

Generalized Relativistic Variational Calculations for Hydrogenic Atoms in Arbitrary Magnetic Fields

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A relativistic basis set composed of products of Slater- and Landau-type functions is introduced and applied to the accurate calculation of the ground-state energy of an electron in a static Coulomb field and a magnetic field of arbitrary strength. The relativistic corrections for strong magnetic fields differ from previous relativistic adiabatic approximations. It is found that *the sign of the relativistic correction changes* from negative to positive; for hydrogen this occurs near $B=10^{11}$ G. The accuracy of the nonrelativistic-limit results matches or exceeds that of previous nonrelativistic calculations.

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Hydrogenic atoms in strong magnetic fields have been studied extensively in nonrelativistic quantum mechanics [1-8] because of considerable interest in astrophysics [9], in solid-state physics [10], and in chaotic studies [11]. Very accurate nonrelativistic numerical results have been obtained recently [3-8] (with a precision better than 10^{-6} a.u. for the binding energy of hydrogen for $B \lesssim 10^{11}$ G). It is therefore necessary to include relativistic corrections [of the order of $(\alpha Z)^2 \approx 10^{-5}$ a.u. for $Z=1$] in such highly accurate calculations. Few relativistic studies of the problem have been performed [12-14], and different approximations have yielded quite different results. The relativistic corrections given by adiabatic approximations [14], for example, are much smaller than those given by a first-order approximation of the Foldy-Wouthuysen transformation to the Dirac equation [12]. Recently, a relativistic finite-basis-set method has been used to calculate the binding energies of hydrogenic atoms to a precision of 10^{-7} a.u. for $B \lesssim 10^{10}$ G [15]. The results are different, both in sign and in magnitude, from previous calculations using adiabatic approximations [14]. For $B \gtrsim 10^{10}$ G, however, the method [15] based on the coupling of Slater-type basis functions with different angular momenta fails to converge to a high enough accuracy to calculate the relativistic corrections. In this paper we generalize the basis set to incorporate Slater- and Landau-type functions so that it contains the exact solutions to the Dirac equation at both $B=0$ and $Z=0$ limits. This enables us to calculate both relativistic and nonrelativistic binding energies with higher accuracy

for arbitrary magnetic fields.

The Dirac Hamiltonian for an electron around a fixed nucleus with charge Ze and in a constant magnetic field \mathbf{B} is

$$H = c\boldsymbol{\alpha} \cdot \left[\mathbf{p} + \frac{e}{c}\mathbf{A} \right] + \beta mc^2 - \frac{Ze^2}{r}, \quad (1)$$

where $\boldsymbol{\alpha}$ and β are the standard Dirac matrices. The vector potential \mathbf{A} can take the form

$$\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r},$$

where $\mathbf{B} = B\hat{z}$. The Hamiltonian commutes with the z component of the total angular momentum and with the parity operator, so that the corresponding quantum numbers μ and π are conserved. In the following discussion atomic units $m = \hbar = e = 1$ will be used. The magnetic field will be given, by convention [2], in units of $(e/\hbar)^3 m^2 c \approx 2.35 \times 10^9$ G. In these units, $B=1$ corresponds to $\hbar\omega_c/(e^2/a_0) = 1$, where a_0 is the Bohr radius and $\omega_c = eB/mc$ is the cyclotron frequency of the electron. When $B \geq 1$, the transverse energy ($\hbar\omega_c$) is bigger than 1 a.u., and in this case, the magnetic field will be called intense.

For intense magnetic fields, the excitation energies of the Landau levels are bigger than those of the Coulomb potential, so that the major contributions to the ground-state energy are the ground state of the Landau levels and many low-lying Coulomb states. Thus, we propose to obtain the variational solutions to the Hamiltonian in Eq. (1) with a basis set of the form

$$\Phi_{n_l k}^{(k)} = r^{\gamma-1} r^n e^{-\lambda r - \beta(r \sin \theta)^2} (\cos \theta)^{l_k} (\sin \theta)^{|\mu - s_k|} e^{i(\mu - s_k)\phi} \chi_k, \quad n=0, 1, \dots, N_r, \quad (2)$$

where χ_k are the four-component spin functions with spin projection s_k . For the ground state (with $\pi=1$, $\mu = -\frac{1}{2}$), the powers l_k for the angular dependence are given by

$$l_1 = 1, 3, \dots, 2N_\theta - 1, \quad l_2 = 0, 2, \dots, 2N_\theta,$$

$$l_3 = 0, 2, \dots, 2N_\theta, \quad l_4 = 1, 3, \dots, 2N_\theta + 1.$$

Note that when $N_\theta=0$, there will be no vectors corre-

sponding to $k=1$; the total number of vectors will be $M = (4N_\theta + 3)(N_r + 1)$. These choices are based on the consideration that the basis set should contain the exact solutions at both the Landau and Coulomb limits. For example, when $B=0$, the spherical harmonics and the Clebsch-Gordon coefficients are produced automatically by the diagonalization procedure. The parameter γ is determined by the boundary condition as $r \rightarrow 0$ to be

$[1 - (\alpha Z)^2]^{1/2}$ for the ground state; and λ and β are nonlinear variational parameters.

The variational procedure is similar to that for the pure Coulomb and the Dirac-Hartree-Fock potentials [16]. The basis set is first orthonormalized by the diagonalization of the overlap matrix $\langle \Phi_{n'l_k}^{(k)} | \Phi_{n'l_k}^{(k)} \rangle$, which yields M orthonormal basis vectors of the form

$$\psi_i^{(k)} = \sum_{n'l_k} b_{in'l_k}^{(k)} \Phi_{n'l_k}^{(k)}. \quad (3)$$

The variational solutions to the Hamiltonian in Eq. (1) are then obtained with trial functions of the form

$$\Psi_{\text{tr}}^i = \sum_{jk} a_{ij}^{(k)} \psi_j^{(k)}. \quad (4)$$

Since we are looking for stationary states, we diagonalize the Hamiltonian in the orthonormal basis vectors to determine the linear variational parameters $a_{ij}^{(k)}$ for certain values of N_r , N_θ , λ , and β . This procedure yields $N_+ + N_- = M$ variational eigenvalues and eigenstates, where N_+ and N_- are the number of basis vectors for positive-energy and negative-energy states, respectively. If the basis set is complete, then in the vicinity of the true energy, the change of the variational eigenvalue $E(\lambda, \beta)$ with the nonlinear parameters λ and β should decrease as the size of the basis set increases. Thus a smoother range of $E(\lambda, \beta)$ against λ and β should be achieved as the powers N_r and N_θ are increased. We therefore determine the optimal value of the energy by searching for the most stable range of the ground-state energy $E(\lambda, \beta)$ against λ and β for certain values of N_r and N_θ . The results obtained in this way have converged to more than seven-significant-digit accuracy for $0 < B \leq 5000$ ($0 < B \leq 10^{13}$ G) with less than 200 basis vectors. Note, however, that there is no upper bound on the energy globally: The convergence can be achieved from both sides of the true energy. We have confirmed that our basis set is approaching completeness as the size of the basis set is increased by means of sum rules [17] and the virial theorem [15,18]. The detailed discussions of the results will be presented in another paper.

A comparison with previous results for hydrogenic atoms is made in Table I. Our relativistic results differ from the previous relativistic calculations which were performed using adiabatic approximations [14]. In the nonrelativistic limit, however, unlike the adiabatic calculations, our results agree with the most accurate nonrelativistic calculations available. Moreover, for $B \geq 20$, our results converge to more significant digits than previous nonrelativistic calculations. Note that, as shown in Table I, the previous nonrelativistic calculations do not agree to the quoted precision for $B \geq 200$.

The nonrelativistic limit for strong B is obtained by taking $\alpha \rightarrow 0$ in the Dirac Hamiltonian but keeping αB fixed. In the framework of the Schrödinger equation, the nonrelativistic binding energies with $Z \neq 1$ can be calcu-

lated by a simple scaling relation [19] for the energy

$$E(Z, B) = Z^2 E(1, B/Z^2). \quad (5)$$

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 .

The dependence of the relativistic corrections on B for the ground state of hydrogen is plotted in Fig. 1. It shows that the relativistic correction changes sign near $B = 40$ ($\approx 10^{11}$ G); thus the absolute value of the correction is decreasing with B for $B \lesssim 40$ and is increasing with B when $B \gtrsim 40$.

The 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 . Using these perturbation methods, the relative relativistic correction can be written as [20,21]

$$\delta E = \frac{E - E_{\text{nr}}}{|E_{\text{nr}}|} = -\frac{1}{2} (\alpha Z)^2 \frac{Z^2/4 - B/3}{Z^2/2 + B/2}, \quad (6)$$

where E and E_{nr} are the relativistic and nonrelativistic ground-state energy, respectively. Figure 1 shows that our variational results agree very well with the perturbation results for the range of B where the perturbation method is valid. Note that although the perturbation results for E and E_{nr} are accurate to 10^{-5} a.u. only for $B \lesssim 10^{-2}$, their difference yields correct results up to $B \lesssim 10^{-1}$.

We have also confirmed our previous relativistic results [15] which were obtained by Slater-type basis functions for $B < 20$. The present method, however, yields higher precision with fewer basis vectors for the full range of values of B . The method provides both accurate nonrelativistic and relativistic results, with an accuracy of more than eight significant digits for magnetic fields in the range $0 \leq B \leq 500$ ($0 < B \lesssim 10^{12}$ G) for $Z = 1$, and higher accuracy for larger Z .

Our calculations indicate the necessity to include relativistic corrections given the current numerical accuracy of the nonrelativistic calculations. The adiabatic approximations used in Ref. [14] are not accurate enough to get relativistic corrections for $0 < B \lesssim 2000$ for hydrogenic atoms, given that the error introduced by the adiabatic approximations can be bigger or of the same order as the relativistic corrections.

In conclusion, we have provided a very efficient and precise technique to calculate the binding energies of a Dirac electron in the presence of a static Coulomb potential and an arbitrary magnetic field. However, for a complete description of a hydrogenic atom to the level of accuracy presented, it is also necessary to include other small effects such as the finite mass and size of the nucleus, the interaction between the magnetic moments of the electron and nucleus, the anomalous magnetic moment of the electron, and other radiative corrections. The

TABLE I. Relativistic ($-E$) and nonrelativistic ($-E_{nr}$) 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_{nr} in column 4 is obtained by the scaling relation of Eq. (5), while $E_{nr}^{(g)}$ is obtained in each case by taking the nonrelativistic limit of the Dirac equation. The relativistic correction is given by $\delta E = (E - E_{nr})/|E_{nr}|$. The numbers in column 4 give the previous most accurate nonrelativistic results.

Z	B	$\delta E^{(a)}$	$-E_{nr}$	$-E_{nr}^{(g)}$	$-E^{(g)}$	$\delta E^{(g)}$
1	0.1		$\left\{ \begin{array}{l} 0.54752648040109 \\ 0.54752648040110 \end{array} \right\}^b$	0.5475264804011	0.5475324083429	-1.08×10^{-5}
1	1		$\left\{ \begin{array}{l} 0.8311688966 \\ 0.8311688973 \end{array} \right\}^b$	0.831168897	0.831173226	-5.21×10^{-6}
1	2	0.57×10^{-6}	$\left\{ \begin{array}{l} 1.022213908 \\ 1.022213910 \end{array} \right\}^b$	1.022213908	1.022218029	-4.03×10^{-6}
1	3		$\left\{ \begin{array}{l} 1.16453299 \\ 1.16453307 \end{array} \right\}^b$	1.164532989	1.164537038	-3.48×10^{-6}
1	20	0.23×10^{-5}	$\left\{ \begin{array}{l} 2.215396 \\ 2.215913 \end{array} \right\}^b$ 2.215398 ^c 2.215393 ^e	2.2153985	2.21540091	-1.15×10^{-6}
1	200	0.77×10^{-5}	4.7266 ^c 4.727134 ^d 4.72708 ^e	4.7271451	4.7271233	4.61×10^{-6}
1	500			6.2570877	6.2570326	8.80×10^{-6}
1	2000	0.215×10^{-4}	$\left\{ \begin{array}{l} 9.2754 \\ 9.3102 \end{array} \right\}^f$ 9.30448 ^c 9.30464 ^e	9.304765	9.304593	1.85×10^{-5}
1	5000			11.87341	11.87308	2.78×10^{-5}
5	25		$\left\{ \begin{array}{l} 0.8311688966 \\ 0.8311688973 \end{array} \right\}^b$	0.831168897	0.831277196	-1.303×10^{-4}
5	50		$\left\{ \begin{array}{l} 1.022213908 \\ 1.022213910 \end{array} \right\}^b$	1.022213908	1.022317006	-1.008×10^{-4}
20	800		$\left\{ \begin{array}{l} 1.022213908 \\ 1.022213910 \end{array} \right\}^b$	1.022213908	1.023879534	-1.629×10^{-3}

^aReference [14].

^bLower and upper bounds in Ref. [8].

^cReference [3].

^dReference [4].

^eReference [7].

^fLower and upper bounds in Ref. [5].

^gPresent results.

finite-nuclear-size correction can be calculated exactly in the context of the method presented here by replacing the Coulomb potential by an appropriate finite-nuclear-size potential. This correction is of the order of $\langle r_n^2 \rangle / \langle r_e^2 \rangle \sim 10^{-10}$ for hydrogen with $B=0$, where $\langle r_n^2 \rangle$ and $\langle r_e^2 \rangle$ are the mean-square radius of the nuclear charge distribution and electron orbital, respectively [21]. Even for an intense magnetic field such as $B \approx 10^{12}$ G, the Landau

radius is reduced by a factor of 15, so that the correction is of the order of 1 part in 10^8 . The case of large Z and B is very interesting due to the large overlap between the electron wave function and the finite nucleus. The finite-nuclear-mass correction to the energy can be obtained to lowest order by introducing the reduced mass in the non-relativistic Hamiltonian. Higher-order corrections such as QED corrections can be calculated perturbatively us-

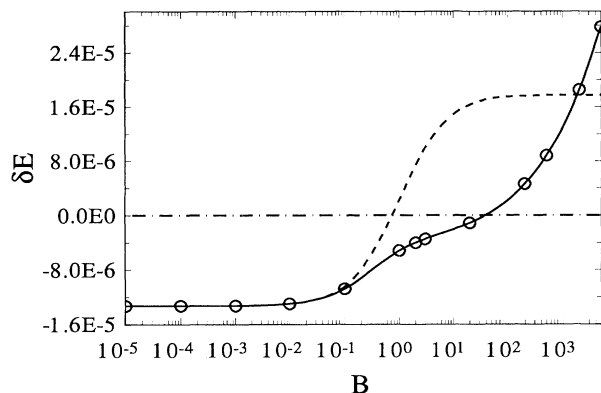


FIG. 1. Relative relativistic correction $\delta E = (E - E_{nr})/|E_{nr}|$ for the ground-state energy of hydrogen as a function of the magnetic field B (in units of 2.35×10^9 G). The results of the present paper are given by open circles and plotted as a solid line. The perturbation result given by Eq. (6), valid for the relativistic correction only for $B \lesssim 10^{-1}$, is plotted as a dashed line.

ing the optimized variational wave functions obtained in the present work. This work is presently in progress.

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