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Finite-element analysis of hydrogen in superstrong magnetic fields

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The ground state of hydrogen in a magnetic field has been analyzed using the finite-element method. Accurate values for the binding energy have been obtained for fields up to 10^{12} G. Unlike other approaches, the computational effort required to obtain converged results is independent of the strength of the magnetic field. Values obtained for the lower bounds on the binding energy at very high fields are the most accurate to date.

I. INTRODUCTION

There is considerable interest in astrophysics and solid-state physics[1] in obtaining accurate values for the ground-state energy of hydrogenic atoms in superstrong magnetic fields. Many numerical and analytical calculations have been reported in the literature.[2-10] Liu and Starace[6] were among the first to recognize the need for rigorous bounds on the binding energy in order to establish the validity of the approximation techniques applied to this problem. Handy *et al.*[9] improved these bounds using the eigenvalue-moment method. The weak-field-expansion calculation by Le Guillou and Zinn-Justin[8] yielded very accurate energies in the transition region between low and high fields. Rosner *et al.*[10] have calculated the energies of the ground state and many excited states via a modified Hartree-Fock approach. In this paper, the ground state of hydrogen in a magnetic field is analyzed using the finite-element method.

II. FINITE-ELEMENT ANALYSIS

The Schrödinger equation for s-state hydrogenic atoms (spin down) in a uniform magnetic field is

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}+\frac{2Z}{(r^2+z^2)^{1/2}}-\frac{B^2r^2}{4}+B+2E\right]\psi(r,z)=0\ , \quad (1)$$

where $r=(x^2+y^2)^{1/2}$. Atomic units are used throughout, with $B=1$ corresponding to 2.35×10^9 G. Since the energy scales for atomic charge Z, it is sufficient to examine the case $Z=1$. The physical solution to Eq. (1) is subject to the asymptotic boundary conditions,

$$\psi(r\to\infty,z)\to0\ , \quad (2a)$$

$$\psi(r,z\to\pm\infty)\to0\ . \quad (2b)$$

In finite-element analysis, Eq. (1) is solved numerically for the ground-state energy E and corresponding wave function $\psi(r,z)$. The approximate energy E is a rigorous upper bound to the exact energy,[11] within the limits of numerical error.

As in any numerical solution of the Schrödinger equation, the infinite coordinate space spanned by r and z is truncated by choosing cutoff values r_c and $\pm z_c$. In this case, cutoff values were selected by requiring that the wave function be at least 6 orders of magnitude smaller in the region of r_c and $\pm z_c$ than at the origin. The finite two-dimensional space is discretized into rectangular elements. The grid points, which are called nodes, form the corners of the elements. Table I gives the values of the nodes used for each calculation. Although no attempt was made to optimize the grid at each field strength, the choice of node sites reflects the anticipated behavior of the wave function. The concentration of nodes is greatest near the origin where the wave function is sharply peaked. For increasing values of $\pm z$, the element size was gradually increased to allow for an accurate approximation of the slowly decaying wave function. In the r direction, the wave function fell off more sharply, particularly at high fields, and the element size was small even near the asymptotic region. The energy was remarkably stable with respect to minor variation in the number and location of nodes. It is an obvious advantage of this algorithm, that for sufficiently dense grids, tedious fine tuning is not required in order to obtain converged results.

In each element n, the wave function is approximated by a local function ψ^n,

$$\psi^n(r,z)=\sum_{i,j=1}^{4}\psi_{ij}^n\phi_i(r)\phi_j(z)\ , \quad (3)$$

where the unknown expansion coefficients ψ_{ij}^n are the values of ψ, $\partial\psi/\partial r$, $\partial\psi/\partial z$, and $\partial^2\psi/\partial z\partial r$ at the four corner nodes; the basis functions are the locally defined cubic Hermite polynomials.[11,12] Substituting Eq. (3) into Eq. (1) and projecting onto the local basis set, one obtains a simple matrix relation for each element,

$$\underline{H}^n\Psi^n=E\underline{U}^n\Psi^n\ . \quad (4)$$

With the exception of the Coulomb interaction in the Hamiltonian, the matrix elements of $\underline{H}^n$ and $\underline{U}^n$ involve integrations of simple polynomials over the area of each element. However, the presence of the Coulomb term necessitates the use of high-accuracy numerical integration. The bound principle of any variational calculation is not applicable if the cumulative numerical error is

TABLE I. Grid points for finite-element analysis.

$B=0,2\times10^{-4},2\times10^{-2},2\times10^{-1}$										
r nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.8
	1	1.2	1.4	1.8	2.2	2.6	3	4	5	6
	7	8	9	10	11	12	13	14	15	16
$\pm z$ nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.8
	1	1.2	1.4	1.8	2.2	2.6	3	4	5	6
	7	8	9	10	11	12	13	14	15	16
$B=2$										
r nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7
	0.8	0.9	1	1.2	1.4	1.6	1.8	2.0	2.2	2.4
	2.6	2.8	3.0	3.4	3.8	4.2	4.6	5.0	5.4	5.8
$\pm z$ nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.8
	1	1.2	1.4	1.8	2.2	2.6	3	3.5	4	4.5
	5	6	7	8	9	10	11	12	13	14
$B=2\times10^{1}$										
r nodes	0	0.025	0.05	0.075	0.1	0.14	0.18	0.22	0.26	0.3
	0.34	0.4	0.46	0.52	0.58	0.64	0.7	0.76	0.82	0.88
	0.94	1	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8
$\pm z$ nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.8
	1	1.2	1.4	1.8	2.2	2.6	3	3.5	4	4.5
	5	5.5	6	6.5	7	8	9	10	11	12
$B=2\times10^{2},3\times10^{2}$										
r nodes	0	0.005	0.01	0.015	0.02	0.03	0.04	0.05	0.06	0.07
	0.08	0.09	0.1	0.12	0.14	0.16	0.18	0.2	0.22	0.24
	0.26	0.28	0.3	0.34	0.38	0.42	0.46	0.5	0.54	0.58
$\pm z$ nodes	0	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.8
	1	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4
	4.4	4.8	5.2	5.6	6	6.4	6.8	7.2	7.6	8
$B=1\times10^{3}$										
r nodes	0	0.005	0.01	0.015	0.02	0.025	0.03	0.04	0.05	0.06
	0.07	0.08	0.09	0.1	0.11	0.12	0.14	0.16	0.18	0.20
	0.22	0.24	0.26	0.28	0.3	0.32	0.34	0.36	0.38	0.40
$\pm z$ nodes	0	0.025	0.05	0.075	0.1	0.15	0.2	0.25	0.3	0.35
	0.4	0.5	0.6	0.7	0.8	0.9	1	1.2	1.4	1.6
	1.8	2	2.2	2.6	3	3.4	3.8	4.2	4.6	5
$B=2\times10^{3}$										
r nodes	0	0.002	0.004	0.006	0.01	0.15	0.02	0.025	0.03	0.035
	0.04	0.045	0.05	0.055	0.06	0.065	0.07	0.08	0.09	0.1
	0.11	0.12	0.13	0.14	0.15	0.16	0.17	0.18	0.19	0.2
$\pm z$ nodes	0	0.025	0.05	0.075	0.1	0.15	0.2	0.25	0.3	0.35
	0.4	0.5	0.6	0.7	0.8	0.9	1	1.2	1.4	1.6
	1.8	2	2.2	2.6	3	3.4	3.8	4.2	4.6	5

large enough to make a significant (positive or negative) contribution to the energy. All integrations were carried out using 16-point Gauss quadrature, which is exact for arbitrary polynomials of degree 31 or less, and for the Coulomb term, provides an approximation equal to using a polynomial of degree 31.

The local approximate wave functions for each element are joined in such a way as to guarantee the continuity of the global wave function and its derivatives across the element boundaries.[11,12] This is achieved by mapping the local matrices $\underline{H}^n$ and $\underline{U}^n$ for each element onto global matrices $\underline{H}$ and $\underline{U}$; similarly, the local vectors $\boldsymbol{\Psi}^n$ are mapped onto a single global vector $\boldsymbol{\Psi}$. The matrices of the global eigenvalue equation,

$$\underline{H}\boldsymbol{\Psi}=E\underline{U}\boldsymbol{\Psi}\ , \tag{5}$$

are symmetric and banded. The eigenvector components are the value of the wave function and its derivatives at the nodes in the mesh.

The boundary conditions are imposed by requiring that components of $\boldsymbol{\Psi}$ corresponding to a node at $r=r_c$ or $z=\pm z_c$ are set equal to zero, which forces the wave func-

TABLE II. Binding energy of the ground state of hydrogen (a.u.).

B	Liu and Starace (Ref. 6) lower bound upper bound	Handy *et al.* (Ref. 9) lower bound upper bound	Finite element lower bound	Le Guillou and Zinn-Justin (Ref. 8)	Rosner *et al.* (Ref. 10)
0			0.499 999 5		
2×10^{-4}			0.500 099 5		0.500 100
2×10^{-2}			0.509 899 5		0.509 900
2×10^{-1}			0.590 381 0	0.590 381 56	0.590 382
2	0.9832 1.0600	1.022 213 8 1.022 214 2	1.022 213	1.022 213 9	1.022 214
2×10^{1}		2.215 325 2.215 450	2.215 393	2.2153	2.215 398
2×10^{2}	4.6462 4.7387	4.710 4.740	4.727 08	4.725	4.7266
3×10^{2}		5.34 5.39	5.360 71	5.355	5.3603
10^{3}		7.55 7.85	7.662 35	7.64	7.6621
2×10^{3}	9.2754 9.3102		9.304 64	9.27	9.304 48

tion and its derivatives to vanish asymptotically. The generalized eigenvalue equation can be solved by standard techniques. Since the global matrices are still quite large, it is extremely inefficient to calculate all but the lowest eigenvalues and corresponding eigenvectors. Subspace iteration[13] is particularly well suited for solving the eigenvalue equations that result from finite-element analysis. Requiring a tolerance of 10^{-12} on the lowest eigenvalue, convergence was obtained in ten iterations or less. Total CPU time for each run (including subspace iteration) was 6.3 min on an IBM 3090 (with vectorization).

III. RESULTS

Values of the binding energy obtained via the finite-element method are given in Table II and compared with the upper and lower bounds obtained by Liu and Starace[6] and Handy *et al.*;[9] results of Le Guillou and Zinn-Justin[8] and Rosner *et al.*[10] are also included. For fields greater than $B=2$, the lower bounds obtained via finite elements are the best calculated to date.

It appears that the finite-element method is ideal for treating atomic systems subject to strong perturbation, where typical global basis functions are a poor approximation to the Schrödinger wave function.

Calculation of the excited-state energies are currently underway. Only the work of Rosner *et al.*[10] provides anywhere near a complete analysis of the excited states in superstrong fields. Even in their work, there is some difficulty in obtaining converged results at intermediate field strengths when the wave function is in transition from spherical to cylindrical symmetry. Since the success of the finite-element method appears to be independent of the strength of the B field, it is anticipated that the excited-state calculations will provide a complete and accurate picture of the energy spectrum.

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