavior as  $k \to 0$  of these prefactors using their forms

$$S(k,\omega) = \frac{\sin \pi \tilde{\mu}_L \theta(\delta\omega) + \sin \pi \tilde{\mu}_R \theta(-\delta\omega)}{\sin \pi (\tilde{\mu}_L + \tilde{\mu}_R)} \frac{2\pi S_1(k) \delta \omega^{\tilde{\mu}_R + \tilde{\mu}_L - 1}}{\Gamma(\tilde{\mu}_R + \tilde{\mu}_L)(v + v_d)^{\tilde{\mu}_L} |v - v_d|^{\tilde{\mu}_R}},$$
$$|\delta\omega| = |\omega - \varepsilon_1(k)| \ll \varepsilon_1(k),$$
$$S(k,\omega) = \theta(\delta\omega) \frac{2\pi S_2(k) \delta \omega^{\tilde{\mu}_R + \tilde{\mu}_L - 1}}{\Gamma(\tilde{\mu}_R + \tilde{\mu}_L)(v + v_d)^{\tilde{\mu}_L} |v - v_d|^{\tilde{\mu}_R}}, \quad \delta\omega = \omega - \varepsilon_2(k) \ll \varepsilon_2(k),$$

and the universal relation for  $S(k, \omega)$  given in Ref. [231],

$$S(k,\omega) = \frac{m_*K}{k}\theta(\frac{k^2}{2m_*} - |\omega - v|k||).$$
(7.198)

The exponents  $\tilde{\mu}_{R(L)} = (F(\pm q|\lambda) + \sqrt{K}/2 + 1/2\sqrt{K})$  and  $m_*$  is the effective mass. In the limit that  $k \to 0$  we have  $\mu_R \to 1, \mu_L \to 0$ . Then from the above relations we obtain

$$\lim_{k \to 0} S_2(k) = S_1(k) = \frac{K}{2\pi}.$$
(7.199)

This asymptote is indicated by the red dotted line.

Numerical results for  $\overline{A^{\pm}(k)}$ ,  $\underline{A^{\pm}(k)}$  as functions of k are obtained from Eqs. (7.194), (7.196) and (7.197), and are plotted in Fig. 7.6 for K = 1.81.

#### 7.6 Conclusions and Summary of Results

We used a general method for obtaining non-universal prefactors of correlation functions by combining field theoretical considerations with form factors of exactly solvable models. The technique relies on the existence of a well defined relationship

Figure 7.4 : (Color online) Results for the Lieb-Liniger model of 1D bosons:  $2\pi^2 A_1$  (dashed black),  $512\pi^{10}A_2$  (solid green) and  $B_0$  (dot-dashed blue),  $-8\pi^2 B_1$  (dotted red) as functions of the Luttinger liquid parameter K. In the limit of strong interaction  $(K \to 1)$  our expressions for  $B_0$  and  $B_1$  agree with the known values [210], while  $A_1 \to 1/2\pi^2, A_2 \to 0$  are in accordance with the density correlator of the free Fermi gas. We also match  $B_0$  in the weakly interacting regime  $(K \gg 1)$  to Popov's result (dashed line) [209], and show some numerical results (crosses) [213].

Figure 7.5 : Plot of  $2\pi S_1$  (blue),  $2\pi S_2$  (orange, dashed) as functions of  $k/k_F$  for K = 1.81. As  $k/k_F \to 0$  they approach K indicated by a dashed red line.

Figure 7.6 : Log-log plot of  $\overline{A^+(k)}$  (black, dashed),  $\overline{A^-(k)}$  (orange),  $\underline{A^+(k)}$  (blue, dashed) and  $A^-(k)$  (red) as functions of  $k/k_F$  for K = 1.81.

between lowest energy form factors of operators and the associated prefactors of their correlation functions, see e.g. Eqs. (7.10)-(??). For example, in the case of equal time correlators, such a relationship can be demonstrated by an effective field theoretical description of the system as a Luttinger liquid, when finite system size is properly accounted for. In fact such relations were already known in a few cases [268]. Moreover using the effective three subband model of a mobile impurity moving in a Luttinger liquid, we also obtained expressions for prefactors of dynamic response functions, see Eqs. (7.21), (7.24) and (7.27). To the best of our knowledge, these latter results are new. In addition to providing various non-universal prefactors for dynamic response function, calculations presented in this paper constitute a stringent microscopic check of the phenomenological impurity Hamiltonians [238], which have been previously justified only in the perturbative regime.

The universality of the field theoretical description of interacting one-dimensional quantum systems of bosons, fermions and spins, allows us to apply the relationship between the correlation prefactors and form factors to a wide variety of systems. It should be emphasized that the method is quite general, requiring only calculable form factors; it does not rely on the integrability of the system considered. With regards to prefactors of singularities in response functions, we note that as long as there exist kinematic thresholds in the system considered, these will manifest as singularities in dynamic response functions whose prefactors can be extracted using the methods we applied here.

Here we focused on two integrable models: the Calogero-Sutherland, and Lieb-Liniger models. We exploited the connection between prefactors and form factors in the case of the aforementioned systems, where explicit expressions for finite-size form factors were already available. We demonstrated how to properly take the thermodynamic limit of such form factors, which contain non-trivial power laws in system size, to obtain numerically tractable analytic expressions for non-universal prefactors of their correlation functions.

We note here that a few of the prefactors we obtained do not represent new results. It was our aim to demonstrate a more direct way to obtain them, with a wider range of applicability, e.g. we obtained the prefactor of the first oscillatory component of the equal-time density-density correlator for the Calogero-Sutherland model without employing the replica method or multiple integrals [215].

We obtained prefactors for dynamic response functions of the Bose gas in the vicinity of threshold singularities which are fundamentally new results. Calculations of the prefactors of singularities in dynamic response functions so far assumed that the field theory of mobile impurities provides an adequate description. The microscopic approach presented here allows one to also explicitly prove the existence of singularities without this assumption. If we consider the total spectral weight in a small interval of energy  $\delta \omega$  in the vicinity of  $\varepsilon_{1(2)}(k)$ , we need to sum over states with

low energy particle-hole excitations. We may use Eq. (7.14), proven in Ref. [218] and the expansion  $C(n_{r(l)}, \mu_{R(L)}) \approx n_{r(l)}^{\mu_{R(L)}-1} / \Gamma(\mu_{R(L)})$  for  $n_{r(l)} \gg 1$  to show that he total spectral weight scales with  $\delta \omega$  as

$$\propto \sum_{|E-\varepsilon_{1(2)}|<\delta\omega/2} \frac{|C(n_r,\mu_R)C(n_l,\mu_L)|}{L^{\mu_R+\mu_L+1}} \propto |\delta\omega|^{1-\mu_R-\mu_L},$$

which proves the existence of the singularity.

Our results represent a significant step towards an analytical calculation of the full correlators.

In the following subsections, we provide a self-contained summary of the results obtained in this paper.

#### 7.6.1 Prefactors of equal-time correlators

The equal time correlators of 1D quantum liquids can be expressed as an asymptotic series with unknown prefactors, see Eqs. (7.1) - (7.3), (??) and (??). From the analysis of the finite size scaling of the field theoretical description of 1D quantum liquids one obtains a correspondence between the prefactors and form factors of the density, creation, annihilation and spin operators, see Eqs. (7.10) - (??). We present below the prefactors of the equal time density and field correlators of the bosonic Lieb-Liniger model followed by prefactors of the spin-spin correlators of the XXZ model.

For the first prefactor  $A_1$  of the oscillatory terms in the density-density correlator (see Eq. (7.1)) of the Calogero-Sutherland model we obtained

$$A_1 = 2 \frac{\Gamma \left(1 + \frac{1}{\lambda}\right)^2}{(2\pi)^{2/\lambda}},\tag{7.200}$$

in agreement with the results of Ref. [215] which were obtained using the replica method.

For the prefactors of the oscillatory terms in the density-density correlator (see Eq. (7.1)) of the Lieb-Liniger model we have from we have from Eq. (7.12),(7.167) and (7.180)

$$A_{m} = 2\gamma^{2} \left(\frac{q\sqrt{K}}{\rho_{0}}\right)^{-2m^{2}K} \left(\frac{4q^{2}+c^{2}}{4c^{2}}\right)^{m^{2}} \left(\frac{G(1+m\sqrt{K})^{2}G(m+1-m\sqrt{K})}{\Gamma(m-m\sqrt{K})^{m}\Gamma(1-m+m\sqrt{K})^{m}G(1-m+m\sqrt{K})}\right)^{2} \exp\left[4mq \int_{-q}^{q} d\lambda \frac{F(\lambda)}{((\lambda+ic)^{2}-q^{2})} - \int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}}\right] \exp\left[2P_{\pm} \int_{-1}^{1} dx \frac{F^{2}(qx)-2mF(qx)}{x^{2}-1} - \frac{1}{2} \int_{-q}^{q} \int_{-q}^{q} d\lambda d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right] \frac{\text{Det}^{2}(1+\hat{Q}_{\pi})}{\text{Det}^{2}\left(1-\frac{K}{2\pi}\right)} \cdot 201)$$

with  $F(\lambda) = m(1 - 2\pi\rho(\lambda))$ , where the quasiparticle distribution function  $\rho(\lambda)$  is given by Eq. (7.55), q is the edge of the quasimomentum distribution and satisfies  $2\pi\rho(q) = K$ , the Luttinger parameter.  $\rho_0$  is the density and c is the strength of the interaction between the bosons, with the associated dimensionless parameter  $\gamma = c/\rho_0$ . G(x) is the Barnes G function defined in Appendix A, and the symbol  $P_{\pm}$ defined in Appendix B is an instruction to evaluate the integral in the principal value sense where the singularity occurs at the edge of the range of integration.  $\hat{G}$  is obtained from Sec. 4.5, Eq. (7.160) while  $K(\lambda) = \frac{2c}{c^2 + \lambda^2}$ . The two determinants are meant to be evaluated as Fredholm determinants, see Appendix D and Ref. [279].

For the prefactors of the oscillatory terms in the Green's function (see Eq. (7.2)) of the Lieb-Liniger model we have from Eq. (7.10), (7.185) and (7.190)

$$B_{0} = q(q\sqrt{K})^{-1/2K}(2\pi)^{-4+2/\sqrt{K}}G(1+F_{-}(-q))^{2}G(1-F_{-}(q))^{2}\Gamma(1+F_{-}(q))^{2}$$

$$\times \exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F_{-}(\lambda)F_{-}(\mu)}{(\lambda-\mu+ic)^{2}} + 2P_{\pm} \int_{-1}^{1} dx \left(\frac{F_{-}^{2}(qx)}{x^{2}-1} + \frac{F_{-}(qx)}{x-1}\right)\right]\right]$$

$$\times \exp\left[-\frac{1}{2} \int_{-q}^{q} \int_{-q}^{q} d\lambda d\mu \left(\frac{F_{-}(\lambda)-F_{-}(\mu)}{\lambda-\mu}\right)^{2}\right] \frac{\text{Det}^{2}(1+\hat{H}^{-})}{\text{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)},$$

$$B_{m>0} = q \frac{(q\sqrt{K})^{-2m^{2}K-1/2K}}{2^{2m^{2}-2m-1}} (2\pi)^{-4+2/\sqrt{K}} \left(\frac{4q^{2}+c^{2}}{c^{2}}\right)^{(m-1)^{2}} \frac{\text{Det}^{2}(1+\hat{H}^{-})}{\text{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)},$$

$$\times \left(\frac{G(m-F_{-}(q))G(m+1-F_{-}(-q)))G(1+F_{-}(-q))}{\Gamma(F_{-}(-q))^{m-1}\Gamma(1-F_{-}(-q))m^{-1}G(1-F_{-}(-q))}\right)^{2}$$

$$\times \exp\left[4(m-1)q \int_{-q}^{q} d\lambda \frac{F_{-}(\lambda)}{((\lambda+ic)^{2}-q^{2})} - \int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F_{-}(\lambda)F_{-}(\mu)}{(\lambda-\mu+ic)^{2}}\right]$$

$$\times \exp\left[2P_{\pm} \int_{-1}^{1} dx \frac{F_{-}^{2}(qx) - 2(m-1/2)F_{-}(qx) + xF_{-}(qx)}{x^{2}-1} - \frac{1}{2} \int_{-q}^{q} \int_{-q}^{q} d\lambda d\mu \left(\frac{F_{-}(\lambda)-F_{-}(\mu)}{\lambda-\mu}\right)^{2}\right].$$
(7.202)

where  $F_{-}(\lambda) = F_{m}(\lambda | \text{Umklapp}) - F(\lambda | q) - \pi \rho(\lambda)$  is the modified shift function defined in Eq. (7.85), K is the Luttinger parameter, q the edge of the distribution of ground state quasimomenta,  $\rho_{0}$  is the density and c is the strength of the interaction between the bosons, with the associated dimensionless parameter  $\gamma = c/\rho_{0}$ . G(x)is the Barnes G function defined in Appendix A, and the symbol  $P_{\pm}$  defined in Appendix B is an instruction to evaluate the integral in the principal value sense where the singularity occurs at the edge of the range of integration.  $\hat{H}^{-}$  is obtained from Sec. 4.5, Eq. (7.166), while  $K(\lambda) = \frac{2c}{c^{2}+\lambda^{2}}$ . The two determinants are meant to be evaluated as Fredholm determinants, see Appendix D and Ref. [279].

By applying the techniques described in Sec. 2 above to the prefactors of singularities in dynamic response functions like the spectral function and dynamic structure factor, we obtained a correspondence between form factors of the creation and annihilation operators and the prefactors of the response functions. We present results for the prefactors of the dynamic response functions of the Lieb-Liniger model below.

#### 7.6.2 Prefactors of the singularities of the dynamic structure factor

The dynamic structure factor  $S(k, \omega)$  defined in Eq. (7.15) shows singular behavior for  $\omega \approx |\varepsilon(k) = \lambda(k^2 - k_F^2)|$ , with prefactor  $S_{\text{CSM}}(k)$  when  $0 < k < 2k_F$ . The prefactor is given by

$$S_{\rm CSM}(k) = \frac{2\pi}{\lambda} \Gamma\left(1 + \frac{1}{\lambda}\right) \left(\frac{2k_F k}{2k_F - k}\right)^{1 - \frac{1}{\lambda}}.$$
 (7.203)

In the case of the Lieb-Liniger model, the dynamic structure factor  $S(k, \omega)$  also shows singular behavior for  $\omega \approx \varepsilon_{1(2)}(k)$ , i.e. near Lieb's modes [224, 242], and the behavior there is described by Eqs. (7.19) and (7.20). For the prefactors  $S_1(k)$  and  $S_2(k)$  in those equations we obtain from Eqs. (7.21) and (7.167)

$$S_{1}(k) = c^{2}\sqrt{K} \left(q\sqrt{K}\right)^{-(F^{2}(q)+F^{2}(-q)-2F(q)+2)} (2\pi)^{F(q)-F(-q)} \left(\frac{G(1+F(-q))G(1-F(q))}{\Gamma(1-F(q))}\right)^{2} \\ \times \exp\left\{P_{\pm} \int_{-1}^{1} dx \frac{2F^{2}(qx)}{x^{2}-1} + P_{+} \int_{-1}^{1} dx \frac{2F(qx)}{x-1} - \frac{1}{2} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right\} \\ \times \exp\left[\int_{-q}^{q} d\lambda \frac{2F(\lambda)(\mu^{+}-q)}{(\lambda-q+ic)(\lambda-\mu^{+}+ic)}\right] \frac{(q-\mu^{+})^{2}+c^{2}}{c^{2}} \left(\frac{F^{2}(q)}{\rho(\mu^{+})(\mu^{+}/q-1)^{2}}\right) \\ \times \exp\left[-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}} - \int_{-q}^{q} d\lambda \frac{2F(\lambda)}{\lambda-\mu^{+}}\right] \frac{\operatorname{Det}^{2}(1+\hat{G})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.204)

Note that the momentum dependence in the above expression is contained in the shift function  $F(\lambda) = F(\lambda|\mu^+) - F(\lambda|q)$ , defined in Eq. (7.56) as well as the terms directly involving  $\mu^+$ , the quasimomentum corresponding to particle excitation (see Eq. (7.44)). We may relate the physical momentum k to the quasimomentum  $\mu^+$ 

using [203, 224]:

$$k = \mu^+ - \pi \rho_0 - \int_{-q}^{q} d\lambda \theta(\mu^+ - \lambda) \rho(\lambda), \qquad (7.205)$$

where,  $\theta(\lambda) = i \log \left(\frac{ic+\lambda}{ic-\lambda}\right)$ , and q is the quasimomentum at the edge of the distribution;  $\rho_0$  is the density and c is the strength of the interaction between the bosons, with the associated dimensionless parameter  $\gamma = c/\rho_0$ . G(x) is the Barnes G function defined in Appendix A, and the symbol  $P_{\pm}$  defined in Appendix B is an instruction to evaluate the integral in the principal value sense where the singularity occurs at the edge of the range of integration.  $\hat{G}$  is obtained from Sec. 4.5, Eq. (7.160), while  $K(\lambda) = \frac{2c}{c^2+\lambda^2}$ . The two determinants are meant to be evaluated as Fredholm determinants, see Appendix D and Ref. [279].

Similarly, we get the following expression for  $S_2(k)$ :

$$S_{2}(k) = c^{2}\sqrt{K} \left(q\sqrt{K}\right)^{-(F^{2}(q)+F^{2}(-q)+2F(q)+2)} (2\pi)^{F(q)-F(-q)} \\ \left(\frac{G(1+F(-q))G(1-F(q))\Gamma(1-F(q))}{\Gamma(1+F(\mu^{-}))\Gamma(1-F(\mu^{-}))}\right)^{2} \\ \times \exp\left[\int_{-q}^{q} d\lambda \frac{2F(\lambda)(q-\mu^{-})}{(\lambda-\mu^{-}+ic)(\lambda-q+ic)}\right] \frac{(q-\mu^{-})^{2}+c^{2}}{c^{2}} \left(\frac{F^{2}(\mu^{-})}{\rho(\mu^{-})(\mu^{-}/q-1)^{2}}\right) \\ \times \exp\left\{-\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{F(\lambda)F(\mu)}{(\lambda-\mu+ic)^{2}} + P_{\pm} \int_{-1}^{1} dx \frac{2F^{2}(qx)}{x^{2}-1} - P_{+} \int_{-1}^{1} dx \frac{2F(qx)}{x-1}\right\} \\ \times \exp\left[P \int_{-1}^{1} dx \frac{2F(qx)}{x-\mu^{-}/q} - \frac{1}{2} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left(\frac{F(\lambda)-F(\mu)}{\lambda-\mu}\right)^{2}\right] \times \frac{\operatorname{Det}^{2}(1-\hat{K})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)}.$$
(7.206)

Here too the dependence on momentum k is carried by  $F(\lambda) = F(\lambda|q) - F(\lambda|\mu^{-})$ and  $\mu^{-}$ , the quasimomentum of the hole excitation (see Eq. (7.44)). This time we relate the quasi momentum of the hole,  $\mu^{-}$ , to the physical momentum, k using

$$-k = \mu^{-} - \pi \rho_{0} - \int_{-q}^{q} d\lambda \theta (\mu^{-} - \lambda) \rho(\lambda).$$
 (7.207)

#### 7.6.3 Prefactors of the singularities of the spectral function

The spectral function  $A(k, \omega)$  defined in Eq. (7.16) also displays singular behavior in the vicinity of Lieb's collective modes [242]. This behavior is described by Eqs. (7.22), (7.25) and the text in that section. There are four associated prefactors defined in Eqs.(7.22) and (7.25) for which we obtain analytic expression below.

 $\overline{A_{\pm}(k)}$ 

We obtain  $\overline{A_+(k)}$  from the creation operator form factor for a Bose gas with a high energy particle, and obtain  $\overline{A_-(k)}$  from the annihilation operator form factor for a Bose gas with one high energy hole. These functions give the prefactors for the spectral function singularities at  $\epsilon_1(k)$  and  $-\epsilon_2(k)$  respectively. We must first relate the quasi momentum of the particle to the momentum k of the excited bosonic state as follows [203, 224]:

$$k = \mu^+ - \pi \rho_0 - \int_{-q}^{q} d\lambda \theta(\mu^+ - \lambda) \rho(\lambda), \qquad (7.208)$$

and for the quasi momentum of the hole

$$-k = \mu^{-} - \pi \rho_0 - \int_{-q}^{q} d\lambda \theta (\mu^{-} - \lambda) \rho(\lambda), \qquad (7.209)$$

where  $\theta(\lambda) = i \log \left(\frac{ic+\lambda}{ic-\lambda}\right)$ , and q is the quasimomentum at the edge of the distribution.

Particle-hole pairs in Eqs. (7.84) and (7.85) are defined with respect to ground states of  $N \pm 1$  particles, so to obtain a state with a single high energy particle (hole), a particle-hole pair needs to contain a hole (particle) at q. Such a procedure results in the following expressions for shift functions  $\overline{F_{\pm}(\lambda)}$ 

$$\overline{F_{+}(\lambda)} = F(\lambda|\mu^{+}) + \pi\rho(\lambda),$$
  
$$\overline{F_{-}(\lambda)} = -F(\lambda|\mu^{-}) - \pi\rho(\lambda).$$
(7.210)

From Eq. (7.24), (7.185) and (7.186) we have

$$\overline{A_{\pm}(k)} = \frac{1}{\rho(\mu^{-})} \left( q\sqrt{K} \right)^{-(\overline{F_{\pm}^{2}(q)} + \overline{F_{\pm}^{2}(-q)})} (2\pi)^{\overline{F_{\pm}(q)} - \overline{F_{\pm}(-q)} - 2} (G(1 + \overline{F_{\pm}(-q)})G(1 - \overline{F_{\pm}(q)}))^{2}$$

$$\times \exp\left\{ P_{\pm} \int_{-1}^{1} dx \frac{2\overline{F_{\pm}^{2}(qx)}}{x^{2} - 1} \mp (P) \int_{-1}^{1} dx \frac{2\overline{F_{\pm}(qx)}}{x - \mu^{\pm}/q} \right\}$$

$$\times \exp\left[ -\int_{-q}^{q} d\mu \int_{-q}^{q} d\lambda \frac{\overline{F_{\pm}(\lambda)}}{(\lambda - \mu + ic)^{2}} \right] \times \frac{\operatorname{Det}^{2}(1 + \hat{H}^{-})}{\operatorname{Det}^{2}\left(1 - \frac{\hat{K}}{2\pi}\right)} \frac{((q - \mu^{\pm})^{2} + c^{2})}{c^{2}}$$

$$\times \exp\left[ \pm 2 \int_{-q}^{q} d\lambda \frac{\overline{F_{\pm}(\lambda)}(\mu^{\pm} - q)}{(\lambda - \mu^{\pm} + ic)(\lambda - q + ic)} \right]$$

$$\times \exp\left[ -\frac{1}{2} \int_{-q}^{q} d\lambda \int_{-q}^{q} d\mu \left( \frac{\overline{F_{\pm}(\lambda)} - \overline{F_{\pm}(\mu)}}{\lambda - \mu} \right)^{2} \right]. \quad (7.211)$$

 $A_{\pm}(k)$ 

Similarly, we obtain the prefactors of the spectral function singularities,  $\underline{A_{+}(k)}$  and  $\underline{A_{-}(k)}$ , near the Lieb modes  $\epsilon_2(k)$  and  $-\epsilon_1(k)$  from the form factors of the creation and annihilation operator respectively. We can obtain the prefactor  $\underline{A_{+}(k)}$  from the creation operator form factor of a system with a high momentum hole and two particles at the right quasi-Fermi point. From the annihilation operator form factor of a system with a high momentum particle and two holes at the right quasi-Fermi point, we obtain the prefactor  $\underline{A_{-}(k)}$ . We again relate the quasimomenta of the particle and hole to the momentum k using, Eqs. (7.191) and (7.192) and determine  $F_{\pm}(\lambda)$  using Eqs. (7.84) and (7.85).

Particle-hole pairs in Eqs. (7.84) and (7.85) are defined with respect to ground states of  $N \pm 1$  particles, so to obtain a state with a single high energy particle (hole), a particle-hole pair needs to contain a hole (particle) at q. Such a procedure results in the following expressions for shift functions  $\underline{F_{\pm}(\lambda)}$ :

$$\underline{F_{+}(\lambda)} = 2F(\lambda|q) - F(\lambda|\mu^{-}) + \pi\rho(\lambda),$$

$$\underline{F_{-}(\lambda)} = F(\lambda|\mu^{+}) - 2F(\lambda|q) - \pi\rho(\lambda).$$
(7.212)

Then using Eqs. (7.27), (7.185) and (7.186) we get the following expressions:

$$\frac{A_{+}(k)}{\rho(\mu^{-})(\mu^{-}/q-1)^{4}} \left(q\sqrt{K}\right)^{-\left(\frac{F_{+}^{2}(q)}{P_{+}^{2}(-q)}-4F_{+}(q)+4\right)} (2\pi)\frac{F_{+}(q)-F_{+}(-q)-2}{(2\pi)^{2}} \\
\times \left(\frac{G(1+F_{+}(-q))G(1-F_{+}(q))\Gamma(1-F_{+}(q))\Gamma(2-F_{+}(q))}{\Gamma(1-F_{+}(\mu^{-}))}\right)^{2} \frac{((q-\mu^{-})^{2}+c^{2})}{c^{2}} \\
\times \exp\left\{P_{\pm}\int_{-1}^{1} dx\frac{2F_{+}^{2}(qx)}{x^{2}-1} - P_{+}\int_{-1}^{1} dx\frac{4F_{+}(qx)}{x-1}\right\} \\
\times \exp\left[P\int_{-1}^{1} d\lambda\frac{2F_{+}(qx)}{x-\mu^{-}/q} - \frac{1}{2}\int_{-q}^{q} d\lambda\int_{-q}^{q} d\mu\left(\frac{F_{+}(\lambda)-F_{+}(\mu)}{\lambda-\mu}\right)^{2}\right] \\
\times \exp\left[-\int_{-q}^{q} d\mu\int_{-q}^{q} d\lambda\frac{F_{+}(\lambda)}{(\lambda-\mu+ic)^{2}}\right] \times \frac{\operatorname{Det}^{2}(1+\hat{H}^{+})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)} \\
\times \exp\left[2\int_{-q}^{q} d\lambda\frac{F_{+}(\lambda)(q-\mu^{-})}{(\lambda-\mu^{-}+ic)(\lambda-q+ic)}\right].$$
(7.213)

$$\frac{A_{-}(k)}{\rho(\mu^{+})(\mu^{+}/q-1)^{4}} \left(q\sqrt{K}\right)^{-(\frac{F^{2}(q)}{2}+\frac{F^{2}(-q)}{2}+4F_{-}(q)+4)} (2\pi)\frac{F_{-}(q)-F_{-}(-q)-2}{\rho(q)-F_{-}(-q)-2} \\
\times \frac{((q-\mu^{+})^{2}+c^{2})}{c^{2}} \left(\frac{G(1+F_{-}(-q))G(1-F_{-}(q))\Gamma(1+F_{-}(q))\Gamma(2+F_{-}(q))}{\Gamma(F_{-}(q))\Gamma(1-F_{-}(q))}\right)^{2} \\
\times \exp\left\{P_{\pm}\int_{-1}^{1} dx\frac{2F^{2}(qx)}{x^{2}-1} + P_{+}\int_{-1}^{1} dx\frac{4F_{-}(qx)}{x-1}\right\} \\
\times \exp\left[-\int_{-q}^{q} d\mu\int_{-q}^{q} d\lambda\frac{F_{-}(\lambda)}{(\lambda-\mu+ic)^{2}} - \int_{-q}^{q} d\lambda\frac{2F_{-}(\lambda)}{\lambda-\mu^{+}}\right] \\
\times \exp\left[2\int_{-q}^{q} d\lambda\frac{F_{-}(\lambda)(\mu^{+}-q)}{(\lambda-q+ic)(\lambda-\mu^{+}+ic)}\right]\frac{\operatorname{Det}^{2}(1+\hat{H}^{-})}{\operatorname{Det}^{2}\left(1-\frac{\hat{K}}{2\pi}\right)} \\
\times \exp\left[-\frac{1}{2}\int_{-q}^{q} d\lambda\int_{-q}^{q} d\mu\left(\frac{F_{-}(\lambda)-F_{-}(\mu)}{\lambda-\mu}\right)^{2}\right] \tag{7.214}$$

In the expressions above, q is the quasimomentum at the edge of the distribution;  $\rho_0$  is the density and c is the strength of the interaction between the bosons, with the associated dimensionless parameter  $\gamma = c/\rho_0$ . G(x) is the Barnes G function defined in the Appendix, and the symbol  $P_{\pm}$  which is also defined in Appendix is an instruction to evaluate the integral in the principal value sense where the singularity occurs at the edge of the range of integration.  $\hat{H}^{\pm}$  is obtained from Eq. (7.166), while  $K(\lambda) = \frac{2c}{c^2 + \lambda^2}$ . The two determinants are meant to be evaluated as Fredholm determinants, see Appendix and Ref. [279].

# Chapter 8

# Quantum quench of interacting 1D Bose gas

### 8.1 Introduction

In this chapter the GGE solution of the 1D Bose gas quenched from a noninteracting initial state to an arbitrary final state will be presented, and will highlight the technical challenges in constructing such a solution: it will be seen that the interplay of contact interactions, which are zero-range in space, and the instantaneous quench, which is zero-range in time, will lead to pathological ultraviolet divergences for the natural choice of conserved charges entering the GGE. Although the divergences can be regularized, the required procedure is highly nontrivial.

The absence of thermalization of a 1D bosonic gas reported in Ref. [164] brought to light the special role of integrability. The observed lack of thermalization was attributed to the fact that the system was very close to an integrable one, the Lieb– Liniger (LL) model [242] which is the subject of the present study. The dynamics of integrable systems are highly constrained by the presence of a large number of conserved charges [188] in addition to the total particle number, momentum, and energy, thus they are not expected to thermalize. The so-called Generalized Gibbs Ensemble (GGE) was proposed [179] to capture the long-time behavior of integrable systems brought out of equilibrium. The density matrix is

$$\hat{\rho}_{\rm GGE} = \frac{e^{-\sum_m \beta_m \hat{Q}_m}}{Z_{\rm GGE}} \,, \tag{8.1}$$

where the generalized "chemical potentials"  $\{\beta_m\}$  are fixed by the expectation values

 $\langle \hat{Q}_m \rangle$  in the initial state, and  $Z_{\text{GGE}} = \text{Tr} \left[ e^{-\sum_m \beta_m \hat{Q}_m} \right]$ . The GGE proposal was tested successfully by various numerical and analytic approaches [180, 181, 182, 183].

#### 8.2 The model

The LL model describes a system of identical bosons in 1D interacting via a Diracdelta potential. The Hamiltonian is given by [242]

$$\hat{H} = -\sum_{i}^{N} \frac{'^{2}}{x_{i}^{2}} + 2c \sum_{i < j} \delta(x_{i} - x_{j}), \qquad (8.2)$$

which in the second quantized formulation takes the form

$$\hat{H} = \int_0^L \mathrm{d}x \, \left( {'}_x \hat{\psi}^{\dagger} {'}_x \hat{\psi} + c \, \hat{\psi}^{\dagger} \hat{\psi}^{\dagger} \hat{\psi} \hat{\psi} \right) \,, \tag{8.3}$$

where c > 0 in the repulsive regime we wish to study, and for brevity we set  $\hbar = 1$ and the boson mass to be equal to 1/2. The dimensionless coupling constant is given by  $\gamma = c/n$ , where n = N/L is the density of the gas. In cold atom experiments  $\gamma$ is a function of the 3D scattering length and the 1D confinement [189]. The exact spectrum and thermodynamics of the model can be obtained via Bethe Ansatz [242, 190]. The many-body eigenfunctions  $\phi(\{x_i\})$  of  $\hat{H}$  satisfy the boundary condition

$$\left(\frac{'}{x_j} - \frac{'}{x_k} - c\right) \phi(x_1, \dots, x_N) \Big|_{x_j = x_k + 0} = 0, \qquad (8.4)$$

whenever the coordinates of two particles coincide, thus the wave functions have cusps. The eigenstates on a ring can be expressed in terms of N quasimomenta  $\{\lambda_j\}$ that satisfy a set of algebraic equations, the Bethe equations. The eigenvalues of the mutually commuting *local* conserved charges can be computed as  $\langle \hat{Q}_m \rangle = \sum_j \lambda_j^m$ , in particular, the energy is simply  $E = \langle \hat{Q}_2 \rangle = \sum_j \lambda_j^2$  [190]. In the thermodynamic limit (TDL), a mixed state is captured by a continuous density of quasimomenta,  $\rho_{\rm LL}(\lambda)$ [191]. All quasimomenta are coupled to each other by the Bethe equations and thus  $\rho_{\rm LL}(\lambda)$  as well as the density of "holes" satisfies integral equations, the Thermodynamic Bethe Ansatz (TBA) equations. This approach was developed for thermal equilibrium but it can be generalized to the case of the GGE [183].

#### 8.3 Divergence of the local conserved charges

The simplest way to bring a system out of equilibrium is a sudden change of one of its parameters, a quantum quench [174]. In a cold atom setting such a quench could be achieved by a rapid change of the transverse confinement or the scattering length. We will compute the predictions of the GGE for a sudden quench of the interaction parameter c starting from the ground state of the c = 0 system, a pure non-interacting BEC (although we expect our results to be also valid for small initial interactions) and compare them with those of the grand canonical ensemble (GCE).

In order to describe the final state in terms of the distribution  $\rho_{\rm LL}(\lambda)$ , one needs to find the expectation values of the conserved charges  $\hat{Q}_m$  right after the quench, i.e. in the BEC-like ground state of free bosons. The density  $\rho_{\rm LL}(\lambda)$  is then found, in principle, by solving the problem of moments defined by  $\langle \hat{Q}_m \rangle = L \int d\lambda \rho_{\rm LL}(\lambda) \lambda^m$ . The first few  $\hat{Q}_m$  can be written in terms of the field operator as  $\hat{Q}_0 = \int dx \hat{\psi}^{\dagger} \hat{\psi}$ ,  $\int \hat{Q}_1 = -i \int dx \hat{\psi}^{\dagger'} x \hat{\psi}$ , and  $\hat{Q}_2 = \hat{H}$  is the Hamiltonian given by Eq. (8.3). Unfortunately, similar second quantized expressions do not exist for the operators  $\hat{Q}_m$  for  $m \ge 4$  [192]. More importantly, their expectation values can be shown to diverge in almost all states other than the eigenstates of  $\hat{H}$ . The reason is that their first quantized expressions contain products of Dirac deltas and higher derivatives [192, 193], and are only meaningful when evaluated on a wave function satisfying the cusp condition (8.4). Clearly, any eigenfunction of the Hamiltonian with a different coupling c, including the BEC wave function, will violate this condition Note that although its expectation value is finite, even the action of the Hamiltonian is singular on such a state as it generates Dirac- $\delta$ 's \*. The diverging expectation values of the charges imply in general that the density  $\rho_{LL}(\lambda)$  has a  $\lambda^{-4}$  power-law tail instead of the usual exponential fall-off. We expect these divergences to be a generic phenomenon for interaction quenches in continuum models which has not been addressed so far.

### 8.4 q-boson regularization

To circumvent the problem of divergences we regularize them by considering an integrable lattice regularization of the LL model, the so-called q-boson hopping model [194]. The Hamiltonian is

$$H_q = -\frac{1}{\delta^2} \sum_{j=1}^{M} \left( B_j^{\dagger} B_{j+1} + B_{j+1}^{\dagger} B_j - 2N_j \right), \qquad (8.5)$$

where  $\delta$  is the lattice spacing of the lattice of length M having periodic boundary conditions. The operators  $B_j$ ,  $B_j^{\dagger}$  and the number operator  $N_j = N_j^{\dagger}$  satisfy the q-boson algebra

$$B_j B_j^{\dagger} - q^{-2} B_j^{\dagger} B_j = 1, \quad q > 1,$$
(8.6)

with  $[N_j, B_j] = -B_j$ ,  $[N_j, B_j^{\dagger}] = B_j^{\dagger}$ , and operators at different sites commute. In the representation on the Fock space generated by the canonical lattice boson operators  $b_j, b_j^{\dagger}$  at each site it is possible to express the q-operators as  $N_j = b_j^{\dagger}b_j$ ,  $B_j = \sqrt{\frac{[N_j+1]_q}{N_j+1}} b_j$ , where  $[x]_q \equiv \frac{1-q^{-2x}}{1-q^{-2}}$ . Note that as  $q \to 1$ ,  $[x]_q \to x$  and therefore

<sup>\*</sup>The divergence can also be verified for N = 2 particles and quenches from the c = 0 ground state by explicitly calculating the overlaps between the new eigenstates and initial state which is a constant. The overlaps scale as  $\lambda^{-2}$  for large  $\lambda$  which implies that  $\langle \hat{Q}_m \rangle$  diverge for  $m \ge 4$ .

 $B_j^{(\dagger)} \to b_j^{(\dagger)}$ . The Hamiltonian is non-polynomial either in the *b* or the *B* operators, thus the model is interacting and the interaction is encoded in the deformation parameter *q*. In the naive limit  $q \to 1$  we recover the system free bosons hopping on a lattice. We are interested instead in the following *continuum limit*: let  $\delta \to 0$ ,  $M \to \infty$ , and  $q \to 1$ , while *L* and *c* are kept constant:

$$L = M\delta, \ c/2 = \kappa\delta^{-1}, \text{ as } M \to \infty \text{ and } \delta, \kappa \to 0,$$
 (8.7)

where  $\kappa$  is related to q as  $q = e^{\kappa}$ . Defining the continuum boson fields  $\hat{\psi}(x = j\delta) = \delta^{-1/2}b_j$ , the q-boson Hamiltonian (8.5) becomes the LL Hamiltonian in the limit (8.7).

The main idea behind our regularized GGE is to use the local conserved charges of the lattice model to determine the density of quasimomenta of q-bosons first, and to take the continuum limit yielding  $\rho_{\text{LL}}(\lambda)$  only as the last step. An infinite set of mutually commuting local charges can be constructed via the Quantum Inverse Scattering Method ( see Appendix D). They are of the form  $I_m = \delta \sum_{j=1}^M \mathcal{J}_j^{(m)}$ , where the operators  $\mathcal{J}_j^{(m)}$  act nontrivially in m + 1 neighboring lattice sites only. These charges are not in one-to-one correspondence with the LL operators  $\hat{Q}_m$ .

Similarly to the LL model, the common eigenstates of all  $I_m$  are defined in the N-particle sector by N quasi-momenta  $\{p_i\}$  which are solutions of the q-boson Bethe equations. Under the limit (8.7) the quasi-momenta should be rescaled as  $\lambda_j = p_j/\delta$  in order to regain the Bethe equations of the LL model. In the thermodynamic limit,  $N, M \to \infty, \nu \equiv N/M = \text{const.}$ , we introduce the quasimomentum distribution function  $\rho_q(p)$ . In terms of  $\rho_q(p)$  the expectation values of the integrals of motion can be written as [195]

$$\rho_m \equiv \frac{|m|\langle I_m \rangle}{M\left(1 - q^{-2|m|}\right)} = \int_{-\pi}^{\pi} \cos\left(mp\right)\rho_q(p)\mathrm{d}p\,,\tag{8.8}$$

for m = 1, 2, ..., and  $\rho_0 = \nu$ , thus the expectation values are essentially the Fourier

series coefficient of  $\rho_q(p)$ . Here we specialized to the case where the parity symmetry is not broken and thus  $\rho_q(p)$  is an even function.

# 8.5 The density $\rho_{LL}(\lambda)$

Let us evaluate now expectation values of  $I_m$  in a q-boson state which reduces to the free boson ground state in the continuum limit, i.e. a BEC state. There is no unique choice but we pick the lattice BEC state  $|\text{BEC}\rangle_N = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{M}} \sum_i b_i^{\dagger}\right)^N |0\rangle$ , where  $b_i^{\dagger}$ are creation operators of *canonical* lattice bosons. Using the explicit expressions of the charge densities  $\mathcal{I}_j^{(m)}$  in terms of the  $B_j^{(\dagger)}$  operators, expanding these in terms of  $b_j^{(\dagger)}$  we obtain series expansions of  $\langle I_m \rangle$  in terms of the small parameter  $\kappa$  (see Appendix D). Combining the lowest orders of the first few  $\langle I_m \rangle$  we confirmed that we obtain the correct value of energy in the limit,  $E/L = n^3\gamma$ . We also find that in the continuum limit  $\hat{Q}_4$  is divergent, as expected.

Based on the first seven charges we conjectured a pattern for the lowest orders in the expansion of the expectation values (see Appendix D). The distribution  $\rho_q(p)$ is obtained by taking the Fourier sum,  $\rho_q(p) = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \rho_m \cos(mp)$ . Summing up the Fourier series order by order in  $\kappa$  and then taking the continuum limit we find

$$2\pi\rho_{\rm LL}(\lambda) = \frac{n^4\gamma^2}{\lambda^4} - \frac{n^6\gamma^3(\gamma - 24)}{4\lambda^6} + \dots$$
 (8.9)

The expansion of the Fourier modes  $\rho_m$  in terms of  $\kappa$  translates into a large momentum expansion of  $\rho_{LL}(\lambda)$  due to the rescaling of momenta,  $\lambda = p/\delta$ . We found the expected  $\lambda^{-4}$  tail together with the subleading  $\lambda^{-6}$  tail.

To find the full  $\rho_{\text{LL}}(\lambda)$  function one needs a pattern for the  $\rho_m$  in all orders in  $\kappa$ . This requires the knowledge of the expectation values of higher charges which are increasingly hard to the compute. However, for observables localized on l neighboring

sites the truncated GGE using the first  $m \gtrsim l$  charges of size  $\leq m + 1$  is expected to give a very good approximation

[227]. Observables localized at a point in the LL model, like  $g_k = \langle :(\hat{\psi}(x)^{\dagger}\hat{\psi}(x))^k:\rangle/n^k$ , are the limits of operators localized on a few neighboring sites in the q-boson lattice system, thus we expect to capture the  $g_k$  using the first few conserved q-boson charges.

To this end, we approximate  $\rho_q(p)$  by the truncated Fourier sum using the Fourier– Padé approximation. Keeping charges up to  $I_4$  and  $I_5$ , Padé-approximants of different types yield the same result in the limit (see Appendix D).

$$\rho_{\rm LL}^{(1)}(\lambda) = \frac{1}{2\pi} \frac{\gamma^2}{(\lambda/n)^4 + \gamma(\gamma/4 - 2)(\lambda/n)^2 + \gamma^2} \,. \tag{8.10}$$

This result changes only when we take into account  $I_6$ : it becomes the ratio of a second and a sixth order polynomial in  $\lambda$ , which we call  $\rho_{LL}^{(2)}(\lambda)$  (see Appendix D). The densities are shown for  $\gamma = 1$  in the inset of Fig. 8.1 together with the GCE density fixed by the energy and particle number only. Let us note that, interestingly, the  $\gamma \to \infty$  limit of both expressions gives the Lorentzian form

$$\lim_{\gamma \to \infty} \rho_{\rm LL}^{(1,2)}(\lambda) = \frac{1}{2\pi} \frac{4}{(\lambda/n)^2 + 4} \,. \tag{8.11}$$

#### 8.6 Correlation functions in the final state.

Knowing the density  $\rho_{\text{LL}}(\lambda)$  allows us to calculate correlation functions. First we compute point-local correlators using the results of Ref. [197] which give analytic expressions for the local two and three-point correlators for arbitrary states that are captured by a continuous  $\rho_{\text{LL}}(\lambda)$ . We compute  $g_2 = \langle :(\hat{\psi}^{\dagger}\hat{\psi})^2 : \rangle/n^2$  and  $g_3 =$  $\langle :(\hat{\psi}^{\dagger}\hat{\psi})^3 : \rangle/n^3$  both for the GGE and the GCE by using the appropriate  $\rho_{\text{LL}}(\lambda)$ . In the latter only the energy and the particle densities are fixed to be the same as for the GGE. The results are shown in the main panel of Fig. 8.1. The values of the correlators computed using the two Padé approximants are very close to each other conforming with the expectation that adding more charges to the thermal GGE does not significantly change the result. This is an important consistency check of our truncation method. The deviations are bigger for  $g_3$  which agrees with the intuition that  $g_3$  is more complex than  $g_2$ . The second observation is that as the difference between the two truncated results decreases for increasing  $\gamma$ , their deviation from the GCE results  $g_k^{\text{th}}$  (dotted lines) grows, the relative difference between the  $g_2$  values being bigger than 20% for  $\gamma > 10$ . For strong interactions the asymptotic behavior of  $g_k$  can be obtained analytically. For  $g_2$  we find  $g_2 \sim 8/(3\gamma)$  and  $g_2^{\text{th}} \sim 4/\gamma$  implying a factor of 3/2 between the two. For  $g_3$  even the power laws are different:  $g_3 \sim 32/(15\gamma^2)$ while  $g_3^{\text{th}} \sim 72/\gamma^3$ .

## 8.7 Strongly interacting final state

For large coupling the system is in the fermionized TG regime since the strong repulsion induces an effective Pauli principle in real space. In the special case of the quench from c = 0 to  $c = \infty$  the overlaps between the initial state and the final TG eigenstates are explicitly known [198]. Only states defined by a set of  $\{\lambda_i, -\lambda_i\}$  pairs have nonzero overlaps which are  $\langle \lambda_i | \text{BEC} \rangle \propto 1/\prod_{\lambda_i>0} \lambda_i$ . The overlaps are the necessary ingredients in the formalism of Ref. [185] to compute the saddle point density. Solving the generalized TBA equations we obtain the simple result  $2\pi\rho_{\text{LL}}(\lambda) = 1/(1+\lambda^2n^2/4)$  (see also Ref. [200]) which exactly matches the  $\gamma \to \infty$  limit of our Padé-approximants, Eq. (8.11). The fact that the two derivations are completely independent gives a strong evidence for the correctness of the result.

Bosonic correlation functions can now be calculated by first fermionizing the field operators using Jordan–Wigner strings,  $\hat{\psi}(x) = \exp[i\pi \int_{-\infty}^{x} \hat{\psi}_{\rm F}^{\dagger}(z)\hat{\psi}_{\rm F}(z)dz]\hat{\psi}_{\rm F}(x)$ , and then exploiting free fermionic correlators of  $\hat{\psi}_{\rm F}$ . Let us consider the equal time correlation  $G(x) = \langle \hat{\psi}^{\dagger}(x)\hat{\psi}(0) \rangle$  in the saddle point distribution of Eq. (8.11). After introducing a lattice discretization, the long chain of operators is amenable to a Wick expansion using as a building block the *fermionic* two point function. Since for  $\gamma = \infty$  the quasimomenta coincide with the physical momenta, this is given by the Fourier transform of the density (8.11),  $G_{\rm FF}(x) = \int d\lambda \rho_{\rm s}(\lambda) e^{i\lambda x} = e^{-2n|x|}$ . The Wick expansion can be recast as a Fredholm-like determinant [199] that finally leads to  $G(x) = e^{-2n|x|}$ . This simple result is drastically different from the corresponding GCE result,  $G_{\rm th}(x) \xrightarrow{\gamma \to \infty} e^{-\gamma (nx)^2/2}$ , which approaches an infinitely narrow Dirac- $\delta$  in the TG limit. Since  $G(x) = G_{\rm FF}(x)$ , the experimentally accessible bosonic momentum distribution,  $n_{\rm B}(k)$ , is thus equal to  $\rho_{\rm LL}(k)$  given by Eq. (8.11), plotted in the inset of Fig. 8.2.

We can also compute the density-density correlation function  $g_2(x) = \langle \hat{\psi}^{\dagger}(x)\hat{\psi}^{\dagger}(0)\hat{\psi}(0)\hat{\psi}(x)\rangle/n^2$ for large final  $\gamma$  using the first few terms of the infinite series given in Ref. [201]. In the large  $\gamma$  limit the leading order for arbitrary  $\rho(\lambda)$  is given by  $g_2(x) \approx 1 - (\int d\lambda \rho(\lambda) e^{i\lambda x})^2$ . Using  $\rho_s(\lambda)$  we obtain  $g_2(x) = 1 - e^{-4n|x|}$ , which agrees very well with the large time result of the numerical solution of the time evolution in Ref. [198] based on the exact overlaps (see main panel of Fig. 8.2). To the best of our knowledge this is one of the first demonstrations in a continuum integrable model that the GGE value of an observable agrees with its actual large time asymptotics.

#### 8.8 Summary

Extending the studies of the post-quench behavior of many-body systems to a nonquadratic continuum model, we investigated the large time behavior of the Lieb– Liniger model after an interaction quench using analytic techniques by combining the Generalized Gibbs Ensemble and Bethe Ansatz integrability of the model and its lattice discretization. We pointed out the divergence of local charges in the initial state that prevents the naive application of the GGE methodology. We expect this to be a generic phenomenon for interaction quenches in continuum models which deserves further study. For a non-interacting initial state and arbitrary final interactions, we evaluated local correlations and found deviations from the thermal predictions. These are experimentally accessible through the measurement of the photoassociation rate  $(g_2)$  and the inelastic three-body loss  $(g_3)$  in cold atom experiments. We computed two-point correlation functions exactly for quenches to the femionized Tonks-Girardeau regime and found excellent agreement with a recent numerical simulation of the time evolution.

Figure 8.1 : Quench from a non-interacting initial state to arbitrary final interactions. *Main panel:* Local correlations  $g_2$  and  $g_3$  as functions of the coupling  $\gamma$ , calculated from the two truncated Generalized Gibbs Ensembles (GGE) (red dashed, blue solid) and from the grand canonical ensemble (GCE) (dot-dashed). The asymptotic behaviors are also shown (dotted). *Inset:* density of quasimomenta,  $\rho_{LL}^{(1)}(\lambda)$ ,  $\rho_{LL}^{(2)}(\lambda)$  in the two truncated GGE (red dashed, blue solid) and  $\rho_{LL}^{th}(\lambda)$  in the GCE (black dotdashed) for  $\gamma = 1$ .

Figure 8.2 : Quench to the TG regime ( $\gamma = \infty$ ). *Main panel:* Equal time densitydensity correlation function. We compare GGE/saddle point (green solid) values with the large time result of a numerical solution of the dynamics of Ref. [198](purple dot-dot-dashed). *Inset:* Momentum distribution function.

Appendices
## Appendix A

## Appendix to impurity in BEC

#### A.1 UV regularization of polaron binding energy

Here we describe the regularization of UV divergences which arise in our model of impurity-BEC interactions

$$H_{\rm int} = \int d\mathbf{x} d\mathbf{x}' g_{\rm IB,\sigma} \delta(\mathbf{x} - \mathbf{x}') \rho_{\rm BEC}(\mathbf{x}) \rho_{\rm I}(\mathbf{x}'), \qquad (A.1)$$

which assumes zero interaction range. Such a model is a reasonable treatment of interactions in dilute atoms [89, 28], that occur predominantly via two-particle collisions. Moreover for low-energy collisions, the two-particle scattering amplitude attains a universal form given by

$$f_{\mathrm{IB},\sigma}(k) = \frac{-1}{1/a_{\mathrm{IB},\sigma} + ik},\tag{A.2}$$

which depends only on the s-wave scattering length,  $a_{IB,\sigma}$ . Consequently the effect of interactions enters all physical observables *only through the measurable s-wave scattering length*, which completely encodes the physics of two-particle collisions, and leads to universality in ultracold atoms.

However, for large enough energies the scattering amplitude (A.2) is no longer universal, and is sensitive to the microscopic details of the true interatomic potential. The appearance of UV divergences in physical observables is a direct consequence of poorly approximating this fundamentally different atomic-scale physics. Indeed, the zero range model Eq. (A.1) pathologically couples short (atomic) distance to long distance degrees of freedom. On the other hand, if one is only interested in universal properties, which are insensitive to microscopic physics, then one requires a means of safely and justifiably decoupling microscopic and macroscopic degrees of freedom. The renormalization group provides the formal means of achieving such a decoupling [104], but in the present case we require only a very trivial example of renormalization, which amounts to "the subtraction of an infinity". We demonstrate this approach, called dimensional regularization, on the binding energy defined in Eq. (4.14).

Consider the limit of a localized impurity  $M \to \infty$  where the binding energy simplifies to

$$E_B^{M \to \infty} = -\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} \xrightarrow{k \gg 1/\xi} -n_0 g_{\mathrm{IB},\sigma}^2 \sum_{\mathbf{k}} \frac{2\mu}{k^2}.$$
 (A.3)

We wish to subtract the leading UV divergence on the right hand side, but this procedure is a priori unjustified. To construct a rigorous prescription we invoke analytic continuity: we take the continuum limit  $\sum_{\mathbf{k}} \rightarrow \int \frac{d^D \mathbf{k}}{(2\pi)^D}$  letting spatial dimension Dtemporarily be a complex valued parameter. We will restore it to integer dimension, e.g. D = 3, at the end of the calculation. Such a procedure leads to the important identity:

$$\int \frac{d^D \mathbf{k}}{(2\pi)^D} \frac{1}{\mathbf{k}^2} = 0, \quad D \in \mathbb{C}.$$
(A.4)

Identity (A.4) allows us to subtract the leading UV divergence from all quantities which require regularization, including the binding energy, since it amounts to the mathematically allowed subtraction of zero by analytically continuing to complex dimension D. Thus we find the following regularized finite expression for the energy

$$E_{B,\text{reg.}}^{M\to\infty} = -\lim_{D\to3} \int \frac{d^D \mathbf{k}}{(2\pi)^D} \left( \frac{V_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} - \frac{2\mu n_0 g_{\text{IB},\sigma}^2}{k^2} \right)$$
$$= -\frac{2\sqrt{2\pi}a_{\text{IB},\sigma}^2 n_0}{\mu\xi} < 0.$$
(A.4)

Moreover, we can use the same prescription to obtain the binding energy of a polaron formed by a finite mass impurity. There, the subtracted quantity retains the form of identity Eq. (A.4), but has a different prefactor. The actual computation of the energy (4.14) needs to be performed numerically in this case.

### A.2 Path integral formulation of time dependent overlap

Here we consider the time-dependent overlap,

$$A(t) = \langle \psi_i | e^{-i\mathcal{H}t} | \psi_i \rangle, \tag{A.5}$$

which describes the return probability of a non-stationary initial state  $|\psi_i\rangle$ , following time-evolution by a Hamiltonian  $\mathcal{H}$ . It typically arises in the context of quantum quenches, where it plays the same role as the partition function in equilibrium statistical mechanics. To take this analogy further, we wish to formulate the time dependent overlap (A.5) as a path integral, which is a standard formulation of the usual partition function.

In addition to being of general theoretical interest, in the present context it provides a practical means of calculating the response of an impurity in a BEC to an RF signal. Indeed, as described in Sec. 3.7 of the main text, the impurity RF response is in fact the Fourier transform of Eq. (A.5).

Specifically, we consider the return amplitude of an initially decoupled impurity-BEC state, after time evolution by an interacting Hamiltonian, leading to the expression

$$A_{p}(t) = \langle 0|e^{-i\int_{0}^{t}\mathcal{H}dt'}|0\rangle \qquad (A.6)$$
$$= \langle 0|e^{-i\left[\frac{1}{2M}\left(\mathbf{p}-\sum_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}\right)^{2}+\sum_{\mathbf{k}}(\omega_{\mathbf{k}}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}+V_{\mathbf{k}}(\hat{b}_{\mathbf{k}}^{\dagger}+\hat{b}_{\mathbf{k}}))\right]^{t}}|0\rangle.$$

This quantity determines the "inverse" RF response, see Sec. 4.4.3 of the main text. Note that by using the Lee-Low-Pines (LLP) transformation outlined in Sec. 4.3.1, we dispensed with the impurity degree of freedom in the Hamiltonian, and mapped the impurity dynamics onto an interaction between phonons. Additionally, the initial state  $|0\rangle$  is simply the phonon vacuum, and is unaffected by the LLP.

Using the Hubbard-Stratonovich (HS) identity

$$= \frac{e^{-\frac{i}{2M}\left(p-\sum_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}\right)^{2}}}{\int_{-\infty}^{\infty}d\varphi(t')e^{i\left[\frac{M}{2}\phi(t')^{2}-i\varphi(t')\cdot\left(\mathbf{p}-\sum_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}\right)\right]dt'}}{\int_{-\infty}^{\infty}d\varphi(t')e^{i\frac{M}{2}\varphi(t')^{2}}},$$
(A.5)

in each interval dt' we introduce a time-dependent classical field  $\varphi(t')$ . This leads to the following path integral formulation of the time-dependent overlap (A.6):

$$A_{p}(t) = \mathcal{N} \int \mathcal{D}[\varphi(t)] e^{i \int_{0}^{t} dt' \frac{M}{2} \varphi(t')^{2}}$$

$$\times \langle 0| e^{-i \int_{0}^{t} dt' \left[\varphi(t') \cdot \left(\mathbf{p} - \sum_{\mathbf{k}} \mathbf{k} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}\right) - \sum_{\mathbf{k}} (\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + V_{\mathbf{k}} (\hat{b}_{\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}})) \right]} |0\rangle,$$
(A.6)

normalized by  $\mathcal{N} = \int \mathcal{D}[\varphi(t)] e^{i \int_0^t dt' \frac{M}{2} \varphi(t')^2}$ .

The path integral notation is a compact representation of the measure

$$\int \mathcal{D}[\varphi(t)] = \lim_{N \to \infty} \prod_{j=1}^{N} \int_{-\infty}^{\infty} d\varphi(t_j),$$

which accounts for our discretization of the time interval t into  $N \to \infty$  infinitesimal windows of size dt'. Correspondingly, we also decomposed the bosonic Hamiltonian

$$H[\hat{b}_{\mathbf{k}}^{\dagger}, \hat{b}_{\mathbf{k}}, \varphi] = \sum_{\mathbf{k}} \left[ (\omega_{\mathbf{k}} - \varphi. \mathbf{k}) \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + V_{\mathbf{k}} (\hat{b}_{\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}}) \right], \qquad (A.6)$$

into a sum of N discrete terms which we rewrote as an integral, to precision dt':

$$e^{i\int_0^t Hdt'} = \prod_{j=1}^N e^{iH[\hat{b}_{\mathbf{k}}^{\dagger},\hat{b}_{\mathbf{k}},\varphi(t_j)]} + \mathcal{O}(dt') = e^{i\int_0^t dt' H[\hat{b}_{\mathbf{k}}^{\dagger},\hat{b}_{\mathbf{k}},\varphi(t')]}$$

Hamiltonian (A.6) contains at most quadratic terms in bosons, enabling us to "integrate them out". We do so by noting that the dynamics of bosons due to such a quadratic Hamiltonian can be exactly described by a decoupled product of timedependent coherent states (c.f. the discussion of localized impurities in Sec. 4.4.3 of the main text). Thus we demand

$$e^{-i\int_0^t dt' H[\hat{b}_{\mathbf{k}}^{\dagger}, \hat{b}_{\mathbf{k}}, \varphi(t')]} |0\rangle = \prod_{\mathbf{k}} |\alpha_{\mathbf{k}}(t)\rangle, \qquad (A.7)$$

with  $|\alpha_{\mathbf{k}}(t)\rangle$  of the coherent state form:

$$|\alpha_{\mathbf{k}}(t)\rangle = e^{i\chi_{\mathbf{k}}(t)}e^{\alpha_{\mathbf{k}}(t)\hat{b}^{\dagger}_{\mathbf{k}} - \alpha^{*}_{\mathbf{k}}(t)\hat{b}_{\mathbf{k}}}|0\rangle.$$
(A.8)

By taking the time derivative of the two sides of Eq. (A.7), and using the explicit form (A.8) to differentiate the right hand side, we obtain differential equations for the coherent state parameters:

$$\dot{\alpha}_{\mathbf{k}}(t) = -i[(\omega_{\mathbf{k}} - \varphi(t).\mathbf{k})\alpha_{\mathbf{k}}(t) + V_{\mathbf{k}}], \qquad (A.9)$$

$$\dot{\chi}_{\mathbf{k}}(t) = -\frac{V_{\mathbf{k}}}{2}(\alpha_{\mathbf{k}}(t) + \alpha_{\mathbf{k}}^{*}(t)), \qquad (A.10)$$

which can be solved by recognizing that Eq. (A.9) contains the total time-derivative of  $\alpha_{\mathbf{k}}(t) \exp\left[-i\mathbf{k} \int_{0}^{t} \varphi(t') dt' + i\omega_{\mathbf{k}}t\right]$ .

Thus we obtain:

$$\alpha_{\mathbf{k}}(t) = -iV_{\mathbf{k}} \int_{0}^{t} dt_{1} e^{-i\mathbf{k} \cdot \int_{t_{1}}^{t} dt'(\omega_{\mathbf{k}} - \varphi(t'))}, \qquad (A.11)$$
  

$$\chi_{\mathbf{k}}(t) = V_{\mathbf{k}}^{2} \int_{0}^{t} dt_{1} \int_{0}^{t_{1}} dt_{2} \sin\left[\int_{t_{2}}^{t_{1}} dt'(\omega_{\mathbf{k}} - \varphi(t').\mathbf{k})\right]. \qquad (A.11)$$

The expectation value

$$E[\varphi(t)] = \langle 0|e^{-i\int_0^t dt' H[\hat{b}_{\mathbf{k}}^{\dagger}, \hat{b}_{\mathbf{k}}, \varphi(t)]}|0\rangle, \qquad (A.12)$$

appearing in Eq. (A.6), can be rewritten using Eq. (A.7) and the coherent state property

$$\langle 0|e^{\alpha b^{\dagger}-\alpha b}|0\rangle = e^{-\frac{1}{2}|\alpha|^2},$$

to yield

$$E[\varphi(t)] = e^{\sum_{\mathbf{k}} \left[ i \chi_{\mathbf{k}}(t) - \frac{1}{2} |\alpha_{\mathbf{k}}(t)|^2 \right]},\tag{A.13}$$

which allows us to rewrite the time-dependent overlap (A.6) in the form:

$$A_{p}(t) = \mathcal{N} \int \mathcal{D}[\varphi(t)] e^{i \int_{0}^{t} dt' \left(\frac{M}{2} \varphi(t')^{2} - \mathbf{p}.\varphi(t')\right)} E[\varphi(t)]$$
  
$$= \mathcal{N} \int \mathcal{D}[\varphi(t)] e^{i \int_{0}^{t} dt' \left(\frac{M}{2} \varphi(t')^{2} - \mathbf{p}.\varphi(t')\right)}$$
  
$$\times e^{\sum_{\mathbf{k}} \left[i\chi_{\mathbf{k}}(t) - \frac{1}{2}|\alpha_{\mathbf{k}}(t)|^{2}\right]}.$$
(A.12)

Eqs. (A.11),(A.11) can be substituted in Eq. (A.12), leading to a path integral over  $\varphi(t)$  alone:

$$A_p(t) = \mathcal{N} \int \mathcal{D}[\varphi(t)] e^{i\mathcal{A}[\varphi(t)]}, \qquad (A.13)$$

with action given by

$$\mathcal{A}[\varphi(t)] = \int_0^t dt' \left[ \frac{M}{2} \varphi(t')^2 - \varphi(t) \cdot \mathbf{p} \right] + i \sum_{\mathbf{k}} V_{\mathbf{k}}^2$$
$$\times \int_0^t dt_1 \int_0^{t_1} dt_2 \exp\left[ -i \int_{t_2}^{t_1} dt' (\omega_{\mathbf{k}} - \varphi(t') \cdot \mathbf{k}) \right].$$
(A.13)

Thus, using the HS identity and the exact solution of the bosonic Hamiltonian (A.6) in terms of decoupled coherent states, we showed that the path integral (A.13) with the action (A.14) is an *exact reformulation* of the time-dependent overlap (A.6).

However further progress requires an approximation scheme to treat the non-Gaussian path integral, which involves a retarded self-interaction of the impurity velocity field  $\varphi(t)$ . To this end we estimate Eq. (A.13) within a saddle point treatment, by extremizing action (A.14) with respect to  $\varphi(t)$ . Thus we obtain the following saddle point equation

$$\varphi_{s}(t') = \frac{\mathbf{p}}{M} + \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{2} \mathbf{k}}{M} \int_{t'}^{t} dt_{1} \int_{0}^{t'} dt_{2} e^{-i \int_{t_{2}}^{t_{1}} dt''(\omega_{\mathbf{k}} - \mathbf{k}.\varphi_{s}(t''))}.$$
(A.12)

The solution of Eq. (A.14) represents a single trajectory that approximates the path integral form of the overlap (A.13) by identifying the most dominant contribution to it. The solution is a time-dependent velocity profile defined up to the propagation time t at which the time-dependent overlap is evaluated. Moreover, as can be seen from Eq. (A.14) it is symmetric around t/2 and  $\varphi_s(0) = \varphi_s(t) = \frac{\mathbf{p}}{M}$ , the bare velocity of the impurity. This unique feature of the velocity profile is due to the requirement of the time-evolving state to return to its initial value, by construction of the quantum propagation amplitude (A.5).

We solved Eq. (A.14) iteratively, taking a lattice of time and momentum points. Moreover in the numerical procedure we dealt with the UV divergence inherent to the zero-range model (see Appendix. A) by introducing a soft cutoff for large momenta, into the interaction of the form  $e^{-k^2/\Lambda^2}$ , and choosing  $\Lambda$  large enough to obtain converged results. The numerical effort required to solve Eq. (A.14) was significantly greater than the mean-field approach outlined in the main text, see Ref. 4.4.3. On the other hand the difference in value of the time-dependent overlap was negligible when computed using the two approaches. Thus we evaluated RF spectra using the time-dependent mean-field approach, confirming its validity based on this agreement.

# Appendix B

# Appendix to correlation prefactors I

### **B.1** Multiplet Summation Rule

Let us now provide an illustration of the multiplet summation rule, Eq. (7.14) of the Chapter, for a few simple cases. The sum rule is given by

$$\sum_{\sum p_i - q_i = n_+} |f(\{p_i\}; \{q_i\})|^2 = C(n_+, \mu_{F,R}),$$
(B.1)

where

$$C(n_r, \mu_{F,R}) = \frac{\Gamma(\mu_{F,R} + n_+)}{\Gamma(\mu_{F,R})\Gamma(n_+ + 1)},$$
(B.1)

and  $f(\{p_i, q_i\})$  is defined in Eq. (6.20). The rules for  $n_-$  are analogous.

Figure B.1 : (Color online) Schematic showing how spectral weights are distributed amongst multiplet of states which are degenerate within  $\propto 1/L$  accuracy. In the inset, we illustrate how spectral weights are distributed within a multiplet for  $n_+ = 2$ , once the degeneracy is lifted by  $\propto 1/L^2$  corrections.

## **B.1.1** $n_+ = 1$

For  $n_{+} = 1$ , the only state which contributes to the multiplet is p = 0, q = -1. Thus the left hand side of Eq. (B.1) is given by

$$|f(\{0,-1\})|^{2} = |f^{+}(0) \times f^{-}(-1)|^{2}$$

$$= \left| \left( \frac{(-\sqrt{\mu_{F,R}})(-\sqrt{\mu_{F,R}}-1)...}{(-\sqrt{\mu_{F,R}}-1)...} \right) \times \left( \frac{(\sqrt{\mu_{F,R}}-1)(\sqrt{\mu_{F,R}}-2)...}{(\sqrt{\mu_{F,R}}-1)(\sqrt{\mu_{F,R}}-2)...} \right) \right|^{2}$$

$$= \mu_{F,R}.$$
(B.-1)

The right hand side of Eq. (B.1) is given by

$$C(n_{+} = 1, \mu_{F,R}) = \left(\frac{(\mu_{F,R})(\mu_{F,R} - 1)...}{(\mu_{F,R} - 1)...}\right) = \mu_{F,R}$$
$$= |f(\{0, -1\})|^{2}.$$
(B.-1)

## **B.1.2** $n_+ = 2$

For  $n_+ = 2$ , there are two states: p = 1, q = -1, and p = 0, q = -2. Consequently the left hand side of Eq. (B.1) is given by

$$|f(+1;-1)|^{2} + |f(0,-2)|^{2} = \left|\frac{1}{2}f^{+}(1)f^{-}(-1)\right|^{2} + \left|\frac{1}{2}f^{+}(0)f^{-}(-2)\right|^{2} \\ = \frac{\mu_{F,R}(\sqrt{\mu_{F,R}}-1)^{2}}{4} + \frac{\mu_{F,R}(\sqrt{\mu_{F,R}}+1)^{2}}{4} \\ = \frac{\mu_{F,R}(\mu_{F,R}+1)}{2}.$$
(B.-3)

And the right hand side of Eq. (B.1) is given by

$$C(n_{+} = 2, \mu_{F,R}) = \left(\frac{(\mu_{F,R} + 1)(\mu_{F,R})(\mu_{F,R} - 1)...}{\Gamma(3)(\mu_{F,R} - 1)...}\right)$$
$$= \frac{\mu_{F,R}(\mu_{F,R} + 1)}{2} = |f(+1; -1)|^{2} + |f(0, -2)|^{2}.$$
(B.-3)

## **B.1.3** $n_+ = 3$

There are three states in the multiplet  $n_+ = 3$ : p = 2, q = -1, p = 1, q = -2 and p = 0, q = -3. The left hand side of Eq. (B.1) is given by

$$|f(+2;-1)|^{2} + |f(+1;-2)|^{2} + |f(0;-3)|^{2}$$

$$= \frac{1}{36}\mu_{R}(2-\sqrt{\mu_{R}})^{2}(1-\sqrt{\mu_{R}})^{2}$$

$$+ \frac{1}{9}\mu_{R}(\sqrt{1-\mu_{R}})^{2}(1+\sqrt{\mu_{R}})^{2}$$

$$+ \frac{1}{36}\mu_{R}(2+\sqrt{\mu_{R}})^{2}(1+\sqrt{\mu_{R}})^{2}$$

$$= \frac{\Gamma(\mu_{R}+3)}{6\Gamma(\mu_{R})} = C(n_{+}=3,\mu_{R}).$$
(B.-6)

Thus once again the summation rule holds.

### **B.2** Identities involving Poly-Gamma functions

The poly-gamma function is defined as  $\psi^{(k)}(z) = \frac{d^k}{dx^k} \log(\Gamma(x))|_{x=z}$ . We have the following summation identity for  $\psi^{(n)}(z)$ :

$$\sum_{k=0}^{N-1} \frac{1}{(k+a)^{n+1}} = \frac{(-1)^n}{n!} (\psi^{(n)}(N+a) - \psi^{(n)}(a)).$$
(B.-5)

We have a few explicit values of the polygamma functions:

$$\psi^{(0)}(1) = -\gamma_E,$$
  
$$\psi^{(1)}(1) = \frac{\pi^2}{6},$$
 (B.-5)

where  $\gamma_E \approx 0.5772...$  is the Euler-Mascheroni constant.

We also have the following asymptotic expansions:

$$\lim_{z \to \infty} \psi^{(0)}(z) = \log(z) - \frac{1}{2z} + O\left(\frac{1}{z^2}\right),$$
$$\lim_{z \to \infty} \psi^{(1)}(z) = \frac{1}{z} + \frac{1}{2z^2} + O\left(\frac{1}{z^3}\right).$$
(B.-5)

# B.3 Principal Value Integrals: Interior and Edge Singularities

We define three distinct types of principal value integrals as follows,

$$P \int_{a}^{b} dx \frac{f(x)}{x-c} = \lim_{\delta \to 0} \left( \int_{a}^{c-\delta} dx \frac{f(x)}{x-c} + \int_{c+\delta}^{b} dx \frac{f(x)}{x-c} \right),$$

$$P_{-} \int_{a}^{b} dx \frac{f(x)}{x-a} = \lim_{\delta \to 0} \left( \int_{a+\delta}^{b} \frac{f(x)}{x-a} + f(a) \log(\delta) \right),$$

$$P_{+} \int_{a}^{b} dx \frac{f(x)}{x-b} = \lim_{\delta \to 0} \left( \int_{a}^{b-\delta} \frac{f(x)}{x-b} - f(b) \log(\delta) \right),$$

$$P_{\pm} \int_{a}^{b} dx \frac{f(x)(b-a)}{(x-a)(x-b)} = P_{+} \int_{a}^{b} \frac{f(x)}{x-b} - P_{-} \int_{a}^{b} \frac{f(x)}{x-a}.$$
(B.-8)

Note also that when we have a multiple integral where all but one of the integrals is analytic and do not need to be evaluated in the special sense above, we will use the notation

$$P_{\pm} \int_{a}^{b} dx \int_{c}^{d} dy \frac{f(x)f(y)}{x - b(a)},$$
 (B.-7)

where we mean that we can freely carry out the inner integration, but the final integration needs to be performed as in Eq. (B.-4).

# Appendix C

# Appendix to correlation prefactors II

## C.1 $\Gamma$ products and Barnes G function

Following are the definition of the Barnes G function and it's relation to the  $\Gamma$ function as well as a few special values and asymptotic expansions:

$$\prod_{i=1}^{n} \Gamma(i+a) = \frac{G(n+a+1)}{G(1+a)},$$
(C.0)  
 $G(1) = 1,$ 

(C.0)

$$\lim_{n \to \infty} \log(\Gamma(n)) = (n - 1/2) \log(n) - n + \frac{1}{2} \log(2\pi)$$
(C.0)

$$+O\left(\frac{1}{n}\right),$$
 (C.0)

$$\lim_{n \to \infty} \log(G(n+1)) = \frac{n^2}{2} \log(n) - \frac{3}{4}n^2 + \frac{n}{2} \log(2\pi)$$
(C.0)

$$-\frac{1}{12}\log(n) + \zeta'(-1) + O\left(\frac{1}{n}\right).$$
 (C.1)

# C.2 Principal Value Integrals: Interior and Edge Singularities

We define three distinct types of principal value integrals as follows,

$$P \int_{a}^{b} dx \frac{f(x)}{x-c} = \lim_{\delta \to 0} \left( \int_{a}^{c-\delta} dx \frac{f(x)}{x-c} + \int_{c+\delta}^{b} dx \frac{f(x)}{x-c} \right),$$
(C.1)  

$$P_{-} \int_{a}^{b} dx \frac{f(x)}{x-a} = \lim_{\delta \to 0} \left( \int_{a+\delta}^{b} \frac{f(x)}{x-a} + f(a) \log(\delta) \right),$$
(C.1)  

$$P_{+} \int_{a}^{b} dx \frac{f(x)}{x-b} = \lim_{\delta \to 0} \left( \int_{a}^{b-\delta} \frac{f(x)}{x-b} - f(b) \log(\delta) \right),$$
(C.1)  

$$P_{\pm} \int_{a}^{b} dx \frac{f(x)(b-a)}{(x-a)(x-b)} = P_{+} \int_{a}^{b} \frac{f(x)}{x-b} - P_{-} \int_{a}^{b} \frac{f(x)}{x-a}.$$
(C.1)

$$P_{\pm} \int_{a}^{b} dx \frac{f(x)(b-a)}{(x-a)(x-b)} = P_{\pm} \int_{a}^{b} \frac{f(x)}{x-b} - P_{-} \int_{a}^{b} \frac{f(x)}{x-a}.$$
(C.1)

(C.2)

Note that we consider all quantities being integrated to be dimensionless, and the bounds of integration to be real numbers with no physical units. All such special principal value integrals evaluated in the text are first made dimensionless by mapping the region of integration to the interval (-1, 1).

## C.3 Special Property of Barnes Function

We will use the following property of the Barnes function,

$$G(1-z) = \frac{G(1+z)}{(2\pi)^z} e^{\int_0^z \pi x \cot(\pi x) dx},$$
 (C.3)

to simplify a group of terms occurring in the final expression for the various form factors.

Now consider the term,

$$\exp\left\{\int_{-q}^{q} d\lambda \pi F(\lambda) F'(\lambda) \cot(\pi F(\lambda))\right\}$$
(C.3)

$$= \exp\left\{\int_{F(-q)}^{F(q)} \mathrm{d}x\pi\mathrm{xcot}(\pi\mathrm{x})\right\}$$
(C.3)

$$= \exp\left\{\int_{0}^{F(q)} \mathrm{dx}\pi\mathrm{xcot}(\pi\mathrm{x}) - \int_{0}^{F(-q)} \mathrm{dx}\pi\mathrm{xcot}(\pi\mathrm{x})\right\}$$
(C.3)

$$= \frac{G(1 - F(q))G(1 + F(-q))(2\pi)^{F(q) - F(-q)}}{G(1 + F(q))G(1 - F(-q))}.$$
 (C.4)

Thus we have

$$G(1+F(q))G(1-F(q))G(1+F(-q))G(1-F(-q))\exp\left[\int_{-q}^{q}d\lambda\pi F(\lambda)F'(\lambda)cot(\pi F(\lambda))\right]$$
(C.4)

$$= G^{2}(1 + F(-q))G^{2}(1 - F(q))(2\pi)^{F(q) - F(-q)}.$$
(C.5)

### C.4 The Fredholm Determinant

Given an integral equation of the form,

$$\phi(x) = f(x) + \lambda \int_{a}^{b} K(x, y)\phi(y)dy, \qquad (C.6)$$

we may construct a Fredholm determinant  $D(\lambda)$  from it by replacing the integral above by a finite sum. The procedure to do so is as follows and is outlined in more detail in Ref. [279]. First we discretize the interval [a, b] into n equal parts of length,  $\delta = (b - a)/n$ . We may index points in the interval using  $x_j = a + j\delta$ , and denote  $\phi_j = \phi(x_j), f_j = f(x_j), K_{jk} = K(x_j, x_k)$  where j, k run from 1 to n. Using these definitions, the discrete version of Eq. (C.6) becomes,

$$\phi_j = f_j + \lambda \delta \sum_{k=1}^n K_{jk} \phi_k, \qquad j = 1, 2, ..., n.$$
 (C.7)

•

We note that the original integral equation in Eq. (C.6) gives rise to a system of n equations in n unknowns,  $\phi_1, ..., \phi_n$ . We may solve the above system by constructing a determinant as per Cramer's theorem of the form, [279], [281],

$$D_n(\lambda) = \begin{vmatrix} 1 - \lambda K_{11}\delta & -\lambda K_{12}\delta & \dots & -\lambda K_{1n}\delta \\ -\lambda K_{21}\delta & 1 - \lambda K_{22}\delta & \dots & -\lambda K_{2n}\delta \\ \dots & \dots & \dots & \dots \\ -\lambda K_{n1}\delta & -\lambda K_{n2}\delta & \dots & 1 - \lambda K_{nn}\delta \end{vmatrix}$$

We wish to obtain the "true" Fredholm Determinant associated with the integral equation in Eq. (C.6) as the continuum limit of Eq. (C.8). One way to proceed is to first expand the determinant in Eq. (C.8) as in Ref. [281],

$$D_{n}(\lambda) = 1 - \lambda \sum_{p_{1}=1}^{n} \delta K_{p_{1},p_{1}} + \dots + \frac{(-\lambda)^{n}}{n!} \sum_{p_{1},\dots,p_{n}=1}^{n} \delta^{n} \begin{vmatrix} K_{p_{1}p_{1}} & K_{p_{1}p_{2}} & \dots & K_{p_{1}p_{n}} \\ K_{p_{2}p_{1}} & K_{p_{2}p_{2}} & \dots & K_{p_{2}p_{n}} \\ \dots & \dots & \dots & \dots \\ K_{p_{n}p_{1}} & K_{p_{n}p_{2}} & \dots & K_{p_{n}p_{n}} \end{vmatrix},$$
(C.6)

and take  $n \to \infty$ . This allows us to replace the finite sums by integrals. Thus we may define the Fredholm determinant as the entire function  $D(\lambda)$ , where

$$D(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{(-\lambda)^n}{n!} d_n,$$
(C.7)

with

$$d_{n} = \int_{a}^{b} dx_{1} \int_{a}^{b} dx_{2} \dots \int_{a}^{b} dx_{n} \begin{vmatrix} K(x_{1}, x_{1}) & K(x_{1}, x_{2}) & \dots & K(x_{1}, x_{n}) \\ K(x_{2}, x_{1}) & K(x_{2}, x_{2}) & \dots & K(x_{2}, x_{n}) \\ \dots & \dots & \dots & \dots \\ K(x_{n}, x_{1}) & K(x_{n}, x_{2}) & \dots & K(x_{n}, x_{n}) \end{vmatrix} .$$
(C.7)

The above derivation also illustrates an elementary numerical method for calculating Fredholm determinants associated with various integral operators.

# Appendix D

# Appendix to Interaction quench of 1D Bose gas

### D.1 Local conserved charges in the *q*-boson hopping model

Integrals of motion of the q-boson hopping model can be constructed using the Quantum Inverse Scattering Method. The L-operator for the model is given by

$$L_j(\lambda) = \begin{pmatrix} e^{\lambda} & \chi B_j^{\dagger} \\ \chi B_j & e^{-\lambda} \end{pmatrix}, \qquad (D.0)$$

where  $\chi = \sqrt{1 - q^{-2}} = \sqrt{1 - e^{-2\kappa}}$ . The monodromy matrix  $T(\lambda)$  is defined as a matrix product of the *L*-operators over all the lattice sites

$$T(\lambda) = L_M(\lambda)L_{M-1}(\lambda)\cdots L_1(\lambda), \qquad (D.1)$$

and the transfer matrix  $\tau(\lambda)$  is given by the trace over the matrix space of the monodromy matrix

$$\tau(\lambda) = \operatorname{Tr} T(\lambda) \,. \tag{D.1}$$

For any  $\lambda$  and  $\mu$  the transfer matrices commute:  $[\tau(\lambda), \tau(\mu)] = 0$ , which implies that  $\tau(\lambda)$  is a generating function of the conserved charges. Many different sets can be generated since any analytic function of  $\tau(\lambda)$  can play the role of the generating function. We consider the set consisting of *local* charges that can be written in the form

$$I_m = \delta \sum_{j=1}^M \mathcal{J}_j^{(m)}, \qquad (D.1)$$

where the operators  $\mathcal{J}_{j}^{(m)}$  act nontrivially in m+1 neighboring lattice sites only. This set is obtained by the formula

$$I_m = \frac{1}{(2m)!} \frac{d^{2m}}{d\zeta^{2m}} \ln \left[ \zeta^M \tau(\zeta) \right] \Big|_{\zeta \to 0} , \qquad m = 1, 2, 3, \dots .$$
 (D.2)

where we introduced the variable  $\zeta = e^{\lambda}$ . The local operators  $\mathcal{J}^{(1)}(n)$ ,  $\mathcal{J}^{(2)}(n)$  and  $\mathcal{J}^{(3)}(n)$  are

$$\mathcal{J}^{(1)}(n) = \frac{1}{\delta} \chi^2 B_j^{\dagger} B_{j+1} ,$$
  
$$\mathcal{J}^{(2)}(n) = \frac{1}{\delta} \chi^2 \left( 1 - \frac{\chi^2}{2} \right) \left( B_j^{\dagger} B_{j+2} - \frac{\chi^2}{2 - \chi^2} B_j^{\dagger} B_j^{\dagger} B_{j+1} B_{j+1} - \chi^2 B_j^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+2} \right) ,$$

and

$$\begin{aligned} \mathcal{J}^{(3)}(n) &= \frac{1}{\delta} \chi^2 \left( 1 - \chi^2 + \frac{\chi^4}{3} \right) \left( B_j^{\dagger} B_{j+3} - \chi^2 B_j^{\dagger} B_j^{\dagger} B_{j+1} B_{j+2} - \chi^2 B_j^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+3} \right. \\ &- \chi^2 B_j^{\dagger} B_{j+1}^{\dagger} B_{j+2} B_{j+2} - \chi^2 B_j^{\dagger} B_{j+2}^{\dagger} B_{j+2} B_{j+3} + \frac{\chi^4}{3 - 3\chi^2 + \chi^4} B_j^{\dagger} B_j^{\dagger} B_j^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+1} B_{j+1} \\ &+ \chi^4 B_j^{\dagger} B_j^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+1} B_{j+2} + \chi^4 B_j^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+2} B_{j+2} \\ &+ \chi^4 B_j^{\dagger} B_{j+1}^{\dagger} B_{j+2} B_{j+2} B_{j+3} \right) . \end{aligned}$$

The integrals  $I_m$  are not Hermitian operators. Using the involution  $[\tau(\zeta)]^{\dagger} = \tau(\zeta^{-1})$  it can be shown that  $[I_m^{\dagger}, I_n] = 0$  for any m, n. As the number operator  $N = \sum_j N_j = \sum_j b_j^{\dagger} b_j$ , is non-polynomial in the  $B_j^{(\dagger)}$  operators while the charges  $I_m$  are, it cannot be expressed as a finite linear combination of the  $I_m$ . However, N commutes with any monomial containing an equal number of the creation and annihilation operators thus  $[N, I_m] = 0$ . It is convenient to use the notation  $N \equiv I_0$ . The Hamiltonian (8.5) can then be written as

$$H_q = -\frac{1}{\chi^2 \delta^2} (I_1 + I_{-1} - 2\chi^2 I_0).$$
 (D.2)

#### D.2 Expectation values of the charges in the initial state

We need to evaluate the expectation values of local charges  $I_m$  in a state which transforms into the continuum BEC-state in the limit (8.7). We pick here the state

$$|\text{BEC}\rangle_N = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{M}} \sum_i b_i^{\dagger}\right)^N |0\rangle, \qquad (D.3)$$

since it has the nice property (established by commuting annihilation operators one by one)

$$b_j^{\alpha}|\text{BEC}\rangle_N = \sqrt{\frac{N}{M}} \cdots \sqrt{\frac{N-\alpha+1}{M}}|\text{BEC}\rangle_{N-\alpha} \approx \nu^{\alpha/2}|\text{BEC}\rangle_{N-\alpha},$$
 (D.4)

where the approximate relation is valid in the thermodynamic limit (TDL) when we are interested in  $\alpha$  that does not scale proportionally to the system size. Note that as long as we are interested in evaluation of expectation values of *normal ordered* operators over BEC state in the TDL, one can also use the coherent state form of the BEC

$$|\text{BEC}, c\rangle = \prod_{j} e^{-\nu/2 + \sqrt{\nu} b_{j}^{\dagger}} |0\rangle , \qquad (D.5)$$

which has the same matrix elements as state (D.4).

In what follows, we compute expectation values of the local charges by computing first the building blocks, on-site monomials, based on expanding  $B_i^{(\dagger)}$  in terms of  $b_i^{(\dagger)}$ and normal ordering. For most of the matrix elements we can only derive expansions in powers of  $\kappa$  (but not making any assumptions about  $\nu$ ). We will start from

$$B_{j} = b_{j}\sqrt{\frac{[N+1]_{q}}{N+1}} \approx b_{j}\left(1 - \frac{\kappa}{2}N_{j} + \frac{\kappa^{2}}{24}N_{j}(5N_{j}+4) + \dots\right)$$
$$= b_{j} - \frac{\kappa}{2}b_{j}^{\dagger}b_{j}b_{j} + \frac{\kappa^{2}}{24}(5b_{j}^{\dagger}b_{j}^{\dagger}b_{j}b_{j}b_{j} + 9b_{j}^{\dagger}b_{j}b_{j}) + \dots$$
(D.5)

The evaluation of its expectation value in the state (D.5) leads to

$$\langle \text{BEC}, c | B_j | \text{BEC}, c \rangle = \sqrt{\nu} - \frac{1}{2} \kappa \nu^{3/2} + \frac{\kappa^2}{24} \left( 9\nu^{3/2} + 5\nu^{5/2} \right) + \dots$$
 (D.6)

In a similar way we obtain

$$\langle \text{BEC}|B_{j}^{\dagger}B_{j}|\text{BEC}\rangle = \nu - \kappa\nu^{2} + \kappa^{2}\nu^{2} - \frac{2}{3}\nu^{2}\kappa^{3} + \frac{2}{3}\nu^{3}\kappa^{2} + \dots$$
 (D.7)

We note that for this combination a closed form expression exists,  $\langle \text{BEC}|B_j^{\dagger}B_j|\text{BEC}\rangle = (1-e^{-(1-q^{-2})\nu})/(1-q^{-2})$ . These and similar on-site matrix elements are the only type needed to systematically evaluate the expectation values of any polynomial of  $B^{(\dagger)}$  operators acting on different sites over the BEC. Indeed, due to the factorization of the wave function on different sites in the coherent state representation (D.5) one can treat different sites separately.

Let us now use these matrix elements to evaluate the first  $\rho_m$ , m = 1, ..., 6. From Eqs. (D.1,D.1) and from the definition (8.8) we have

$$\rho_{1} = \frac{1}{M} \sum_{j} \langle B_{j}^{\dagger} B_{j+1} \rangle,$$
  

$$\rho_{2} = \frac{1}{M} \sum_{j} \left\langle B_{j}^{\dagger} B_{j+2} - \frac{\chi^{2}}{2 - \chi^{2}} B_{j}^{\dagger} B_{j}^{\dagger} B_{j+1} B_{j+1} - \chi^{2} B_{j}^{\dagger} B_{j+1}^{\dagger} B_{j+1} B_{j+2} \right\rangle, \text{ et(D.7)}$$

Due to translational invariance we need to evaluate the expectation value only for a

single value of j. We find

$$\begin{split} \rho_1 &= \nu - \frac{1}{2} \gamma \nu^3 + \frac{3}{16} \gamma^2 \nu^4 + \left(\frac{1}{6} \gamma^2 - \frac{7}{192} \gamma^3\right) \nu^5 - \frac{11}{96} \gamma^3 \nu^6 + \dots, \\ \rho_2 &= \nu - 2\gamma \nu^3 + \frac{15}{16} \gamma^2 \nu^4 + \left(\frac{5}{3} \gamma^2 - \frac{55}{192} \gamma^3\right) \nu^5 + \left(-\frac{51}{32} \gamma^3 + \frac{1}{16} \gamma^4\right) \nu^6 + \dots, \\ \rho_3 &= \nu - \frac{9}{2} \gamma \nu^3 + \frac{43}{16} \gamma^2 \nu^4 + \left(\frac{15}{2} \gamma^2 - \frac{73}{64} \gamma^3\right) \nu^5 + \left(-\frac{859}{96} \gamma^3 + \frac{73}{192} \gamma^4\right) \nu^6 + \dots, \\ \rho_4 &= \nu - 8\gamma \nu^3 + \frac{95}{16} \gamma^2 \nu^4 + \left(\frac{68}{3} \gamma^2 - \frac{619}{192} \gamma^3\right) \nu^5 + \left(-\frac{3137}{96} \gamma^3 + \frac{269}{192} \gamma^4\right) \nu^6 + \dots, \\ \rho_5 &= \nu - \frac{25}{2} \gamma \nu^3 + \frac{179}{16} \gamma^2 \nu^4 + \left(\frac{325}{6} \gamma^2 - \frac{1423}{192} \gamma^3\right) \nu^5 + \left(-\frac{2953}{32} \gamma^3 + \frac{379}{96} \gamma^4\right) \nu^6 + \dots, \\ \rho_6 &= \nu - 18\gamma \nu^3 + \frac{303}{16} \gamma^2 \nu^4 + \left(111\gamma^2 - \frac{949}{64} \gamma^3\right) \nu^5 + \left(-\frac{21049}{96} \gamma^3 + \frac{299}{32} \gamma^4\right) \nu^6 + \dots, \end{split}$$

where we use  $\nu$  as small parameter by the relation

$$\kappa = \gamma \nu / 2 \,. \tag{D.9}$$

Naively, combining various  $\rho_m$  and taking the limit one can obtain moments of the  $\rho_{LL}(\lambda)$  density, i.e. the expectation values of the charges  $\hat{Q}_m$  of the LL model. However, this must be done with care. First, the limits of integration are strictly speaking not  $\pm \infty$ , but  $\pm \pi/\delta$ , which matters if the LL moments are divergent (as expected). Second, the scaling limit (8.7), Eq. (D.9) as well as the relations  $\lambda = p/\delta$ and  $\rho_{LL}(\lambda) = \rho_q(\delta \lambda)$  may have higher order corrections which would mix the orders.

In spite of the problems mentioned above, the energy can be obtained if the  $\rho_{\rm LL}(\lambda)$ 

has at most a  $\lambda^{-4}$  tail:

$$-\frac{1}{4}(\rho_{1}+\rho_{-1}-2\rho_{0}) = \int_{-\pi}^{\pi} dp \left(p^{2}-\frac{1}{6}p^{4}+\dots\right)\rho_{q}(p) = \int_{-\pi/\delta+\dots}^{\pi/\delta+\dots} d\lambda(\delta+\dots)(\delta^{2}\lambda^{2}-\frac{1}{6}\lambda^{4}\delta^{4}+\dots)(\rho_{LL}(\lambda)+\dots), \quad (D.9)$$

where the dots stand for higher order terms in  $\delta$ . The first parenthesis comes from the unknown higher order terms of the relation  $p = \delta \cdot \lambda + \ldots$ , this also generates terms in the middle parenthesis. Now let us make the *assumption* that this relation, as well as the relation between  $\rho(p)$  and  $\rho_{LL}(\lambda)$  does not have higher powers of  $\lambda$ . Under this assumption each power  $\lambda^{2n}$  comes with at least  $\delta^{2n+1}$  in the integrand which implies that although the integrals of higher powers seem to diverge, with the  $\delta$ -powers in their coefficients all of them scale as  $\delta^4$ , while the quadratic term scales as  $\delta^3$ . Thus it is safe to take the  $\delta \to 0$  limit after dividing by  $\delta^3$  and we are left with

$$-\frac{1}{2\delta^3}(\rho_1 - \rho_0) \to \int_{-\infty}^{\infty} \mathrm{d}\lambda \,\rho_{\mathrm{LL}}(\lambda)\lambda^2\,. \tag{D.10}$$

Since  $\lim_{\delta\to 0} \left[ -\frac{1}{2\delta^3} (\rho_1 - \rho_0) \right] = n^3 \gamma$ , the energy density is correctly reproduced, as expected.

In a similar fashion, one can formulate a condition on whether the 2*n*-th moment of the  $\rho_{\text{LL}}(\lambda)$  distribution is divergent. For this one again needs to pick the right combination of  $\rho_m$  with  $m \leq n$ . In particular,  $Q_4$  is divergent if

$$\rho_2 + \rho_{-2} - 2\rho_0 - 4(\rho_1 + \rho_{-1} - 2\rho_0) \propto \delta^4, \qquad (D.11)$$

as opposed to  $\propto \delta^5$ . From the expansion in Eqs. (D.8) we find

$$\rho_2 - \rho_0 - 4(\rho_1 - \rho_0) = \frac{3}{\gamma^2} \kappa^4 + \dots,$$
(D.12)

thus  $\int d\lambda \rho_{\rm LL}(\lambda) \lambda^4 = \langle Q_4 \rangle / L$  is divergent.

#### D.3 Pattern for expectation values in the BEC state

Based on the Taylor expansions in Eqs. (D.8) one can find a pattern for the coefficients of the different orders. They turn out to be low order polynomials in m:

$$\rho_m = \nu - \frac{m^2}{2} \gamma \nu^3 + \frac{m^3 + 2m - \frac{3}{4}}{12} \gamma^2 \nu^4 + \left(\frac{m^2(m^2 + 1)}{12} \gamma^2 - \frac{m^4 + 4m^2 - 3m + \frac{3}{2}}{96} \gamma^3\right) \nu^5 + \left(-\frac{m^5 + 5m^3 - \frac{5}{2}m^2 + \frac{2}{3}m + \frac{5}{12}}{40} \gamma^3 + \frac{m^5 + \frac{20}{3}m^3 - \frac{15}{2}m^2 + \frac{29}{6}m - 5}{960} \gamma^4\right) \nu^6 + \mathcal{O}(\nu^7).$$

The reasonably simple rational coefficients and their structure provide strong evidence that the polynomial dependence on m is correct. The order of the coefficient polynomial of  $\nu^k$  is k - 1 and, interestingly, the subleading orders  $(m^{k-2})$  are always missing. As we will show now, the first property is necessary in order to have a finite scaling limit of the  $\rho(p)$  function, i.e. a finite  $\rho_{LL}(\lambda)$ .

The  $\rho(p)$  distribution function is the Fourier sum of the  $\rho_m$ . It is clear that the scaling limit and this Fourier transformation do not commute: if we take the limit before computing the sum we get  $\rho_m \equiv 0$ . For the computation of the Fourier sum order by order in  $\nu$  one needs to calculate the building blocks

$$\sum_{m=-\infty}^{\infty} m^{2l} \cos(mp) = 0,$$
  
$$\sum_{n=-\infty}^{\infty} m^{2l-1} \cos(mp) = \frac{\sum_{j=0}^{l-1} c_j \cos(jp)}{\sin^{2l} \left(\frac{p}{2}\right)} \longrightarrow \frac{2^{2l} \sum_{j=0}^{l-1} c_j}{\delta^{2l} \lambda^{2l}},$$

where the  $c_j$  are real numbers. This must be multiplied by  $\delta^{2l}$  to be neither divergent nor zero. Thus the fact that in Eq. (D.3) the highest power of m in the coefficient of  $\nu^k$  is k - 1 implies that  $\rho_{LL}(\lambda)$  is finite. Moreover, only the highest powers of min the coefficient polynomials of the even orders of  $\nu$  contributes. This is important, because we know the relation  $\kappa = \gamma \nu/2$  only to leading order. Adding potential subleading terms,  $\kappa = \gamma \nu/2 + a_1 \nu^2 + a_2 \nu^3 + \dots$ , generates terms in each order of  $\nu$  which however have a sub-leading m-dependence, thus they will do not affect the result in the continuum limit.

Taking the Fourier sum we obtain

$$2\pi\rho(p) = \rho_0 + 2\sum_{m=1}^{\infty} \rho_m \cos(mp) = \nu + 2\sum_{m=1}^{\infty} \left(\frac{1}{12}\gamma^2 \nu^4 m^3 + \frac{\gamma^3(\gamma - 24)}{960}\nu^6 m^5\right) + \dots$$
$$= \nu + 2\left(\nu^4 \frac{\gamma^2}{12} \frac{2 + \cos(p)}{8\sin^4(p/2)} - \nu^6 \frac{\gamma^3(\gamma - 24)}{960} \frac{33 + 26\cos(p) + \cos(2p)}{32\sin^6(p/2)} + \dots\right).$$

Taking the continuum limit (8.7) together with  $p = \delta \lambda$  we find

$$\rho_{\rm LL}(\lambda) = \frac{n^4 \gamma^2}{\lambda^4} - \frac{n^6 \gamma^3 (\gamma - 24)}{4\lambda^6} + \dots \qquad (D.13)$$

We see that the expansion of the Fourier modes  $\rho_m$  in terms of  $\delta$  or  $\nu$  is equivalent to a *large momentum expansion* of the LL density of roots  $\rho_{\rm LL}(\lambda)$ . We did find the expected  $\lambda^{-4}$  tail together with the subleading  $\lambda^{-6}$  tail.

Observe that going to higher charges and to higher powers in  $\nu$  go side by side: if one only expands the  $\rho_m$  up to a fixed order in  $\nu$  then one does not gain anything from considering many more charges because the polynomial pattern found from the lower ones already determines them. Conversely, having only a few charges does not allow one to determine the high order polynomial coefficients of the higher orders of  $\nu$ .

A key step in all the above is the rescaling of momenta,  $\lambda = p/\delta$ . This is how lower orders of  $\nu$  may eventually disappear and arbitrary high powers of  $\nu$  may survive in the limit. Consequently, the large momentum expansion structure can be heuristically understood by realizing that we need to resolve the vicinity of p = 0 very well, because this region will be blown up to be the entire domain in  $\lambda$ . Thus it is not very surprising that many Fourier modes are necessary and one needs to know them very precisely. Any truncation or approximation affects the small  $\lambda$  region, so perturbatively we approach from large  $\lambda$ .

### D.4 Padé–Fourier approximation

Let us consider the truncated Fourier sum,

$$\rho^{[l]}(p) = \rho_0 + 2\sum_{m=1}^{l} \rho_m \cos(mp) = \left(\frac{\rho_0}{2} + \sum_{m=1}^{l} \rho_m e^{imp}\right) + \{p \to -p\}$$
$$= \left(\frac{\rho_0}{2} + \sum_{m=1}^{l} \rho_m z^m\right) + \{z \to 1/z\},$$
(D.13)

where we introduced  $z = e^{ip}$ . The parenthesis is a truncated Taylor expansion to which we apply the Hermite–Padé approximation technique: we find a rational function of z such that the first l terms in its Tayor expansion matches our truncated expansion. The (n, m)-type Padé-approximant is a ratio of an nth order and an mth order polynomial (n + m = l). We reintroduce the variable p in the approximants and then we take the continuum limit. The (2, 2), (3, 2), (2, 3), (4, 2) and (2, 4)Padé-approximants all give the same result, Eq. (8.10):

$$\rho_{\rm LL}^{(1)}(\lambda) = \frac{1}{2\pi} \frac{\gamma^2}{(\lambda/n)^4 + \gamma(\gamma/4 - 2)(\lambda/n)^2 + \gamma^2} \,. \tag{D.14}$$

Comparing with Eq. (D.13) this has the correct  $\lambda^{-4}$  tail but not the  $\lambda^{-6}$  one. The latter is reproduced by the Padé-approximant of type (3, 3):

$$\rho_{\rm LL}^{(2)}(\lambda) = \frac{1}{2\pi} \frac{4\gamma^2 \left(\bar{\lambda}^2 + \gamma(\gamma + 2)\right)}{\left(4\bar{\lambda}^2 + \gamma^2\right) \left(\bar{\lambda}^4 + (\gamma - 4)\gamma \,\bar{\lambda}^2 + 4\gamma^2\right)},\tag{D.15}$$

where  $\bar{\lambda} = \lambda/n$ . The  $\gamma \to \infty$  limit of both  $\rho^{(1)}(\lambda)$  and  $\rho^{(2)}(\lambda)$  is given by Eq. (8.11).

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$$[156] \ \mu_{n,\pm,R(L)} = \left[ n\sqrt{K} - (+)\frac{(1\pm1)}{2\sqrt{K}} - \frac{\delta_{+(-)}(k_n)}{2\pi} \right]^2, \\ \mu_{n,\pm,R(L)}^b = \left[ \frac{(2n+1)\sqrt{K}}{2} - (+)\frac{(1\pm1)}{2\sqrt{K}} - \frac{\delta_{+(-)}(k_n^*)}{2\pi} \right]^2, \\ \mu_{n,R(L)} = \left[ \frac{(2n+1)\sqrt{K}}{2} + (-)\frac{1}{2\sqrt{K}} + \frac{\delta_{+(-)}(k_n^*)}{2\pi} \right]^2, \text{ in the notations of Ref. [232].}$$

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