Energy levels of a hydrogen atom in a magnetic field

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A finite-basis-set variational method with the two-limit basis functions proposed to calculate the states $1s_0$ and $2p_{-1}$ by Chen and Goldman [Phys. Rev. A **45**, 1722 (1992)] is used to calculate the energy levels of a hydrogen atom in a magnetic field. The accurate energy eigenvalues for the eigenstates with major quantum numbers less than or equal to 3 are obtained. The finite-basis-set method with the two-limit basis functions can be used to obtain accurate results not only for the ground state but also for any excited state.

The discovery of strong magnetic fields of intensity up to 10^9 T in astrophysics has attracted many investigators to the problem of a hydrogen atom in an intense magnetic field. The problem becomes even more interesting when one finds its applications in solid-state physics. Electrons in a semiconductor medium have an effective mass lower than that of a free electron and are subjected to a weaker Coulomb field because of the static dielectric constant of the medium. These two factors enhance the effect of a magnetic field on the electrons of the shallow donors in a semiconductor medium, so that the shallow donors in a magnetic field of moderate intensity can be considered as a hydrogen atom in an intense magnetic field. Different methods have been applied to the problem, including the variational method [1–4], Hartree-Fock method [5], finite-element method [6], Kato's method [7], and eigenvalue-moment method [8].

Recently, Chen and Goldman [2] calculated the energy levels of the eigenstates $1s_0$ and $2p_{-1}$ of a hydrogen atom in a magnetic field. Considering the limit of zero magnetic field and the limit of zero Coulomb field, they proposed a new type of basis functions for calculation and obtained results with an accuracy better than 1 part in 10^{16} for $B \leq 10^4$ T and better than 1 part in 10^7 for $B \sim 10^9$ T. The high accuracy of their results for the states $1s_0$ and $2p_{-1}$ raises the question whether the basis functions they proposed can be used to find accurate results for other states, such as the state $3d_0$, which has the same magnetic quantum number and the same parity as that of the state $1s_0$. In this paper, we use their type of basis functions to calculate all the states of a hydrogen atom with major quantum numbers less than or equal to 3. Accurate results are obtained for the excited states with 20 basis functions.

If the effective rydberg $R_0 = m^* e^4 / 2\epsilon^2 \hbar^2$ is the energy unit, the effective Bohr radius $a_B = \epsilon \hbar^2 / m^* e^2$ is the length unit, and the vector potential $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ with $\mathbf{B} = B\hat{\mathbf{z}}$, the Hamiltonian of the problem can be written as

$$H = \frac{1}{2m^*}\left[-i\hbar\nabla - \frac{e\mathbf{A}}{c}\right]^2 - \frac{e^2}{\epsilon r}$$

$$= -\nabla^2 - \frac{2}{r} - i\gamma\frac{\partial}{\partial\phi} + \tfrac{1}{4}\gamma^2\rho^2 , \quad (1)$$

where $\gamma = \epsilon^2\hbar^3 B / e^3(m^*)^2 c$ and $\rho^2 = x^2 + y^2$. For a hydrogen atom, $\gamma = 4.25 \times 10^{-6}B$, $R_0 = 13.6$ eV, where B has Tesla as the unit. For a hydrogenic impurity in GaAs, $\gamma = 0.158B$, $R_0 = 5.48$ meV.

In the finite-basis-set variational method, the wave function is expanded in a set of basis functions as follows:

$$\Psi = \sum_{nl} c_{nl}\psi_{nl} . \quad (2)$$

The basis functions Chen and Goldman [2] proposed are

$$\psi_{nl} = e^{-a\rho^2 - br + im\phi}r^n(\cos\theta)^l(\sin\theta)^{|m|} ,$$

$$n = 0, 1, 2, \ldots, N_r . \quad (3)$$

For even-parity states, l takes even non-negative integers up to $2N_\theta$. For odd-parity states, l takes odd positive integers up to $2N_\theta + 1$. For a given set of a and b, the energy $E = \langle\Psi|H|\Psi\rangle / \langle\Psi|\Psi\rangle$ is minimized by letting $\partial E / \partial c_{nl} = 0$. This results in a matrix eigenvalues equation

$$HC = EUC , \quad (4)$$

where H and U are the Hamiltonian and overlap matrices with matrix elements $H_{ij} = \langle\psi_{nl}|H|\psi_{n'l'}\rangle$ and $U_{ij} = \langle\psi_{nl}|\psi_{n'l'}\rangle$. C is a column matrix consisting of c_{nl}. Equation (4) will be solved to obtain eigenvalues and c'_{nl}'s for eigenstates. The nonlinear parameters a and b will then be determined by minimizing the wanted eigenvalue through step-by-step optimization. The calculation is performed with 20 basis functions. By the nature of variational method, the obtained results will be upper bound of the exact results.

Table I shows the energy levels of a hydrogen atom in a magnetic field. The eigenvalues of eigenstates with positive $|m|$ are related to the corresponding eigenvalues for $-|m|$ eigenstates by

$$E_{|m|} = E_{-|m|} + 2|m|\gamma .$$

We limit our calculation to the eigenstates with major quantum numbers less than or equal to 3, although any eigenstates can, in principle, be calculated. Twenty basis functions are used to calculate each eigenvalue. Howev-

TABLE I. Energy levels in effective rydbergs of a hydrogen atom in a uniform magnetic field. The numbers without brackets are the results of the present work. The numbers in parentheses represent the results of Rösner *et al.* [5] and the ones in square brackets the exact results for a hydrogen atom without a magnetic field.

γ	0	1	10	100	1000
$1s_0$	$-1.000\,000$	$-0.662\,338$	$6.504\,41$	92.4204	984.6754
	$[-1.000\,000]$	$(-0.662\,338)$	$(6.504\,41)$	(92.4219)	(984.6759)
$2s_0$	$-0.250\,000$	$0.679\,065$	$9.582\,10$	99.4881	999.4102
	$[-0.250\,000]$	$(0.679\,062)$	$(9.582\,23)$	(99.4877)	(999.4083)
$3d_0$	$-0.111\,111$	$0.867\,544$	$9.845\,88$	99.8276	999.8137
	$[-0.111\,111]$	$(0.867\,98)$	$(9.845\,71)$	(99.8262)	(999.8113)
$3s_0$	$-0.111\,111$	$0.928\,563$	$9.920\,62$	99.9153	999.9105
	$[-0.111\,111]$	$(0.928\,72)$	$(9.920\,45)$	(99.9135)	(999.9083)
$2p_0$	$-0.250\,000$	$0.479\,987$	$9.234\,70$	99.0728	999.0150
	$[-0.250\,000]$	$(0.479\,987)$	$(9.234\,70)$	(99.0728)	(999.0150)
$3p_0$	$-0.111\,111$	$0.819\,558$	$9.780\,41$	99.7590	999.7518
	$[-0.111\,111]$	$(0.819\,559)$	$(9.780\,31)$	(99.7589)	(999.7518)
$2p_{-1}$	$-0.250\,000$	$0.086\,807$	$7.749\,16$	94.7305	988.7232
	$[-0.250\,000]$	$(0.086\,806)$	$(7.749\,16)$	(94.7305)	(988.7232)
$3p_{-1}$	$-0.111\,111$	$0.749\,060$	$9.635\,42$	99.5310	999.4441
	$[-0.111\,111]$	$(0.749\,078)$	$(9.635\,40)$	(99.5305)	(999.4422)
$3d_{-1}$	$-0.111\,111$	$0.586\,914$	$9.322\,28$	99.1144	999.0261
	$[-0.111\,111]$	$(0.586\,865)$	$(9.322\,09)$	(99.1143)	(999.0260)
$3d_{-2}$	$-0.111\,111$	$0.293\,932$	$8.183\,63$	95.6238	990.3906
	$[-0.111\,111]$	$(0.293\,904)$	$(8.183\,58)$	(95.6237)	(990.3898)

er, more basis functions may be used for more accurate results. The results of Rösner *et al.* [5] are widely accepted and include many excited states. Their results are also listed in Table I to compare with the present results. The present results agree with those of Rösner *et al.* with small differences. In some occasions, such as E_{3d_0} and E_{3s_0} at $\gamma = 1$, our eigenvalues are lower than those of Rösner *et al.* In these cases, our eigenvalues are within the ranges of uncertainty reported for the corresponding

eigenvalues of Rösner *et al.* [5] The two-limit basis functions proposed by Chen and Goldman converge fast. Therefore, accurate results can be obtained with a relatively small number of basis functions. With only two nonlinear variational parameters in the basis functions, the amount of numerical computation is significantly reduced. The finite-basis-set method with the two-limit basis functions can be used to obtain accurate results not only for the ground state but also for any excited state.

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