Relativistic calculations for hydrogenic atoms in strong magnetic fields with Slater-type basis functions

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A relativistic finite-basis-set method is used to calculate the ground-state energy of hydrogenic atoms in strong magnetic fields with B up to 10^{12} G, for several values of the nuclear charge Z. A modified Slater-type basis set with different values of the total angular momentum is used. Both accurate relativistic and nonrelativistic binding energies of hydrogen can be obtained with this basis set, with more than seven significant digits accuracy for magnetic fields in the range $0 \leq B \leq 10^{10}$ G. The relativistic corrections are found to differ substantially from previous calculations based on adiabatic approximations. In the case $Z = 1$, $B = 4.7 \times 10^9$ G, for example, our calculation yields a relativistic correction that is a factor of 7 larger, and of the *opposite sign*, than the previous result. For very strong B and small Z, a basis set that mixes Slater- and Landau-type functions is required to avoid a large expansion in angular momenta.

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I. INTRODUCTION

Hydrogenic atoms in strong magnetic fields have been the subject of intensive study because of the existence of strong magnetic fields on neutron stars [1] ($B \sim 10^{11} - 10^{13}$ G), and on white dwarfs [2] ($B \sim 10^6 - 10^9$ G). The strong-field effects also exist for excitons (they behave like hydrogenic atoms) in condensed matter at laboratory fields [3, 4]. There is a mixture of spherical and cylindrical symmetry in the problem, so that the Dirac or Schrödinger equations are not separable in any coordinate system. The problem has been attacked by many authors [5–11]. Very accurate nonrelativistic numerical results have been obtained recently [6, 8–11]. These include Hartree-Fock calculations [6], variational calculations [8], finite-element analysis [10], and rigorous bounds by the moment method [9] and by Kato's method [11]. (For example, the precision in the calculation of the ground-state energy of hydrogen with a magnetic field $B = 4.7 \times 10^9$ G is about 10^{-9} a.u. [11].) The relativistic corrections are, however, of the order of $(\alpha Z)^2 \approx 10^{-5}$ a.u. for a nuclear charge $Z = 1$, where $\alpha \approx 1/137.036$ is the fine-structure constant. It is therefore necessary to include relativistic corrections in such highly accurate calculations. To our knowledge, there have not been relativistic calculations performed to this level of accuracy yet.

There are two purposes for this paper, one is to get accurate relativistic binding energies for hydrogenic atoms in strong magnetic fields, and the other is to explore the relativistic variational method for one electron in the presence of a highly nonspherically symmetric potential.

Several theorems and techniques have been developed in recent years to overcome the difficulties associated with relativistic variational methods [12]. These difficulties include the problems of variational collapse, spurious roots, and, in the many-electron case, of continuum dissolution. It has been shown [13, 14] that the problems of variational collapse and spurious roots can be avoided by an appropriate choice of basis sets (i.e., by constraining the basis functions using boundary conditions), and a rigorous proof of bounds can even be obtained for the Coulomb case [13]. As a result, finite-basis-set techniques have been very successful for calculations involving the one-electron Dirac-Coulomb Hamiltonian (e.g., relativistic two-photon decay rates [15]) or the many-electron Dirac-Hartree-Fock Hamiltonian (based on screened central potential approximations) [13].

These techniques have not been applied yet to the case of a nonspherically symmetric potential. It is therefore interesting to analyze the behavior of these methods in this case as well as to apply them to a test case, namely the problem of hydrogenic atoms in strong magnetic fields. The potential in this problem is highly nonspherically symmetric and the Dirac equation has different boundary conditions from those in the case of the Coulomb or the Dirac-Hartree-Fock potentials.

Notice that in the nonrelativistic case, a simple scaling relation for the energy

$$E(Z, B) = Z^2 E(1, B/Z^2) \tag{1}$$

follows from the Schrödinger equation [16]. Thus it will suffice to consider only the case $Z = 1$ for the nonrelativistic results. In the case of the Dirac equation, however, there is no such scaling relation and it is then necessary to perform separate calculations for different values of Z.

In this paper we calculate the relativistic ground-state binding energies of hydrogenic atoms in magnetic fields with $0 \leq B \leq 10^{12}$ G for several values of the nuclear charge Z. Our method provides both accurate nonrelativistic and relativistic results, with more than seven significant digits accuracy for magnetic fields in the range $0 \leq B \leq 10^{10}$ G for $Z = 1$, and higher accuracy for larger Z. In the nonrelativistic limit (taking $\alpha \to 0$), our results

agree (to the quoted precision) with the most accurate nonrelativistic calculations available. Our method gives, however, accurate relativistic corrections that differ substantially from previous estimates based on adiabatic approximations [7]. The method has also been checked to be accurate to the precision quoted by means of the virial theorem and the relativistic low B limit where comparison can be made with perturbation results.

II. FINITE-BASIS-SET METHOD

The Dirac equation for an electron in the field of a fixed-point nucleus with charge Ze and in a constant magnetic field $\mathbf{B}$ is

$$H\psi = E\psi,$$

with the Hamiltonian H given by

$$H = H_0 + e\boldsymbol{\alpha}\cdot\mathbf{A}, \tag{2}$$

where

$$H_0 = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 - \frac{Ze^2}{r} \tag{3}$$

is the Hamiltonian for the pure Coulomb field, and $\boldsymbol{\alpha}$ and β are the standard Dirac matrices. The vector potential $\mathbf{A}$ can take the form

$$\mathbf{A} = \tfrac{1}{2}\mathbf{B}\times\mathbf{r}, \tag{4}$$

where $\mathbf{B} = B\hat{z}$. In the following discussion atomic units $m = \hbar = e = 1$ will be used, and by convention, the magnetic field will be given in units of $(e/\hbar)^3 m^2 c \approx 2.35\times 10^9$ G. The Hamiltonian commutes with the z component of the total angular momentum, so that the corresponding quantum number μ is conserved.

Since the total angular momentum j is no longer a conserved quantum number, coupling between sets with different total angular momenta is required for a representation of the energy eigenstates. The variational solutions to the Hamiltonian in Eq. (2) are then obtained with trial functions of the form

$$\Psi^{\mu}_{\rm tr} = \sum_{I}^{2N}\sum_{\kappa}^{K_{\max}} a^{\kappa}_{I}\psi^{\kappa\mu}_{I}, \tag{5}$$

where κ is the Dirac quantum number defined as $\kappa = \pm(j+\frac{1}{2})$ for $l = j\pm\frac{1}{2}$, $K_{\max}$ is the largest absolute value of κ in the expansion, and a^{κ}_{I} are linear variational coefficients. The orthonormal basis vectors

$$\psi^{\kappa\mu}_{I} = \sum_{J=1}^{2N} b^{\kappa}_{IJ}\Phi^{\kappa\mu}_{J} \tag{6}$$

are obtained by the diagonalization of the overlap matrix $<\Phi^{\kappa\mu}_{I}|\Phi^{\kappa\mu}_{J}>$ between basis vectors of the form

$$\Phi^{\kappa\mu}_{n} = \varphi^{\kappa}_{n}\begin{pmatrix} i\chi_{\kappa\mu}/r \\ 0\end{pmatrix},$$

$$\Phi^{\kappa\mu}_{N+n} = \varphi^{\kappa}_{n}\begin{pmatrix} 0 \\ -\chi_{\kappa\mu}/r\end{pmatrix}, \tag{7}$$

where $\chi_{\kappa\mu}$ is a two-component spherical spinor and $n = 1,2,...,N$. Three types of radial functions in the basis set are chosen.

(i)

$$\varphi^{\kappa}_{n} = \frac{1}{\sqrt{N_n}} e^{-\lambda r} r^{\gamma_\kappa + n - 1}, \tag{8a}$$

(ii)

$$\varphi^{\kappa}_{n} = \frac{1}{\sqrt{N_n}} e^{-\lambda r} r^{\gamma_n}, \tag{8b}$$

(iii)

$$\varphi^{\kappa}_{n} = \frac{1}{\sqrt{N_n}} e^{-\lambda r - \beta r^2} r^{\gamma_n}, \tag{8c}$$

where $\gamma_\kappa = [\kappa^2 - (\alpha z)^2]^{1/2}$, $\gamma_n = [n^2 - (\alpha z)^2]^{1/2}$ for the ground state, N_n is a normalization constant, and λ and β are nonlinear variational parameters. The choice of type-(ii) and -(iii) basis functions are based on consideration of symmetry in the basis set, and in these cases $K_{\max}$ is taken to be N. It turns out that type-(ii) basis functions are more efficient than type-(i) and type-(iii); the disadvantage of type-(iii) basis functions is that the optimization with two nonlinear parameters takes much more computer time. [In the following discussion, we will consider, for simplicity, only the case with type-(ii) basis functions given by Eq. (8b) with $K_{\max} = N$.] The radial functions are similar to those for a pure Coulomb potential; the effect of the magnetic field is accounted for by the couplings between different values of κ.

The matrix elements for H_0 in the basis set of Eq. (7) can be evaluated analytically [12] and they are diagonal with respect to κ. The matrix elements of $\boldsymbol{\alpha}\cdot\mathbf{A}$ can be written as

$$<\Phi^{\kappa\mu}_{n}|\boldsymbol{\alpha}\cdot\mathbf{A}|\Phi^{\kappa'\mu}_{N+n'}> = \frac{B}{2} r^{\kappa\kappa'}_{nn'} A_{\kappa,\kappa'}, \tag{9}$$

where

$$r^{\kappa\kappa'}_{nn'} = \int_0^\infty r\phi^{\kappa}_{n}(r)\phi^{\kappa'}_{n'}(r)dr \tag{10}$$

is a radial matrix element and

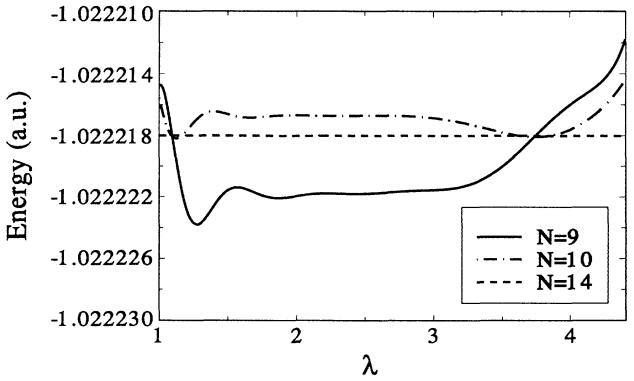

FIG. 1. The variational energy of the ground state of hydrogen for $B = 4.7\times 10^9$ G plotted against nonlinear variational parameter λ.

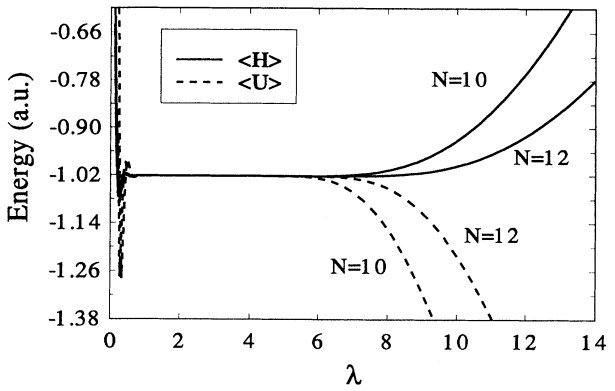

FIG. 2. The variational energies $< H >$ and $< U >$ defined in Eq. (14) plotted against the nonlinear variational parameter λ for the ground state of hydrogen with $B = 4.7 \times 10^9$ G.

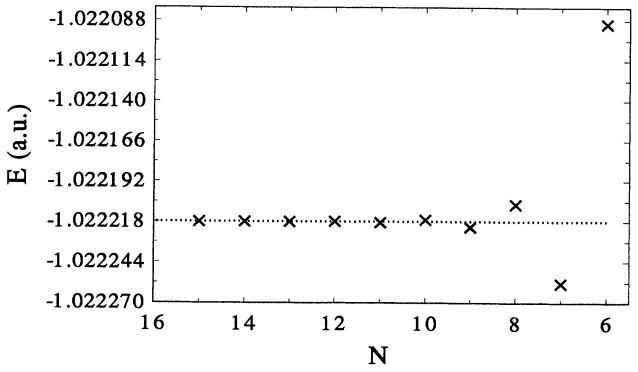

FIG. 3. The ground-state variational energy for $Z = 1$ and $B = 4.7 \times 10^9$ G as a function of the size $2N^2$ of the basis set.

$$A_{\kappa,\kappa'} = -i \int d\Omega < \chi_{\kappa\mu} | (\boldsymbol{\sigma} \times \hat{\mathbf{r}})_z | \chi_{-\kappa'\mu} > \qquad (11)$$

is an angular integral involving the two-component spherical spinors $\chi_{\kappa\mu}$. Similar to the calculations of the general Paschen-Back effect from the Dirac equation [17, 18], the nonvanishing matrix elements can be calculated (after some angular momentum algebra) to be

$$A_{\kappa,\kappa} = \frac{4\kappa\mu}{4\kappa^2 - 1}$$

and

$$A_{\kappa,-\hat{\kappa}(|\kappa|+1)} = \hat{\kappa} \frac{[(|\kappa| + \frac{1}{2})^2 - \mu^2]^{1/2}}{2|\kappa| + 1}, \qquad (12)$$

with $\hat{\kappa} = \kappa/|\kappa|$. Since the operator $\boldsymbol{\alpha} \cdot \mathbf{A}$ transforms under rotations like a first-rank tensor, it can connect states with angular momentum j' and j satisfying the triangle relation $j' = j,\ j \pm 1$. The matrix elements of the Hamiltonian [Eq. (2)] in the orthonormal basis vectors are then obtained by the transformation given by Eq. (6).

Since we are looking for the stationary states, in a way similar to the work [13] for the pure Coulomb and the Dirac-Hartree-Fock potentials, we diagonalize the Hamiltonian in the orthonormal basis vectors to obtain the variational energies and eigenvectors for certain values of N, λ.

If the basis set is complete when $N \to \infty$, then in the vicinity of the true energy, the change of the variational energy $E(\lambda)$ with the nonlinear parameter λ should be minimum and decrease as the size of the basis set increases. Thus a smoother range of $E(\lambda)$ against λ should be achieved as the power N is increased. We will use this property to determine the energy as given by the most stable region of $E(\lambda)$ in the case where the basis set cannot give an upper bound to the energy.

Since the variational energy may not converge to the exact one if the basis set is not complete as $N \to \infty$, the virial theorem is used to provide an additional check. It follows from the Dirac Hamiltonian that [18]

$$< H > = < \beta > mc^2 + 2e < \boldsymbol{\alpha} \cdot \mathbf{A} >, \qquad (13)$$

TABLE I. Relativistic (E) and nonrelativistic ($E_{\rm NR}$) binding energies (divided by Z^2, in atomic units) of hydrogenic atoms in a strong magnetic field B (in units of 2.35×10^9 G). For $Z \neq 1$, $E_{\rm NR}$ is obtained by the scaling relation of Eq. (1). The relativistic correction is given by $\Delta\epsilon = (E - E_{\rm NR})/E_{\rm NR}$.

Z	B	E [a]	$\Delta\epsilon$ [a]	$E_{\rm NR}$ [b]	$E_{\rm NR}$ [c]	E [d]	$\Delta\epsilon$ [d]
1	0.1			0.547 526 480 401 1		0.547 532 408	1.08×10^{-5}
1	1			0.831 168 897	0.831 14	0.831 173 226	5.2×6^{-6}
1	2	0.899 777 12	-5.7×10^{-7}	1.022 213 91	1.022 214	1.022 218 0	4.0×10^{-6}
1	3			1.164 533	1.164 39	1.164 537	3.4×10^{-6}
1	10			1.747 8	1.747 22	1.747 8	
5	25			0.831 168 897	0.831 14	0.831 277 196	1.303×10^{-4}
5	50			1.022 213 91	1.022 214	1.022 317 0	1.008×10^{-4}
5	250			1.747 8	1.747 22	1.747 9	6×10^{-5}
20	800			1.022 213 91	1.022 214	1.023 879 5	1.63×10^{-3}

[a] Reference [7].
[b] The binding energies are obtained by the lower and upper bounds in Ref. [11].
[c] Reference [8].
[d] Present results.

where $< >$ denotes the expectation value for a stationary state. It is then necessary, but not sufficient, for a variational state to be a good approximation of the energy eigenstate, that the difference $| < H > - < U > |$, where

$$< U >=< \beta > mc^2 + 2e < \alpha \cdot \mathbf{A} >, \quad (14)$$

should approach zero when N approaches infinity.

Other checks are made by taking the nonrelativistic limit ($\alpha \rightarrow 0$) and comparing with other accurate nonrelativistic calculations, and by taking the relativistic low B limit where comparison can be made with perturbation results.

III. RESULTS AND DISCUSSIONS

We have diagonalized the Hamiltonian in Eq. (2) to obtain the linear coefficients in Eq. (5) and energy eigenvalues for different values of N, and the nonlinear parameters λ in the basis sets of Eq. (7). This procedure leads to N^2 (more generally $NK_{\max}$) positive energies and N^2 negative energies for each value of the nonlinear parameter in the basis set. The dependence of the ground-state energy of hydrogen on λ with basis functions of the form Eq. (8b) is given in Fig. 1. The diagram shows that the energy dependence on λ gets smoother as N increases. However, there is no upper bound on the energy. We determine the optimal variational energy for each N by searching for the minimum absolute value of the first and second derivatives of $E(\lambda)$ with respect to λ [i.e., the most stable region of $E(\lambda)$] as well as the minimum absolute value of the difference between $< H >$ and $< U >$ from the virial theorem in Eq. (13). The energy determined in this way converges to the same value as N increases, when any of the three types of radial functions of Eq. (8) are used in the basis set. The dependence of $< H >$ and $< U >$ on λ for the ground state of hydrogen is shown in Fig. 2. The difference between $< H >$ and $< U >$ decreases as N increases and tends to zero as $N \rightarrow \infty$. The convergence of the variational energy with N for $B = 4.7 \times 10^{10}$ G using an arbitrary fixed $\lambda = 2$ [close to the most stable region of $E(\lambda)$] is shown in Fig. 3. The convergence is achieved from both sides of the true energy, so that no bound is preserved in the calculations.

A comparison with previous results for hydrogenic atoms is made in Table I. For $B < 10^{10}$ G, our calculated relativistic ground-state energies of hydrogen are deeper than the corresponding nonrelativistic energies, while previous relativistic calculation based on the adiabatic approximation [7] gave a different sign and a different magnitude for the relativistic correction for $B = 4.7 \times 10^9$ G. Our results in the nonrelativistic limit agree, to the accuracy we achieved (eight significant digits for $B \leq 5 \times 10^9$ G and $Z = 1$), with the most accurate nonrelativistic calculations, and the accuracy is good enough to obtain the relativistic corrections in this case. The adiabatic results, on the other hand, agree only to two significant digits in the nonrelativistic limit with the most accurate nonrelativistic calculations. Our variational results are also checked by comparing with the relativistic perturbation results (relativistic general Paschen-Back effect) of hydrogen for low and intermediate magnetic field B. Table II shows that they agree very well for the range of B where the perturbation method is valid.

TABLE II. Comparison of the relativistic binding energy E_{var} of hydrogen, calculated in the present paper, with relativistic hydrogenic perturbation results $E^{\text{P}}_{\text{rel}}$ for low and intermediate magnetic field B (in units of 2.35×10^9 G).

B	$E^{\text{P}}_{\text{rel}}$	E_{var}
0	0.500 006 656 6	0.500 006 656 6
10^{-7}	0.500 006 706 6	0.500 006 706 6
10^{-5}	0.500 011 656 5	0.500 011 656 5
10^{-3}	0.500 506 647 7	0.500 506 398
10^{-1}	0.550 005 769 1	0.547 532 408
1	0.999 997 781 3	0.831 173 226
2	1.499 988 905 9	1.022 218 0
3	1.999 980 030 6	1.164 537

Our calculations indicate the necessity to include relativistic corrections given the current numerical accuracy of the nonrelativistic calculations. The previous relativistic calculations based on adiabatic approximations, however, are not accurate enough for intermediate strong magnetic fields and low Z atoms or for very strong magnetic fields and high Z atoms.

Besides the lack of bounds on the energy, the basis set used above is not very efficient for very strong B and small Z. For $B \geq 10^{10}$ G and $Z = 1$, the calculations with the present basis sets fail to converge to the required accuracy to obtain the relativistic corrections. Since the orbitals will be more similar to the Landau orbitals than the Coulomb orbitals, it is necessary to include many couplings of κ in order to get good convergence. A better basis set would be one that is exact in both limiting cases $B = 0$ and $B \rightarrow \infty$. These generalizations will be presented in a second paper.

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