

Magnetic and Ising quantum phase transitions in a model for isoelectronically tuned iron pnictides

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Considerations of the observed bad-metal behavior in Fe-based superconductors led to an early proposal for quantum criticality induced by isoelectronic P for As doping in iron arsenides, which has since been experimentally confirmed. We study here an effective model for the isoelectronically tuned pnictides using a large- N approach. The model contains antiferromagnetic and Ising-nematic order parameters appropriate for J_1 - J_2 exchange-coupled local moments on an Fe square lattice, and a damping caused by coupling to itinerant electrons. The zero-temperature magnetic and Ising transitions are concurrent and essentially continuous. The order-parameter jumps are very small, and are further reduced by the interplane coupling; consequently, quantum criticality occurs over a wide dynamical range. Our results reconcile recent seemingly contradictory experimental observations concerning the quantum phase transition in the P-doped iron arsenides.

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I. INTRODUCTION

Iron pnictide and chalcogenide materials not only show high-temperature superconductivity [1], but also feature rich phase diagrams. For the undoped parent iron arsenides, the ground state has collinear $(\pi, 0)$ magnetic order [2]. Because superconductivity occurs at the border of this antiferromagnetic (AF) order, a natural question is whether quantum criticality plays a role in the phase diagram. Early on, it was proposed theoretically that tuning the parent iron arsenide by isoelectronic P-for-As doping induces quantum criticality associated with the suppression of both the $(\pi, 0)$ AF order and an Ising-nematic spin order [3]. This proposal was made within a strong-coupling approach, which attributes the bad-metal behavior of iron arsenides [4–7] to correlation effects that are on the verge of localizing electrons [8–10] along with their associated magnetic moments. The P doping increases the in-plane electronic kinetic energy (as P is smaller than As), and thus the coherent electronic spectral weight while leaving other model parameters little changed [11,12]. This weakens both the magnetic order and the associated Ising-nematic spin order [3,13].

Experimental evidence for a quantum critical point (QCP) has since emerged in the P-doped CeFeAsO [14,15] and P-doped BaFe₂As₂ [16–20]. In the phase diagram of the P-doped BaFe₂As₂, an extended temperature and doping regime has been identified for non-Fermi-liquid behavior [16–19]. An Ising-nematic order, inferred from the tetragonal-to-orthorhombic structural distortion, is suppressed around the same P-doping concentration ($x_c \approx 0.33$) at which the AF order disappears. While there is evidence for a QCP “hidden” inside the superconducting dome [18], quantum criticality has now been observed and studied in the normal state when superconductivity is suppressed by a high field [19,20]. We note that the bad-metal behavior persists through x_c [16].

Recently, evidence for a weakly first-order nature of the transition has come from the neutron-scattering experiments in the P-doped BaFe₂As₂ [21]. It is in seeming contradiction with the accumulated experimental evidence for quantum criticality. This puzzle calls for further theoretical analyses on the underlying quantum phase transitions. More generally, the

interplay between the magnetic and nematic orders exemplifies the kind of competing or coexisting orders that is of general interest to a variety of strongly correlated electron systems.

In this paper, we study the zero-temperature phase transitions in the appropriate effective Ginzburg-Landau field theory that was introduced earlier [3,13] to describe the low-energy properties of a J_1 - J_2 model of local moments on a square lattice coupled to coherent itinerant electrons [3,8,22–24]. The theory contains antiferromagnetic (vector) and Ising-nematic (scalar) order parameters as well as a damping term. Since it is important to establish the nature of quantum criticality in the absence of superconductivity [14,19,20], we will focus on the transitions in the normal state and will not consider the effect of superconductivity [25]. Using a large- N approach [26,27], we demonstrate that the AF and Ising-nematic transitions are concurrent at zero temperature both for the case of a square lattice and in the presence of interlayer coupling. Moreover, both transitions are only weakly first order in accordance with the marginal nature of the relevant coupling, with jumps in both order parameters that are very small, which implies a large dynamical range for quantum criticality. Our results provide a natural resolution to the aforementioned puzzle.

II. THE MODEL

The proximity of a bad metal to a Mott transition can be measured by a parameter w , the percentage of the single-electron spectral weight in the coherent itinerant part [3,8,9,28]. This approach has been successful in describing the spin excitation spectrum of the iron pnictides [29–32], and in understanding the fact that T_c in the iron-based superconductors with purely electron Fermi pockets is at least comparably high compared with those with nested Fermi surfaces of co-existing hole and electron pockets [33–39]. At the zeroth order in w , all the single-electron excitations are incoherent; integrating out the corresponding charge excitations leads to couplings J_1 and J_2 among the residual local moments:

$$H = \sum_{\langle i,j \rangle} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\langle\langle i,j \rangle\rangle} J_2 \vec{S}_i \cdot \vec{S}_j, \quad (1)$$

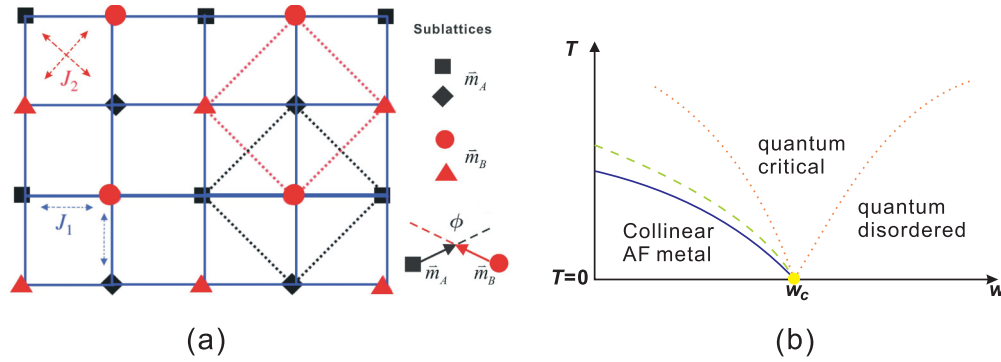


FIG. 1. (a) Illustration of the J_1 - J_2 model on a square lattice. The staggered magnetizations $\vec{m}_A$ and $\vec{m}_B$ are defined on two interpenetrating Néel square lattices. (b) Schematic phase diagram proposed for the P-doped iron arsenides [3]. P doping increases w , the spectral weight of the coherent itinerant electrons. The yellow dot denotes the tuning parameter w_c for the QCP. The purple solid line and the green dashed one respectively mark the AF and structural transitions.

where $\langle \dots \rangle$ and $\langle\langle \dots \rangle\rangle$ respectively denote the nearest-neighbor and next-nearest-neighbor sites [see Fig. 1(a)]. Both general considerations [8] and first-principles calculations [40,41] suggest that $J_2 > J_1/2$. In this regime, we consider two interpenetrating sublattices [the dotted squares in Fig. 1(a)], having independent staggered magnetizations with Néel vectors $\vec{m}_A$ and $\vec{m}_B$. While the mean-field energy is independent of the angle ϕ between $\vec{m}_A$ and $\vec{m}_B$, this degeneracy is broken by quantum or thermal fluctuations. It leads to the collinear order with $\phi = 0$ or π [22,42]. Thus $\vec{m}_A \cdot \vec{m}_B = \pm 1$ becomes an Ising variable.

At nonvanishing orders in w , the coherent itinerant electrons provide Landau damping. This leads to the following Ginzburg-Landau action [3,13]:

$$S = S_2 + S_4 \quad (2)$$

with

$$\begin{aligned} S_2 &= \sum_{\vec{q}, i\omega_l} \{ \chi_0^{-1}(\vec{q}, i\omega_l) [|\vec{m}_A(\vec{q}, i\omega_l)|^2 + |\vec{m}_B(\vec{q}, i\omega_l)|^2] \\ &\quad + 2v(q_x^2 - q_y^2) \vec{m}_A(\vec{q}, i\omega_l) \cdot \vec{m}_B(-\vec{q}, -i\omega_l) \}, \\ S_4 &= \int_0^\beta d\tau \int d\vec{r} \{ u_1 (|\vec{m}_A|^4 + |\vec{m}_B|^4) \\ &\quad + u_2 |\vec{m}_A|^2 |\vec{m}_B|^2 - u_I (\vec{m}_A \cdot \vec{m}_B)^2 \}. \end{aligned} \quad (3)$$

The $\vec{m}_{A/B}$ are in either momentum and Matsubara frequency space (S_2) or real space and imaginary time (S_4). In S_2 , the inverse susceptibility is

$$\chi_0^{-1}(\vec{q}, i\omega_l) = r + \omega_l^2 + cq^2 + \gamma|\omega_l|, \quad (4)$$

where c is the square of the spin-wave velocity and in S_4 , the coupling $u_I > 0$ [3,22]. The parameter v leads to the anisotropic distribution of the spin spectral weight in momentum space, which is observed in neutron scattering [31,32]. It is described by the ellipticity

$$\epsilon \equiv \sqrt{(c-v)/(c+v)}, \quad (5)$$

which goes from full isotropy $\epsilon = 1$ ($v = 0$) to extreme anisotropy $\epsilon = 0$ ($v = c$). In addition, γ is the (Landau)

damping rate and $r = r_0 + wA_Q$, where r_0 is negative, reflecting ground-state order in the absence of damping, and $A_Q > 0$ is related to a quasiparticle susceptibility at $\mathbf{Q} = (\pi, 0)$ or $(0, \pi)$ [3]. The mass r vanishes at $w = w_c$, the point of quantum phase transition. When the damping is present, the effective dimensionality of the fluctuations is $d + z = 4$. From a renormalization-group (RG) perspective, because “ $-u_I$ ” is negative, it is marginally relevant with respect to the underlying QCP at $d + z = 4$ [3,43]. So unlike thermally driven transitions or the case of a zero-temperature transition in the absence of damping (where u_I is relevant), the marginal nature of the coupling is expected to yield only a small change to the underlying QCP; this leads to a qualitative phase diagram shown in Fig. 1(b) [3,13].

Given the aforementioned experimental observations, we shall study the phase transitions beyond qualitative RG-based considerations. Our focus is on the zero-temperature limit, and we place particular emphasis on the effect of damping. We note that the effect of damping on the transitions and dynamics at nonzero temperatures has been studied before [30]. The action S is a functional of the (vector) magnetization fields $\vec{m}_{A/B}$ and we may derive the free-energy density from $\mathcal{F} = -\ln \int \mathcal{D}\{m\} \exp(-S(\{m\}))$.

III. LARGE- N APPROACH

To study the phase transitions for the two-sublattice action of Eq. (3) beyond mean-field theory, we generalize the spin symmetry of the model to $O(N)$ ($\vec{m}_{A/B}$ will have N components) and study it through a $1/N$ expansion. Our goal is to investigate general properties, including issues of universality and the order of the phase transitions of the present setting, which contains *two* order parameters possibly competing or coexisting. We note that the well-known large- N approach has proved fruitful for many problems in statistical physics [26,27].

To proceed, we rescale the quartic couplings in $S(\{m\})$ by a factor $1/N$ and in the functional integral over e^{-S} for $\mathcal{F}$, we decompose them in terms of Hubbard-Stratonovich fields $\lambda_{A/B}$ and Δ_I . For details, refer to the Supplemental Material (SM) [44]. To leading order in $1/N$, $i\lambda_{A/B} = \langle m_{A/B}^2 \rangle \equiv m^2$ contribute to the renormalization of the mass (coefficient of

the quadratic term in the action S_2) and $\Delta_I = \langle \vec{m}_A \cdot \vec{m}_B \rangle$ is the Ising order parameter. We carry out our analysis from the ordered side, and set $\vec{m}_{A/B} = (\sqrt{N}\sigma_{A/B}, \vec{\pi}_{A/B})$ with $\sigma_{A/B}$ and $\vec{\pi}_{A/B}$ as the static order and fluctuation fields of sublattices A and B , respectively. To order $O(1/N)$ we can integrate out $\vec{\pi}_{A/B}$, which yields an effective free energy density $\mathcal{F}(\sigma, m^2, \Delta_I)$ that depends parametrically on the damping strength γ , the square of the spin-wave velocity c , the anisotropy parameter v , and the quartic coupling constants $u_I, 2u_1 + u_2$. From SM, Eqs. (S6) and (S7), we have the free-energy density

$$\mathcal{F} = \frac{\Delta_I^2}{u_I} - \frac{(m^2 - r)^2}{2u_1 + u_2} + (m^2 \pm \Delta_I)\sigma^2 + g(m^2, \Delta_I) \quad (6)$$

with

$$g(m^2, \Delta_I) = \frac{1}{2\beta V} \sum_{\vec{q}, l} \ln \{ (D_{0, \vec{q}, l}^{-1} + m^2)^2 - [v(q_x^2 - q_y^2) + \Delta_I]^2 \}, \quad (7)$$

where $D_{0, \vec{q}, l}^{-1} = \chi_{0, \vec{q}, l}^{-1} - r$, containing γ [see Eq. (4)]. The two cases $\sigma_A = \sigma_B = \sigma$ [+ sign in Eq. (6)] and $\sigma_A = -\sigma_B = \sigma$ [- sign] correspond to $\mathbf{Q} = (0, \pi)$ and $(\pi, 0)$ AF orders, respectively.

Then we have variational equations with respect to σ , m^2 , and Δ_I ,

$$\frac{\partial \mathcal{F}}{\partial \sigma} = \frac{\partial \mathcal{F}}{\partial \Delta_I} = \frac{\partial \mathcal{F}}{\partial m^2} = 0, \quad (8)$$

which in turn correspond to [see SM, Eqs. (S9)–(S11)] [44]

$$(m^2 - |\Delta_I|)\sigma = 0, \quad (9)$$

$$\frac{\Delta_I}{u_I} = \frac{m^2 - r}{2u_1 + u_2} - 2\sigma^2 - G_+, \quad (10)$$

$$\frac{\Delta_I}{u_I} = -\frac{m^2 - r}{2u_1 + u_2} + G_-. \quad (11)$$

Here $G_{\pm}$ are given by

$$G_{\pm} = \frac{1}{2\beta V} \sum_{\vec{q}, l} \frac{1}{D_{0, \vec{q}, l}^{-1} \pm v(q_x^2 - q_y^2) + m^2 \pm \Delta_I}. \quad (12)$$

Several limits provide a check on our approach. From Eqs. (10) and (11), setting $u_I = 0$ will lead to $\Delta_I = 0$; this is consistent with the Ising order being driven by the interaction u_I . In the absence of coupling to coherent itinerant fermions, i.e., setting $\gamma^2/|\Delta_I| = 0$ and $w = 0$, we have a nonzero Ising order at zero temperature, which is what happens for the pure J_1 - J_2 model [22,42]. The detailed analysis of these saddle-point equations is in SM, Eqs. (S12)–(S15). It follows that the vanishing of the Ising order implies a vanishing magnetic order. The converse can also be shown explicitly by analyzing Eq. (S15) of the SM, and is numerically confirmed (see below).

IV. NATURE OF THE MAGNETIC AND ISING TRANSITIONS AT ZERO TEMPERATURE

We are now in position to address the concurrent magnetic and Ising transition at $T = 0$. The RG argument we described earlier suggests that there will be a jump of the order parameters across the transition, but the jump will be smaller as the damping parameter γ increases. To see how the damping affects the transition, we first consider the parameter regime where analytical insights can be gained in our large- N approach. When γ is sufficiently large so that $x, y \ll 1$, Eq. (10) simplifies to be [44]

$$A(\eta) = a\eta - \eta \ln \eta = \mu(w) \quad (13)$$

with $\eta = |\Delta_I|/\gamma^2$, and

$$a = -\frac{8\pi^2 \Gamma (a_I - a_0)}{\epsilon + 1/\epsilon} - \ln 2 - 1/2, \\ \mu(w) = \frac{8\pi^2 a_0}{(\epsilon + 1/\epsilon)\Gamma} \frac{r(w)}{c\Lambda_c^2} + \frac{\tan^{-1}(2/\Gamma)}{\Gamma} - \frac{1}{4} \ln \left(1 + \frac{4}{\Gamma^2} \right), \quad (14)$$

where $\Gamma = \frac{\gamma}{c^{1/2}\Lambda_c}$ is the normalized damping rate, while $a_0 = \frac{\Lambda_c c^{3/2}}{2u_1 + u_2}$ and $a_I = \frac{\Lambda_c c^{3/2}}{u_I}$ relate to the normalized interactions. As described in detail in the SM [44], it follows from this equation that the transition is first order, with the jump of the order parameter decreasing as the damping rate Γ is increased. The jump is exponentially suppressed when Γ becomes large.

To study the transition more quantitatively, we have solved the large- N equations numerically. Figure 2 shows how the Ising and magnetic order parameters change when tuning w , where, for comparison, we assume r can still be tuned even at $\gamma = 0$. The jump of the order parameters is seen to be very small, even for the case of a relatively large anisotropy: of ellipticity $\epsilon \approx 0.27$.

As explained in the SM (and verified numerically: compare Fig. 2 and Fig. S2 for a case of extreme anisotropy with $\epsilon \approx 0.025$), the order-parameter jump decreases with decreasing anisotropy (i.e., increasing ellipticity ϵ). Experiments in the iron arsenides observe an ellipticity of $\epsilon \approx 0.7$ [30,31], i.e., an anisotropy weaker than that shown in Fig. 2. We then expect even smaller jumps of the order parameters across the quantum phase transition.

V. EFFECT OF THE THIRD-DIMENSIONAL COUPLING

Iron pnictides have a finite Néel temperature, which results from an interlayer exchange coupling. In order to understand the role of this coupling on the quantum phase transition, we have studied the effective field theory in three-dimensional space. The details of the model are described in the SM [44], and the results for the case with the spin-wave velocity on the third dimension being equal to the in-plane velocity at $v = 0$ are shown in Figs. S3 and S4. The AF and Ising transitions are still concurrent, and become genuinely continuous. Again, this is consistent with the RG considerations: given that the effective dimensionality in this case is $d + z = 5$, the quartic coupling $-u_I$ becomes irrelevant with respect to

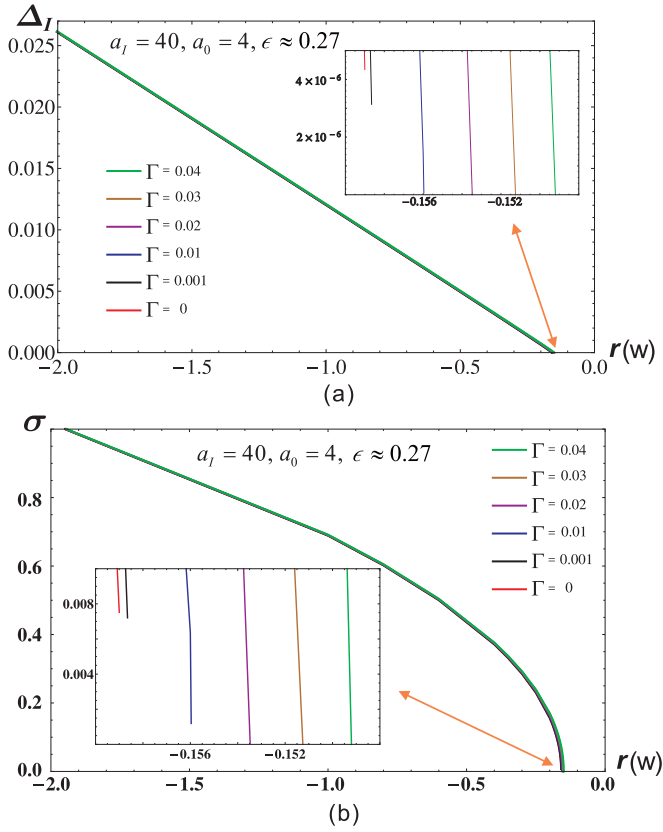


FIG. 2. The evolution of the Ising order parameter Δ_I (a) and the collinear AF order parameter σ (b) vs the control parameter at different damping rates [$\Gamma = \gamma/(c^{1/2}\Lambda_c)$] at a relatively large anisotropy $\epsilon \approx 0.27$, with fixed values of the normalized interactions a_I and a_0 . Each order parameter is normalized so that its value deep in the ordered phase is 1. The transition is very weakly first order, with jumps in the order parameters (insets) that are very small and decrease with damping: already for relatively small damping rate, the jump is on the order of 10^{-6} (and 10^{-3}) for the nematic (and AF) order parameter.

the underlying QCP and will therefore not destabilize the continuous nature of the transition.

In the more general case, with a varying third-dimensional coupling, it is more difficult to solve the large- N equations. However, the RG considerations imply that turning on the interlayer coupling from the purely two-dimensional limit will further suppress the jump in the order parameters.

VI. DISCUSSION

Our results imply that the model for the isoelectronically doped iron pnictides yields quantum phase transitions of the AF and Ising-nematic orders that are concurrent, and essentially second order. In other words, while in two dimensions

the transition is eventually first order, the jumps of the order parameters are small enough to allow a large dynamical range for quantum criticality; the smallness of the jumps is ultimately traced to the marginal nature of the relevant coupling in the effective field theory. In three dimensions, the transition is continuous. Our conclusion reconciles the recent observations of quantum criticality in the normal states of P-doped BaFe_2As_2 [19,20] on the one hand, and the neutron-scattering determination of the weakly first-order nature of the quantum transition [21].

In addition, the extremely small jump of the order parameters across the quantum phase transition in the two-dimensional case is also important for understanding other experimental observations. It implies that quantum criticality occurs over a wide dynamical range, with two-dimensional character. The logarithmic divergence of the effective mass expected from such quantum critical fluctuations [3,13] has received considerable experimental support in the P-doped BaFe_2As_2 . It fits well the P-doping dependence of the effective mass as extracted from the de Haas–van Alphen measurements [45], as well as that of the square root of the T^2 coefficient of the electrical resistivity [19]. Finally, initial dynamical evidence for quantum critical fluctuations in the antiferromagnetic and Ising-nematic channels has come from inelastic neutron scattering measurements in the electron-doped BaFe_2As_2 detwinned by uniaxial strain [46,47]; it would be very instructive to explore similar effects in the P-doped BaFe_2As_2 .

VII. CONCLUSION

We studied zero-temperature magnetic and Ising transitions in a model for isoelectronically tuned iron pnictides using a large- N approach. We demonstrated that the two transitions are concurrent at zero temperature. We also showed that the transition in the presence of damping is essentially continuous; jumps in the order parameters are extremely small, and are further suppressed by an interplane coupling. Our results imply the occurrence of quantum criticality in the isoelectronically doped iron pnictides, and reconcile several seemingly contradictory experimental observations in the P-doped iron arsenides.

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