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Brief Reports

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Comparisons of approximate bases for hydrogen in a magnetic field

Myron L. Zimmerman,* Randall G. Hulet, and Daniel Kleppner
Research Laboratory of Electronics and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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Solutions to the diamagnetic Hamiltonian for Rydberg states of hydrogen are studied in the low-magnetic-field regime where term mixing can be ignored. Several recently proposed approximate bases are compared by calculating the overlap integrals with an accurate numerically generated basis.

I. INTRODUCTION

The problem of hydrogen in a strong magnetic field has received a great deal of attention, but general solutions are still lacking. The investigations of the highly excited states has been stimulated by recent experimental advances.[1,2] Evidence of an approximate symmetry[3] has led to at least a partial theoretical understanding of the origin of this symmetry.[4–8]

In the course of our own study we have investigated a number of analytic basis sets which are approximations to the true zero-field eigenstates of the diamagnetic Hamiltonian when n mixing (n being the principal quantum number) is neglected (i.e., in the limit of low magnetic field). The goal is twofold: First is the hope that identification of approximate eigenstates will give insight into the nature of the symmetry; beyond this is the need to obtain better analytic representations for numerical attacks on problems of current interest. We present here a comparison of the precise numerically generated eigenfunctions with three sets of approximate eigenfunctions: a set identified by Clark,[4] one proposed by Labarthe,[5] and a set which we discovered during our own investigation. We should point out that the work by Clark was devoted to understanding the nature of the general solution, rather than to achieving numerical accuracy, so that the comparison we make below is not in the spirit with which the basis was presented. However, we feel that the comparison can give some insight into the different regions of validity.

II. METHOD

Comparing wave functions by examining expectation values of particular operators gives different weights to different regions in wave-function space. Energy eigenvalues, for instance, can be unreliable for discriminating between bases, since states with the same energy can have completely different wave functions. The most direct comparison involves examining matrix elements of the unitary operator, that is, evaluating their overlap. Therefore we have opted to compare the approximate bases by projecting them onto a precise set of numerically generated eigenstates. The results of this procedure are conveniently represented as a matrix of dot products. The states are arranged in order according to their energies in low magnetic field. An accurate basis will have diagonal elements which are close to unity and off-diagonal elements which are near zero.

III. BASES

The diamagnetic Hamiltonian for spinless, nonrelativistic hydrogen in a uniform magnetic field is (in atomic units)

$$H=\tfrac{1}{2}p^2-\frac{1}{r}+\tfrac{1}{8}\alpha^2B^2r^2\sin^2\theta \quad . \tag{1}$$

We have suppressed the linear Zeeman term. An accurate set of basis states was numerically generated by diagonalizing this Hamiltonian in a spherical basis with a given principal quantum number n.[9] The results are valid in the limit of vanishing magnetic field where n mixing is negligible, that is, fields in which the diamagnetic energy is small compared to the energy separation between levels with different principal quantum numbers. (In the case of electric fields, the analogous basis is the familiar parabolic basis.) We label these states $|n,K,m\rangle_0^{\pm}$, where m is

the magnetic quantum number. The index K has integral values from 0 to $n-|m|-1$; it labels the states within an n,m manifold in order of decreasing energy. Because the Hamiltonian is symmetric under inversion about the origin, parity is a good quantum number. The parity of each eigenstate is denoted by the superscript + or −, and K is even or odd according to whether the parity is even or odd, respectively.

Clark[4] has generated the matrix elements of the Hamiltonian, Eq. (1), in the parabolic basis. Because parabolic states lack inversion symmetry they must be transformed into a parity-conserving basis. Clark defines the following set of definite parity states:

$$|n,K,m\rangle_C^{\pm}=\frac{1}{\sqrt{2}}[\,|n,n_1,n_2,m\rangle\pm(-1)^m|n,n_2,n_1,m\rangle\,]\ . \tag{2}$$

The kets $|n,n_1,n_2,m\rangle$ represent parabolic states.[10] There are only three independent quantum numbers since the parabolic numbers are constrained by $n=n_1+n_2+|m|+1$.

In order to compare the states $|n,K,m\rangle_C^{\pm}$ with our numerical results, it is necessary to transform them to a spherical basis. The transformation from parabolic to spherical representations is[11]

$$|n,n_1,n_2,m\rangle=\sum_{l=|m|}^{n-1}(\kappa,\kappa,\mu,\nu|l,m)|n,l,m\rangle\ , \tag{3}$$

where $\kappa=(n-1)/2$, $\mu=(m+n_1-n_2)/2$, and $\nu=(m-n_1+n_2)/2$. The factors $(j_1,j_2,m_{j1},m_{j2}|j_3,m_{j3})$ are Clebsch-Gordan coefficients. Using this result, we can express the basis $|n,K,m\rangle_C^{\pm}$ in a spherical representation:

$$|n,K,m\rangle_C^{\pm}=\sqrt{2}\sum(\kappa,\kappa,\mu,\nu|l,m)|n,l,m\rangle\ . \tag{4}$$

The sum is over l even or odd, according to the parity.

The second basis we investigate was identified by Labarthe.[5] He approximates the diamagnetic term of the Hamiltonian, Eq. (1), by components of the Runge-Lenz vector $\vec{A}$. Within a given n manifold, $\vec{r}$ and $\vec{A}$ are related by $\vec{r}=-\frac{3}{2}n\vec{A}$. The approximation is made that $r^2\sin^2\theta\rightarrow A_x^2+A_y^2$. The eigenfunctions of this Hamiltonian are

$$|n,\lambda m\rangle_L^{\pm}=\sum_{\mu,\nu}(-1)^{\kappa-\mu}(\kappa,\kappa,\mu,\nu|\lambda,m)|n,n_1,n_2,m\rangle\ , \tag{5}$$

where the approximate quantum number $\lambda=|m|$, $|m|+1,\ldots,n-1$ is associated with the angular momentum $\vec{\Lambda}=(A_x,A_y,L_z)$. The parity of the $|n,\lambda,m\rangle_L^{\pm}$ is $(-1)^{n+1+\lambda+m}$. The values of λ are related to K: $\lambda=n-K-1$ for m even and both parities; $\lambda=n-K-2$ for m odd and even parity; $\lambda=n-K$ for m odd and odd parity. Using Eq. (3) we can rewrite the states $|n,\lambda,m\rangle_L^{\pm}$ in terms of spherical states:

$$|n,\lambda,m\rangle_L^{\pm}=\sum_{l,\mu,\nu}(-1)^{\kappa-\mu}(\kappa,\kappa,\mu,\nu|\lambda,m)\times(\kappa,\kappa,\mu,\nu|l,m)|n,l,m\rangle\ . \tag{6}$$

In the course of our investigations we found that a phase rotation of the basis $|n,K,m\rangle_C^{\pm}$ produced a useful approximate basis, the "M" basis $|n,K,m\rangle_M^{\pm}$, by

$$\begin{aligned}|n,K,m\rangle_M^{+}&=\sqrt{2}\sum_l(-1)^{l/2}(\kappa,\kappa,\mu,\nu|l,m)|n,l,m\rangle\quad(l\text{ even})\ ,\\ |n,K,m\rangle_M^{-}&=\sqrt{2}\sum_l(-1)^{(l+1)/2}(\kappa,\kappa,\mu,\nu|l,m)|n,l,m\rangle\quad(l\text{ odd})\ .\end{aligned} \tag{7}$$

TABLE I. The matrix ${}_C^{+}\langle n,K,m|n,K',m\rangle_0^{+}$ for the basis from Ref. 4 and the numerically generated eigenstates of the diamagnetic Hamiltonian. The states are $n=20$, $m=0$, even parity. See text for explanation of the quantum number K.

${}_C^{+}\langle 20,K,0\vert$ \ $\vert 20,K',0\rangle_0^{+}$	K' 0	2	4	6	8	10	12	14	16	18
0	0.71	0.46	0.35	0.28	−0.22	0.16	−0.10	−0.04	0	0
2	0.57	−0.02	−0.27	−0.40	0.43	−0.40	0.29	0.12	0.02	0
4	0.36	−0.49	−0.44	0.14	−0.19	0.40	−0.42	−0.21	−0.04	0
6	−0.18	0.59	−0.09	−0.45	0.29	0.14	−0.44	−0.32	−0.07	0
8	0.07	−0.41	0.54	0.12	0.42	−0.26	−0.30	−0.42	−0.13	−0.01
10	0.02	−0.18	0.50	−0.48	0.12	0.44	−0.02	0.47	0.23	0.02
12	0	−0.06	0.24	−0.50	−0.50	−0.06	0.37	−0.39	−0.38	−0.06
14	0	0.01	−0.06	0.21	0.43	0.54	0.37	−0.03	−0.56	−0.15
16	0	0	−0.01	0.04	0.13	0.28	0.41	−0.52	0.58	0.37
18	0	0	0	0	−0.01	−0.04	−0.09	0.16	−0.36	0.91

TABLE II. The matrix ${}^{+}_{L}\langle n,\lambda,m\,|\,n,K',m\rangle^{+}_{0}$ for the basis from Ref. 5 and the numerically generated eigenstates of the diamagnetic Hamiltonian. The states are $n=20$, $m=0$, even parity. See text for the relationship between λ and K.

${}^{+}_{L}\langle 20,\lambda,0\|$ \ $\|20,K',0\rangle^{+}_{0}$	K' 2	4	6	8	10	12	14	16	18	
λ 0	−1.0	0.04	0	0	0	0	0	0	0	0
2	0.04	0.99	−0.11	0.01	0	0	0	0	0	0
4	0	−0.11	−0.98	0.18	0.03	0	0	0	0	0
6	0	0.01	0.18	0.95	0.26	0.05	0.01	0	0	0
8	0	0	−0.02	−0.26	0.89	0.35	0.10	−0.03	0.01	0
10	0	0	0	0.05	−0.36	0.79	0.45	−0.20	0.07	−0.01
12	0	0	0	−0.01	0.09	0.47	0.61	−0.56	0.30	−0.07
14	0	0	0	0	−0.02	0.16	−0.58	−0.37	0.66	0.26
16	0	0	0	0	0	−0.04	0.27	0.63	0.38	0.61
18	0	0	0	0	0	0.01	−0.10	−0.34	−0.57	−0.74

This basis is related to the basis $|n,K,m\rangle^{\pm}_{C}$ by a simple phase rotation.

IV. OBSERVATIONS

We have examined manifolds of states with n between 6 and 40, $m=0$ and 1, and both parities. We display in Tables I–III matrices of dot products for Clark's , Labarthe's, and the "M" bases, respectively, for the $n=20$, $m=0$, even-parity manifold. If there were an exact correspondence between the magnetic and the approximate bases, the diagonal matrix elements would be unity and the off-diagonal elements would vanish. A random correlation would give average values of 0.33, since there are ten states in this manifold. The tables reveal that Clark's basis best approximates the highest-K state in this manifold while the other bases better approximate the lower-K states. The basis $|20,\lambda,0\rangle^{+}_{L}$ is especially good for the lowest-K state (which is localized in the x-y plane).

We have investigated more than 20 other manifolds of states with different values of n, m, and parity. In Table IV we summarize the results by displaying the absolute value of the mean, and the maximum and the minimum diagonal elements for the manifolds with $n=6$, 20, and 40, $m=0$ and 1, and both parities. The data of Table IV are generally consistent with our observations of the $n=20$ matrices. The Labarthe and "M" bases provide, on the average, better representations of the spatial behavior of

TABLE III. The matrix ${}^{+}_{M}\langle n,K,m\,|\,n,K',m\rangle^{+}_{0}$ for the "M" basis defined by Eq. (7) and the numerically generated eigenstates of the diamagnetic Hamiltonian. The states are $n=20$, $m=0$, even parity.

${}^{+}_{M}\langle 20,K,0\|$ \ $\|20,K',0\rangle^{+}_{0}$	K' 0	2	4	6	8	10	12	14	16	18
K 0	0.94	0.27	−0.16	0.10	0.07	0.05	0.04	−0.04	0.04	−0.04
2	−0.20	0.93	0.19	−0.16	−0.10	−0.07	−0.05	0.05	−0.05	0.04
4	−0.15	0.11	−0.95	−0.11	−0.16	−0.11	−0.08	0.05	−0.06	0.05
6	0.12	−0.12	0.04	−0.96	0	0.14	0.11	−0.09	0.08	−0.07
8	0.10	−0.09	0.11	0.04	−0.95	−0.13	0.09	−0.12	0.11	−0.09
10	0.09	−0.08	0.08	−0.12	0.14	−0.91	−0.29	−0.01	0.13	−0.13
12	−0.08	0.07	−0.07	0.07	0.14	−0.27	0.79	−0.48	0.07	0.15
14	0.08	−0.06	0.06	−0.07	−0.06	−0.20	0.41	0.63	−0.61	−0.04
16	0.08	−0.06	0.06	−0.06	−0.07	−0.04	−0.30	−0.50	−0.70	0.38
18	0.08	−0.06	0.06	−0.06	−0.06	−0.07	−0.01	0.30	0.31	0.89

TABLE IV. Absolute value of the mean, maximum, and mininum dot products of diagonal elements of the magnetic basis with the three analytic bases, for several manifolds. Note that the $n=6$, $m=1$, even-parity manifold has only two states for which the Labarthe and "M" bases are exact.

			$\lvert n,K,m\rangle_C$			$\lvert n,\lambda,m\rangle_L$			$\lvert n,K,m\rangle_M$		
n	m	Parity	Mean	Max.	Min.	Mean	Max.	Min.	Mean	Max.	Min.
40	0	e	0.27	0.92	0.02	0.59	1.0	0.04	0.63	0.96	0.05
40	0	o	0.28	0.92	0.04	0.55	1.0	0.07	0.44	0.95	0.02
40	1	e	0.24	0.84	0.02	0.58	1.0	0.07	0.63	0.99	0.06
40	1	o	0.28	0.84	0.02	0.56	1.0	0.04	0.54	0.78	0.08
20	0	e	0.44	0.91	0.02	0.77	1.0	0.37	0.87	0.96	0.63
20	0	o	0.35	0.91	0	0.65	1.0	0.10	0.57	0.95	0.14
20	1	e	0.43	0.83	0.20	0.78	1.0	0.36	0.84	0.99	0.43
20	1	o	0.35	0.83	0.11	0.69	1.0	0.14	0.69	0.82	0.55
6	0	e	0.89	0.92	0.83	0.99	1.0		0.96	0.97	0.95
6	0	o	0.62	0.84	0.43	0.95	1.0	0.92	0.88	0.96	0.82
6	1	e	0.89			1.0			1.0		
6	1	o	0.59	0.71	0.40	0.99	1.0	0.98	0.85	0.92	0.80

the exact eigenstates than the Clark basis. It is interesting to note, however, that the functions $\lvert n,K,m,\rangle_C^{\pm}$ provide the best approximation of the highest-K states. Such states which are localized along the z axis are least understood theoretically and experimentally. Thus any approximation method for them is particularly valuable.

The differences in overlap of the bases $\lvert n,\lambda,m\rangle_L^{\pm}$ and $\lvert n,K,m\rangle_M^{\pm}$ with the magnetic basis are not pronounced. In general, $\lvert n,K,m\rangle_L^{\pm}$ provides slightly better approximations of the odd-parity states, while $\lvert n,K,m\rangle_M^{\pm}$ provides a better representation of the even-parity eigenstates. There is little difference in accuracy for different n's or m's; both bases approximate even-parity states better than odd. Consistent with the results of Tables II and III, both bases are most accurate for the highest-energy (i.e., low-K) states.

Herrick[6] has recently obtained a solution to the diamagnetic Hamiltonian which is valid in the limit that n mixing can be neglected. Herrick's results are represented in momentum space, and to our knowledge the spatial wave functions have not yet been obtained. Herrick does make an approximate transformation to spatial wave functions in the limit of low K, however, and our results suggest that both Herrick's and Labarthe's approximate bases give accurate wave functions for the lowest-K state. It is interesting to note that this state, which has the minimum extension along the z axis and the maximum extension in the x-y plane, gives rise to the quasi-Landau resonances. Its energy can be accurately calculated by the WKB approximation and related approximations based on a two-dimensional treatment of the system.[2,12] This observation, however, should be regarded as cautionary: Success in predicting the energy or eigenfunctions for these states provides little insight into the general solution.

The method of direct comparison of approximate bases with numerically exact bases can provide a quick test of other bases yet to be proposed. It is disappointing, though perhaps not unexpected, that none of the bases tested here are accurate over the whole range of states in a manifold. However, for many calculational tasks they can be adequate.

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*Present address: Venturcom, Inc., 139 Main Street, Cambridge, MA 02142.

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