Finite element calculation of low-lying states of hydrogen in a superstrong magnetic field

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Abstract

The finite-element method has been applied to the problem of hydrogen in a superstrong magnetic field. Binding energies have been calculated for the low-lying states ($1s_0, 2s_0, 2p_0$, and $2p_{-1}$) for a range of magnetic field from 10^5 to 10^{12} G. This calculation establishes highly accurate lower bounds for the binding energy of the excited states.

I. Introduction

The finite-element method (FEM) for eigenvalue problems is a numerical algorithm based on a variational principle.[1] Unlike conventional variational schemes, the FEM does not require predetermined, globally defined trial functions. Rather, the continuum is discretized into small elements, and the eigenfunction is approximated locally by a simple polynomial. This flexible approach yields well-converged eigenvalues.

It was recently established that the FEM could be used to provide extremely accurate values for the binding energy of the ground state of hydrogen in a magnetic field.[2] In this paper we extend the analysis to obtain values for the binding energy of the $2s_0$, $2p_0$, and $2p_{-1}$. While such an extension is simple in theory, in practice one is faced with diagonalizing formidably large matrices.

We introduce here two innovations which reduce the computational effort needed to obtain converged results. In the standard implementation of the FEM, the unknown function is approximated piecewise by linear, quadratic, or cubic polynomials. We have found that the use of fifth-degree polynomials results in a marked increase in accuracy and more rapid convergence of the energy. Second, because the wave functions are known to be of even or odd parity with respect to z, the range $(-z_c, z_c)$ can be replaced by the half-range $(0, z_c)$, with the appropriate boundary conditions at $z = 0$. Although two calculations (even and odd z parity) must now be performed for each value of m and B, this is still more efficient than using the full range $(-z_c, z_c)$ and obtaining both even and odd states simultaneously.

In Sec. II details for the finite-element calculation are presented. Results of the calculations are reported in Sec. III. Tables II-IV compare the finite-element results with the upper and lower bounds obtained by

Liu and Starace[3] and the energies obtained by Rosner et al.[4] In all cases, the FEM lower bounds for the binding energy of the excited states are the most accurate to date.

II. FINITE-ELEMENT CALCULATION

The Schrödinger equation for hydrogen in a magnetic field parallel to the z direction is

$$(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}+\frac{2}{\sqrt{r^2+z^2}}-\frac{B^2r^2}{4}-\frac{m^2}{r^2}-Bm+B+2E)\Psi(\mathbf{r},z)=0, \tag{1}$$

where r and z are the cylindrical coordinates, m is the magnetic quantum number, and B is the magnetic field strength; atomic units are used throughout, where $B=1$ corresponds to $2.35\times10^9 G$. The unknown function $\psi(r,z)$ is required to vanish as $r\to\infty$ and $\pm z\to\infty$. For a given value of m and B, Eq. (1) can be solved using finite elements for the complete spectrum of bound states.

The inifinite continuum is truncated by choosing cutoff values for r and z where it is appropriate to set the wave function and its derivatives equal to zero. We used the criterion that the wave function should be about five orders of magnitude smaller near the cutoff values than at its maximum value. In the r direction, the wave function decays asymptotically as $r^{n-1}exp(-r/n)$ in the presence of a weak field; for strong fields $(B>1)$, the wave function decays as a Gaussian, $exp(-Br^2/4)$. In either case, choosing an appropriate value for r_c for a given value of B is quite straightforward.

In the z direction, parallel to the field, the wave function decays asymptotically as $z^{n-1}exp(-|z|/n)$ in the presence of a weak field. The effect of a strong magnetic field $(B>1)$ is subtle and depends on the quantum numbers and z parity of the state. Rosner[4] has shown that the tightly bound states are compressed in the z direction, while some states with higher quantum numbers are slightly elongated in the z direction. In the finite element calculation, the value of z_c was adjusted to accommodate the compression and elongation of the wave function where appropriate.

The truncated space is discretized into rectangular elements. Each element contains nine nodes in a symmetric 3×3 array. (The number of nodes in each element is determined by the degree of the interpolation function.) The accuracy of the finite element calculation depends on the number of elements and the discretization of the grid. There is a trade-off between increasing the number of elements and keeping the CPU time manageable. One of the goals of this calculation has been to show that accuracy of one part in 10^5 or better is obtainable with only 100 elements, without find tuning the grid for each calculation.

Calculations were first carried out (in cylindrical coordinates) for the case $B=0$ to determine the accuracy of the finite element results. As expected, the s states required a higher concentration of nodes in the region between 0 and a_0 since the wave function is strongly peaked near the origin. The p states were extremely insensitive to the location of the nodes. Values for the discretization of the grid are given in Table I. Identical grids were used for all calculations in low magnetic fields.

For fields $B>1$, the wave function in the r direction is approximately Gaussian; the grid was discretized into even intervals along r for both s and p states. In the z direction, the p states are slightly compressed towards the origin, and less extended in space. As z_c was decreased, additional nodes were placed at small values of z, retaining the overall number of elements. For the s states, the situation is slightly more complicated. The $1s$ state is strongly compressed in the z direction, and rapidly falls of to zero. Although the $2s$ state is also compressed near the origin, the exponential tail of the wave function is actually elongated slightly. Hence it is difficult to construct a grid with 100 elements that has an adequate number of nodes near $z=0$ and a sufficiently large value of z_c. This problem becomes more pronounced as the field strength increases. As a result, the value obtained for the binding energy of the $2s$ state at $B=1000$ is slightly less accurate than the other results.

Once the finite element grid is established, the Schrödinger equation is solved in each element by approximating the unknown wave function with a simple polynomial. To facilitate this process, a local coordinate system is introduced into each element N which has the range -1 to 1 in both directions. Given that the size of the element is $h_r^N\times h_s^N$, it is simple to show that the local coordinates x and y are related to their respective global coordinates r and z by

$$\begin{aligned} r &= r_0^{(N)}+h_r^{(N)}(1+x)/2\ , \\ z &= z_0^{(N)}+h_z^{(N)}(1+y)/2 \end{aligned} \tag{2}$$

where r_0^N and z_0^N are the global coordinates at the corner $x = -1, y = -1$ of element N. In terms of the local coordinates, the nine nodes are located at points where x and y have the value 0 and ± 1.

The wave function in element N is approximated by a sum of products of fifth degree Hermite polynomials in x and y,

$$\Psi^N(r,z) = \sum_{i,j=1}^{6} {\psi_k}^N \phi_i(x)\phi_j(y), \;\; k = 6(i-1)+j. \tag{3}$$

These polynomial interpolates have the special property that the 36 expansion coefficients are the values of ψ,$\partial\psi/\partial r$, $\partial\psi/\partial z$, and $\partial^2\psi/\partial r\partial z$ at the nine nodes in the element. Substituting Eq. (3) into Eq. (1) and projecting onto the local basis functions, we obtain

$$H^N \mathbf{\Psi}^N = EU^N \mathbf{\Psi}^N \tag{4}$$

where H^N and U^N are symmetric matrices of order 36 and the vector $\mathbf{\Psi}^N$ contains the unknown expansion coefficients for element N.

All of the integrations (over the element volume) in Eq. (4) can be done exactly with the exception of the Coulomb potential term. In performing the calculation, all integrations were done numerically using 16-point Gauss quadrature, which is exact for polynomials up to degree 31. This may appear to be overkill, since all of the integrals with the exception of the Coulomb term are polynomials of degree 13 or less. However, the binding energy is extremely sensitive to the error in evaluating the Coulomb term, particularly near the origin. Using eight-point Gauss quadrature (which is exact for all integrals but the Coulomb term) may result in an error in the final energy as large as 1 part in 10^5 for the $1s_0$ state, but significantly less for the excited states. Since numerical error in integration can raise or lower the energy, it is critical that this numerical integration error does not lead to false "rigorous bounds." By comparing the FEM energy at $B = 0$ with the exact value, we verified that the error in the energy due to numerical integration of the Coulomb term with 16-point Gauss quadrature is less than 1 part in 10^6 for the state and even less for the excited states.

Once the local matrix equations have been calculated for each element, the elements must be joined in such a way that the wave function and its derivatives are continuous at the boundaries. Such continuity of the wave function is achieved by mapping the local matrix equations for each element onto a single global matrix equation,

$$H\mathbf{\Psi} = EU\mathbf{\Psi}. \tag{5}$$

Equation (5) has the form of a standard generalized eigenvalue problem, where the components of the vector ψ are the values of the wave function and its derivatives at all the nodes in the grid. The global matrices H and U are symmetric and banded.

In order to satisfy the boundary conditions, components of the vector ψ which correspond to $r = r_c$ or $z = z_c$ are set equal to zero. This guarantees that the wave function (and its derivatives) vanish asymptotically. Since we are working on the half-range $(0, z_c)$, boundary conditions must also be imposed at $z = 0$, depending on the z parity of the state. For the odd $z - parity$ state $2p_0$, the wave function (and $\partial\psi/\partial r$)must vanish at $z = 0$; for the even $z - parity$ states, the derivative of the wave function with respect to z (and $\partial^2\psi/\partial z\partial r$) are set equal to zero. These boundary conditions are quite trivial to implement, and result in a further reduction of the size of the global matrices, without destroying symmetry or bandedness.

The reduced global matrices can now be solved by standard algorithms. Subspace iteration,[5] a route developed for finite element calculations, is particularly efficient, exploiting both the symmetry and banded nature of the matrices. It is more efficient than vector iteration, because it does not require orthogonalization of the eigenvectors until the approximate subspace has converged to the subspace spanned by the lowest eigenvectors.

III. RESULTS

Equation (1) was solved for the four low lying states: $m = 0$, even z parity, $1s, 2s; m = 0$, odd z parity, $2p_0$; $m = -1$, even z parity $2p_{-1}$; with values of B corresponding to $10^5 - 10^{12}G$. The energies reported in the tables are rigorous lower bounds to the binding energy, but the last digit is not necessarily converged. Tables

II-V compare the results obtained using finite elements to the calculation of Liu and Starace[3] and Rosner et al.[4] The results of Larsen,[6] Santos and Brandi,[7] and Baldereschi and Bassani[8] are not included in the tables because they are significantly less accurate than the recent works and cover only a small range of magnetic fields. Nevertheless, they are noteworthy calculations because they mark the first attempts to calculate rigorous bounds for the excited states.

Tables II-IV clearly show that the lower bounds obtained via the FEM are far superior to those obtained using a conventional variational approach. (Note that the upper bound obtained by Liu and Starace[3] for the state at $B = 100$ is incorrect.) Although the modified Hartree-Fock approach of Rosner et al.[4] does not guarantee rigorous bounds to the true energy, it is interesting to note that their values agree extremely well with the finite element results for fields up to $B = 1$. For higher fields, the finite element results lie between the upper and lower limits of the Hartree-Fock energy.[4] It is apparent that the results of the Rosner group are accurate as they have claimed. In conclusion, we have shown that the use of piecewise interpolation functions for solving the Schrödinger equation is clearly superior to the standard variational approach when the wave function cannot be readily approximated by simple global basis functions. In other works, the FEM succeeds in cases where standard variational and perturbative calculations fail.

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Table 1: Finite-element discretization.

						$B = 0, 0.0001, 0.001, 0.01, 0.1$						
s	r,z	0	0.25	0.5	1	2	4	8	12	16	20	24
p	r,z	0	1	2	4	8	12	16	20	24	28	32
						$B = 1$						
	r	0	0.5	1	1.5	2	2.5	3	4	5	6	7
s	z	0	0.25	0.5	1	2	4	8	12	16	20	24
p	z	0	1	2	4	8	12	16	20	24	28	32
						$B = 10$						
	r	0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2	2.25	2.5
s	z	0	0.25	0.5	1	2	4	8	12	16	20	24
p	z	0	0.5	1	2	4	8	12	16	20	24	28
						$B = 100$						
	r	0	0.07	0.14	0.21	0.28	0.35	0.42	0.49	0.56	0.63	0.7
s	z	0	0.125	0.25	0.5	1	2	4	8	12	18	24
p	z	0	0.25	0.5	1	2	4	8	12	16	20	24
						$B = 1000$						
	r	0	0.025	0.05	0.075	0.1	0.125	0.15	0.175	0.2	0.225	0.25
s	z	0	0.0625	0.125	0.25	0.5	1	2	4	8	16	24
p	z	0	0.125	0.25	0.5	1	2	4	8	12	16	20

Table 2: Binding energy of the $1s_0$ state.

B	Liu and Starace lower bound upper bound	Rosner *et al.* lower upper	Finite element lower bound
0.0			0.499 999
0.0001			0.500 049
0.001		0.500 500	0.500 499
0.01		0.504 975	0.504 974
0.1	0.5474	0.547 526	0.547 525
1.0	0.8167	0.831 169	0.831 168
	0.8418		
10		1.747 797	1.747 79
100	3.7360	3.789 1	3.789 78
	3.8027	3.790 3	
1000		7.662 1	7.662 36
		7.662 7	

Table 3: Binding enery of the $2s_0$ state.

B	Liu and Starace lower bound upper bound	Rosner *et al.* lower upper	Finite Element lower bound
0.0			0.125 000
0.0001			0.125 050
0.001		0.125 4965	0.125 496
0.01		0.129 6516	0.125 651
0.1	0.0873	0.148 0892	0.148 089
	0.1503		
1.0	0.1357	0.160 4689	0.160 469
	0.1549		
10		0.208 89	0.208 951
		0.208 99	
100	0.2555	0.256 170	0.256 179
	0.2565	0.256 189	
1000		0.295 855	0.295 85
		0.295 859	

Table 4: Binding energy of the $2p_0$ state.

B	Liu and Starace lower bound upper bound	Rosner *et al.* lower upper	Finite element lower bound
0			0.125 0000
0.0001			0.125 0500
0.001		0.125 4985	0.125 4985
0.01		0.129 8504	0.125 8504
0.1		0.162 4104	0.162 4100
1	0.2577	0.260 0066	0.260 0065
	0.2622		
10		0.382 6487	0.382 6498
		0.382 6518	
100	0.4637	0.463 6177	0.463 6177
	0.4638		
1000		0.492 4950	0.492 4950

Table 5: Binding energy of the $2p_{-1}$ state.

B	Liu and Starace lower bound upper bound	Rosner *et al.* lower upper	Finite element lower bound
0.0			0.125 0000
0.0001			0.125 1000
0.001		0.125 9970	0.125 9970
0.01		0.134 7012	0.134 7011
0.1	0.1882	0.200 8457	0.200 8456
	0.2013		
1	0.4524	0.456 5971	0.456 5969
	0.4595		
10		1.1225 422	1.125 422
100		2.634 74	2.634 758
		2.634 80	
1000		5.638 41	5.638 416
		5.638 44	