Hydrogen atom in a high magnetic field

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The low-lying energy levels of a hydrogen atom in a uniformly strong magnetic field B ($B < 10^{10}$ G) are calculated in a simple perturbative variational approach which combines the spirit of the variational principle and the conventional perturbation method. The total Hamiltonian is separated into four parts: a one-dimensional hydrogen-atom system; a two-dimensional harmonic-oscillator system; a z-component angular-momentum operator; and a perturbation part which contains an undetermined variable parameter but is independent of B. The first three parts can be solved exactly. The variational parameter introduced in the Hamiltonian can be determined by requiring the energy-correction expansion to converge as fast as possible. It is found that our calculated ground-state energy is in good agreement with those obtained by the previous works that used the wave-function-expansion approach for high magnetic fields up to $\gamma = 7$ (i.e., 10^{10} G for atoms).

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I. INTRODUCTION

The problem of hydrogenlike systems in an external magnetic field is fundamental in various domains of physics and has received a great deal of attention in recent years [1-11]. Calculations of the energy levels of a hydrogenlike atom are essential for astrophysics [12–15] and solid-state physics involving excitons or shallow donors [16,17]. The possible existence of extremely high magnetic fields in white dwarfs and neutron stars has motivated the investigation of their effects on the electronic structure and spectrum of atoms. This field reaches an intensity of $10^{10} - 10^{13}$ G. It is known that in the low-field limit, the conventional perturbation and variational methods have been proved to be valid, while in the high-field limit the expansion perturbation and variation method [1,4,7,9] and adiabatic techniques [10,11] were usually employed. In the past few years, a great deal of work has been devoted to obtaining the energy values and the wave functions of the whole range of field strength. Praddaude [1] expanded the wave functions of the hydrogen atom under a magnetic field (up to $\gamma = 3.0$) in terms of Laguerre polynomials. Kaschiev et al. [3] solved bound states of the H atom by using the finite-element method in a strong magnetic field B with $10^9 < B < 10^{13}$ G. Chen et al. [9] proposed an expansion variational method to study the energy spectrum of a hydrogenlike system in an arbitrary magnetic field (up to 10^{10} G). After optimizing two variational parameters, they found the numerical results were accurate in the case of both low- and highfield limit. Liu and Starace [10] performed an adiabaticapproximation calculation on the low-lying energy levels of an atomic hydrogen for fields above 10^9 G in cylindrical coordinates. Both upper and lower bounds on the true level energies and binding energies were obtained.

Although the variational approach can provide reasonable results, the accuracy of the variational methods depends on the choice of the trial wave functions. But in the usual cases, to select a "good" trial wave function sometimes yields the problem of how to balance between simplicity and accuracy. In the expansion wave function or expansion variational methods, many expansion terms have to be included to obtain a reasonably accurate result. These approaches involve intrinsically huge numerical complication and thus make the problem become very tedious. Dai and Chuu [17] performed a variational perturbative approach to study the donor impurity states of cadmium sulfide semiconductor in the magnetic field. In their approach the energy correction due to the magnetic field was treated as the perturbation which is able to be optimized by varying the parameter introduced in the Hamiltonian. Therefore their treatment can be essentially applied to the case of lower magnetic field strength. In this work, we improve their treatment and present a simpler approach which not only combines the spirit of the conventional variational and perturbative approaches but also can be applied to the case of higher magnetic field strength. The numerical procedures involved in the calculation are very simple and easy to handle. The results reported here are accurate up to about 10^{10} G, which covers not only the whole range of laboratory accessible fields but also an important part of the range of astrophysical interest. This paper is organized as follows: in Sec. II we present the theory; in Sec. III we report our numerical results. A short summary will be given in the last section.

II. THEORY

The hydrogen atom in a uniformly high magnetic field **B** can be accurately described over a large range of field strengths B by the simple nonrelativistic single particle Hamiltonian

$$H = -\nabla^2 - \frac{2}{r} + \gamma L_z + \frac{\gamma^2}{4} (x^2 + y^2), \qquad (1)$$

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where the energy is expressed in terms of the effective Rydberg $R_0^* = \frac{\mu e^4}{2\hbar^2 \epsilon^2}$ where ϵ is the static dielectric constant and μ is the reduced mass of the system and the length is expressed in terms of the effective Bohr radius $a_0^* = \frac{\epsilon \hbar^2}{\mu e^2}$. The z component of the angular-momentum operator L_z is defined as $-i\partial/\partial\varphi$ and the dimensionless parameter γ is the reduced field strength and can be expressed as $\gamma = e\hbar B/2c\mu R_0^*$. $\gamma = 1$ for $H = 2.35 \times 10^5$ T in the case of the hydrogen atom in vacuum. In the above expression, we have neglected the relativistic correction and the effects of spin-orbit coupling. This is because it is known that the relativistic correction is negligible for fields with $\gamma < 10^4$ and the effects of spin-orbit coupling can be neglected for fields with $\gamma > 10^{-4}$ and in this work the only interesting range of γ lies in $0.0002 < \gamma < 7$.

It is known that the eigenvalue problem described by the Hamiltonian in Eq. (1) cannot be solved exactly. As mentioned above, we will treat this problem in a rather different way by introducing a parameter λ into H by adding and subtracting a term $\frac{-2\lambda}{|z|}$ to make the Hamiltonian separable into four parts:

$$H = H_{\rm I} + H_{\rm II} + H_{\rm III} + H_{\rm IV} ,$$
 (2)

where

$$H_{\rm I} = -\frac{\partial^2}{\partial z^2} - \frac{2\lambda}{\mid z \mid} , \qquad (3)$$

$$H_{\rm II} = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{\gamma^2}{4}(x^2 + y^2), \qquad (4)$$

$$H_{\rm III} = \gamma L_z \ , \tag{5}$$

and

$$H_{\rm IV} = \frac{2\lambda}{|z|} - \frac{2}{r} . \tag{6}$$

The parameter λ plays essentially the same role as the "effective-charge" parameter commonly used in the molecular calculation. The solutions for $H_{\rm I}$ are onedimensional hydrogenic wave functions:

$$\psi_{\rm I}(z,\lambda) = N e^{-\sqrt{2}\lambda z} z \, _1F_1(1-n;2;2\sqrt{2}\lambda z), \qquad (7)$$

where N is the normalization constant. The eigenvalues can be expressed as $E_{\rm I}^{(0)}(\lambda) = -\frac{\lambda^2}{n^2}$, n = 1, 2, ..., where $_1F_1$ is the degenerate hypergeometric function.

The solutions of the term $H_{\rm II}$ are the two-dimensional harmonic-oscillator wave functions:

$$\psi_{\rm II} = N_n N_m H_n(\beta x) H_m(\beta y) e^{-\gamma (x^2 + y^2)}, \qquad (8)$$

where $\beta = \sqrt{2\gamma}$. The normalization constant N_n is defined as $(\frac{l}{2^n n! \sqrt{\pi}})^{1/2}$. The corresponding eigenvalues $E_{\mathrm{II}}^{(0)} = (n+m+1)\gamma, \, n,m = 0, 1, 2, \dots$

The solution of $H_{\rm III}$ is the z-component angularmomentum wave functions, i.e., the spherical harmonic functions:

$$\psi_{\rm III} = Y_m^l(\theta, \varphi), \tag{9}$$

with eigenvalues $E_{\text{III}}^{(0)} = \gamma m, \ m = 0, 1, 2, ...$ The last term H_{IV} is now treated as the perturbation part. By using $\psi_{\rm I}(z,\lambda)\psi_{\rm II}(x,y)\psi_{\rm III}(\theta,\varphi)$ as the unperturbed eigenfunctions, the energy correction of $H_{\rm IV}$ can be evaluated as the conventional perturbation method. For illustration only, we present here the first-order energy correction for the ground state:

$$\Delta E_{1,0,0}^{(1)}(\lambda) = 2\lambda^2 + 2^{\frac{7}{4}}\lambda^3(4\gamma)\sqrt{4\gamma}\frac{\pi}{2}\int_0^\infty \rho^3 e^{-2\gamma\rho^2} \left[\left(H_0(2\sqrt{2}\rho) - \frac{1}{2\sqrt{2}\lambda\rho}H_1(2\sqrt{2}\lambda\rho) \right) - \left(N_0(2\sqrt{2}\lambda\rho) - \frac{1}{2\sqrt{2}\lambda\rho}N_1(2\sqrt{2}\lambda\rho) \right) \right] d\rho,$$
(10)

where $H_n(2\sqrt{2}\lambda\rho)$ and $N_n(2\sqrt{2}\lambda\rho)$ are the *n*th-order Struve and Neuman functions. The second term of the right hand side of the above equation contains the following types of integrals:

$$\int_0^\infty \rho^3 e^{-2\gamma\rho^2} H_0(2\sqrt{2\lambda\rho}) \, d\rho,\tag{11}$$

$$\int_0^\infty \rho^2 e^{-2\gamma\rho^2} H_1(2\sqrt{2}\lambda\rho) \, d\rho,\tag{12}$$

$$\int_0^\infty \rho^3 e^{-2\gamma\rho^2} N_0(2\sqrt{2}\lambda\rho) \, d\rho,\tag{13}$$

$$\int_0^\infty \rho^2 e^{-2\gamma\rho^2} N_1(2\sqrt{2}\lambda\rho) \, d\rho. \tag{14}$$

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The first two integrals can be evaluated as

$$\int_{0}^{\infty} \rho^{s-1} e^{-\alpha^{2}\rho^{2}} H_{\nu}(\beta\rho) \, d\rho = \frac{\beta^{\nu+1} \Gamma(\frac{1}{2} + \frac{s}{2} + \frac{\nu}{2})}{2^{\nu+1} \sqrt{\pi} \alpha^{\nu+s+1} \Gamma(\nu + \frac{3}{2})} \, {}_{2}F_{2}\left(1, \frac{\nu+s+1}{2}; \frac{3}{2}, \nu + \frac{3}{2}; -\frac{\beta^{2}}{4\alpha}\right),\tag{15}$$

where ${}_{p}F_{q}$ is the generalized hypergeometric functions and can be expressed as the following series:

$${}_{p}F_{q}(\alpha_{1},\alpha_{2},\ldots,\alpha_{p};\beta_{1},\beta_{2},\ldots,\beta_{q};z) = \sum_{k=0}^{\infty} \frac{(\alpha_{1})_{k}(\alpha_{2})_{k}\cdots(\alpha_{p})_{k}z^{k}}{(\beta_{1})_{k}(\beta_{2})_{k}\cdots(\beta_{q})_{k}k!} , \qquad (16)$$

where $(\alpha_p)_k = (\alpha_p)(\alpha_p + 1)\cdots(\alpha_p + k)$. The last two terms can be evaluated as

$$\int_{0}^{\infty} \rho^{3} e^{-2\gamma \rho^{2}} N_{0}(2\sqrt{2}\lambda\rho) \, d\rho = -\frac{1}{4\pi\gamma^{2}} e^{-\frac{\lambda^{2}}{\gamma}} \left(1 + \frac{-\frac{3}{2}}{\frac{1}{2}} f_{1}(\gamma,\lambda) + \frac{(-\frac{3}{2})(-\frac{1}{2})(\frac{1}{2})}{\frac{1}{2}(\frac{1}{2})(\frac{3}{2})} \frac{1}{2!} f_{2}(\gamma,\lambda) + \frac{(-\frac{3}{2})(-\frac{1}{2})(\frac{1}{2})}{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})} \frac{1}{3!} f_{3}(\gamma,\lambda) + \cdots \right),$$
(17)

where

$$f_n(\gamma,\lambda) = \left(\frac{2\lambda^2}{\gamma}\right)^n \frac{1}{2^{2n+1}} \left\{ \sum_{k=0}^{n-1} \left[2C_k^{2n} K_{n-k}\left(\frac{\lambda^2}{\gamma}\right) \right] + C_n^{2n} K_0\left(\frac{\lambda^2}{\gamma}\right) \right\},\tag{18}$$

the Kramer function $K_{\nu}(z)$ is defined as

$$K_{\nu}(z) = \int_0^\infty e^{-z \cosh \nu t} \cosh \left(\nu t\right) dt , \qquad (19)$$

 and

$$\int_{0}^{\infty} \rho^{2} e^{-2\gamma\rho^{2}} N_{1}(2\sqrt{2}\lambda\rho) \, d\rho = -\frac{\lambda}{\sqrt{2}\pi\gamma^{2}} e^{-\frac{\lambda^{2}}{\gamma}} \left(1 + \frac{-\frac{1}{2}}{\frac{3}{2}} g_{1}(\gamma,\lambda) + \frac{(-\frac{1}{2})(\frac{1}{2})(\frac{3}{2})}{(\frac{3}{2})(\frac{5}{2})} \frac{1}{2!} g_{2}(\gamma,\lambda) + \frac{(-\frac{1}{2})(\frac{1}{2})(\frac{3}{2})}{(\frac{3}{2})(\frac{5}{2})(\frac{7}{2})} \frac{1}{3!} g_{3}(\gamma,\lambda) + \cdots \right),$$
(20)

where

$$g_n(\gamma,\lambda) = \left(\frac{2\lambda^2}{\gamma}\right)^n \frac{1}{2^{2n+3}} \left\{ \sum_{k=0}^n \left[2C_k^{2n+2} K_{n+1-k}\left(\frac{\lambda^2}{\gamma}\right) \right] + C_{n+1}^{2n+2} K_0\left(\frac{\lambda^2}{\gamma}\right) \right\}.$$
(21)

 $K_{\nu}(z)$ is the Kramer function.

The higher-order energy corrections $\Delta E_{nlm}^{(2)}$, $\Delta E_{nlm}^{(3)}$,... can be obtained in the same way. After evaluating the correction $\Delta E_{nlm}^{(1)}$, the total energy can be expressed as

$$E_{nlm}(\lambda) = E_{\rm I}^{(0)} + E_{\rm II}^{(0)} + E_{\rm III}^{(0)} + \Delta E_{nlm}^{(1)} + \Delta E_{nlm}^{(2)} + \Delta E_{nlm}^{(2)} + \cdots$$
(22)

There are several ways to choose the parameter λ .

(i) The suitable value of the parameter λ can be chosen to make the perturbation expansion expressed in Eq. (22) converge most quickly so that only the first few terms will be enough. Hence λ is to be determined by the condition

$$|\Delta E_{nlm}^{(1)}(\lambda)/E_{nlm}(\lambda)| = \text{minimum}$$
 (23)

This can be satisfied by requiring the parameter λ to satisfy [18]

$$\Delta E_{nlm}^{(1)}(\lambda) = 0. \tag{24}$$

(ii) Another method to choose λ is to set [17]

$$\frac{\partial E_{nlm}(\lambda)}{\partial \lambda} = 0. \tag{25}$$

This is because, in spite of the appearance of λ , the exact result described by the total Hamiltonian H is independent of the parameter λ . However, in most cases only the approximation result is accessible; in order to obtain the approximation which most closely mimics the exact result's independence of λ , the parameter should be chosen so as to minimize the $E_{nlm}(\lambda)$'s sensitivity to small variations in its value.

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γ	λ	BE (units	Ground-state energy (units of R_0^*)						
		of R_0^*)	This work	Ref. [9]	Ref. [17]	Ref. [18]	Ref. [19]	Ref. [20]	Ref. [21]
0.02	1.420	1.018	-0.998		-1.000			-0.998	
0.10	1.445	1.095	-0.995		-0.995			-0.995	
0.20	1.470	1.181	-0.981	-0.981	-0.981	-0.979	-0.981	-0.981	-0.981
0.50	1.513	1.394	-0.894	-0.894		-0.888	-0.894	-0.894	
1.00	1.525	1.662	-0.662	-0.661	-0.642	-0.649	-0.659	-0.662	-0.662
2.00	1.447	2.047	-0.047	-0.041	0.029	-0.013	-0.035	-0.044	-0.045
3.00	1.288	2.329	0.671	0.676	0.755	0.718	0.686	0.671	0.671
4.00	1.060	2.562	1.438	1.446	1.549	1.498	1.459	1.438	1.438
5.00	0.719	2.759	2.241	2.249	2.465	2.310	2.265		2.239
6.00	0.467	2.891	3.109						
7.00	0.098	3.505	3.495						

TABLE I. The ground-state energy (in units of effective rydberg R_0^*) and binding energy (BE) (in units of effective rydberg R_0^*) $\gamma - E^{(g)}$ for a hydrogen atom in a uniform magnetic field with $\gamma = 0.02 - 7.0$. The corresponding values of the variational parameter λ are also shown.

In this work, we determine λ by using Eq. (24). For ground state, the above condition is reduced to solve the following algebraic equation for the parameter λ :

$$\frac{3\lambda}{8\sqrt{\pi}\gamma^{\frac{5}{2}}} \left[1 + \frac{\frac{5}{2}}{(\frac{3}{2})(\frac{3}{2})} \left(-\frac{\lambda^{2}}{2\gamma^{2}} \right) + \frac{2(\frac{5}{2})(\frac{7}{2})}{(\frac{3}{2})(\frac{5}{2})(\frac{3}{2})(\frac{5}{2})} \frac{1}{2!} \left(-\frac{\lambda^{2}}{2\gamma^{2}} \right)^{2} + \cdots \right] \\
- \frac{\lambda}{8\sqrt{\pi}\gamma^{\frac{5}{2}}} \left[1 + \frac{\frac{5}{2}}{(\frac{3}{2})(\frac{3}{2})} \left(-\frac{\lambda^{2}}{2\gamma^{2}} \right) + \frac{2(\frac{5}{2})(\frac{7}{2})}{(\frac{3}{2})(\frac{5}{2})(\frac{7}{2})} \frac{1}{2!} \left(-\frac{\lambda^{2}}{2\gamma^{2}} \right)^{2} + \cdots \right] \\
+ \frac{1}{4\sqrt{\pi}\gamma^{2}} e^{-\frac{\lambda^{2}}{\gamma}} \left(1 + \frac{-\frac{3}{2}}{\frac{1}{2}} f_{1}(\gamma,\lambda) + \frac{(-\frac{3}{2})(-\frac{1}{2})}{(\frac{1}{2})(\frac{3}{2})} \frac{1}{2!} f_{2}(\gamma,\lambda) + \cdots \right) \\
- \frac{1}{4\sqrt{\pi}\gamma^{2}} e^{-\frac{\lambda^{2}}{\gamma}} \left(1 + \frac{-\frac{1}{2}}{\frac{3}{2}} g_{1}(\gamma,\lambda) + \frac{(-\frac{1}{2})(\frac{1}{2})}{(\frac{3}{2})(\frac{5}{2})} \frac{1}{2!} g_{2}(\gamma,\lambda) + \cdots \right) + \frac{1}{4\sqrt{2}\lambda\gamma} = 0.$$
(26)

III. RESULTS AND DISCUSSION

The lower-lying state energies of the hydrogenlike atom under a uniformly arbitrary magnetic field with strength ranging from $\gamma \sim 0$ to 7.0 (i.e., 10¹⁰ G) are calculated by using the perturbative variational technique. The dimensionless parameter γ is the reduced field strength $\frac{e\hbar B}{2cm^*R_0^*}$). It measures the magnetic field strength $(\gamma =$ in units of 2.35×10^5 T. Table I presents the groundstate energies and binding energies of the hydrogenlike atom for magnetic field ranges from $\gamma = 0.02$ to 7.0. In general, it is quite difficult to estimate the error present in a calculation of any approximation approach. To see how accurate our results are, we compare our results with those of other previous works. We will be mainly concerned with the states of $n \leq 3$ manifolds, for which they have already been published. In Table I, our calculated binding energy and ground-state energy are presented in the third and fourth columns; several previous results



FIG. 1. Ionization energy (in eV) of the ground state of a hydrogenlike atom as a function of the magnetic field (in T; solid line). Dotted line was calculated by Chen and Gil (Ref. 19) and broken line was obtained by Gallas (Ref. 20).

State	λ	Excited-state energies (units of R_0^*)					
		This work	Ref. [18]	Ref. [20]	Ref. [17]		
$2s_0$	1.088	-0.096	-0.096	-0.098	-0.097		
$2p_{-1}$	1.097	-0.301	-0.300	-0.301	-0.302		
$2p_0$	1.217	-0.170	-0.170	-0.170	-0.170		
$2p_{+1}$	1.095	0.100	0.100	0.101			
$3s_0$	0.737	0.132	0.121	0.117	0.254		
$3p_{-1}$	0.569	0.019	0.024	0.018	0.020		
$3p_0$	1.095	0.050	0.052	0.050	0.060		
$3p_{+1}$	0.846	0.421	0.424	0.418			
$3d_{-2}$	0.644	-0.161	-0.162	-0.163	-0.161		
$3d_{-1}$	0.710	-0.063	-0.063	-0.064	-0.062		
$3d_0$	1.073	0.056	0.056	0.055	0.058		
$3d_{+1}$	0.710	0.337	0.337	0.336			
$3d_{+2}$	0.805	0.638	0.638	0.637			

TABLE II. The lower-lying excited-state energies (in units of effective rydberg R_0^*) for a hydrogen atom in a magnetic field with $\gamma = 0.2$. The variational parameter λ is shown in the second column. For comparison, some previous results are listed in the last three columns.

[9,17,19–22] are listed also in Table I for comparison. The ionization energy is defined as the difference between the energies of the lowest bound state and lowest free state. The results indicate that the dependence of the energy on B is rather weak for $\gamma \leq 0.1$. At $B = 4.7 \times 10^9$ G (i.e., $\gamma = 2.0$), the ground-state binding energy is 27.84 eV (i.e., $2.047R_0^*$), compared to 27.03 eV obtained by Peek and Katriel [2] using numerical solving of a pair of selfconsistent equations in prolate spherical coordinates, and 27.8 eV obtained by Surmelian and O'Connell [23] using a linear combination of Slater type orbitals. Clearly, one can see from Table I that our calculated results are superior to those of Gallas's work [20], which used the wavefunction-expansion method by making a calculation with mixing eigenfunction up to 20 terms in the interesting range of magnetic strength. One can also note that our methods are also in good agreement with the results of other previous work [19] using the expansion variational method. Gallas [20] used the variational approach with a simple hydrogenic basis while our approach contains also

the perturbative correction which will be dominant in the intermediate magnetic field strength. One can note that Gallas's work [20] loses accuracy as the energies go above the ionization limit; however, our approach can improve them, needing no huge numerical elaboration. One of the best previous theoretical works was performed by Rösner *et al.* [21]; however, one can see from Table I that our results are as good as theirs

Figure 1 presents the ionization energy for a hydrogenlike atom under a uniform magnetic field for field strength from 4.0×10^3 T to 2.0×10^6 T. For comparison, we also present the calculated results of previous works [19,20] in Fig. 1. One can see from Fig. 1 that our calculated ionization energy agrees quite well with those obtained by the expansion variation method. For a magnetic field larger than 2.0×10^6 T, the present results deteriorate rapidly. This clearly indicates that our approach is valid for moderate high magnetic fields such as those typical of white dwarfs, but not for the much higher magnetic fields of neutron stars or pulsars.

TABLE III. The lower-lying excited state energies (in units of effective rydberg R_0^*) for a hydrogen atom in a magnetic field with $\gamma = 1.0$. The variational parameter λ is shown in the second column. For comparison, some previous results are listed in the last three columns.

State	λ	Exci	Excited-state energies (units of R_{c}^{2}	of R_0^*)
		This work	Ref. [18]	Ref. [20]
$2s_0$	1.131	0.680	0.686	0.679
$2p_{-1}$	1.911	0.087	0.089	0.087
$2p_0$	1.442	0.480	0.481	0.480
$2p_{+1}$	1.710	2.088	2.089	2.087
$3s_0$	0.314	0.930	0.934	0.928
$3p_{-1}$	1.000	0.750	0.745	0.749
$3p_0$	1.183	0.825	0.822	0.820
$3p_{+1}$	1.000	2.750	2.755	2.748
$3d_{-2}$	1.011	0.295	0.297	0.294
$3d_{-1}$	1.285	0.857	0.588	0.587
$3d_0$	1.020	0.870	0.871	0.868
$3d_{+1}$	1.284	2.588	2.588	2.587
$3d_{+2}$	1.203	4.295	4.297	4.294



FIG. 2. Calculated excited energies (in units of effective rydberg R_0^*) for the lowest 14 energy states.

Tables II and III present our calculated excited states for a hydrogenlike atom under the uniform magnetic field for field strengths $\gamma = 0.2$ and $\gamma = 1.0$. The state labelings are adopted as those for the hydrogen energy levels in the absence of a magnetic field. For comparison, we also list the calculated results of some previous works [19,21,17]. The second columns in Tables II and III present the variational parameter λ we used in our calculation, the third columns list our results, and the remaining three columns present the calculated results of Chen and Gil [19], Rösner et al. [21], and Dai and Chuu [17]. One can see from Table II that our calculated excited energy levels are better than the results of Chen and Gil [19], which used complicated expansion variational method of the trial function up to the lowest six even-parity hydrogenlike basis functions. Our results are as good as the work of Rösner et al. [21], which used the wave-function-expansion method. The variation of our calculated state energies for the lower 14 states with the magnetic field strength γ from 0 to 6 is shown in Fig. 2. One can see from the figure that there exist a number of energy level crossings as a function of γ . This happens when the Coulomb levels lose their identity and start to resemble the pure magnetic levels. For example, the crossing of the $3d_{-2}$ and the $2p_0$ levels occurs because the large magnetic moment of the $3d_{-2}$ level makes the upturn due to the second-order magnetic effect more difficult. Since the $2p_0$ level has no magnetic moment, the second-order effect of the magnetic field is the only one operative. One can also note from the figure that some excited states are degenerate and all the state energies increase as the magnetic field increases.

Figure 3 shows the variational parameter λ as a function of magnetic field strength γ . One can note from Fig. 3 that the parameter λ first increases as magnetic



FIG. 3. The variational parameter λ as a function of magnetic strength γ .

field strength γ increases, then it decreases as magnetic field increases more strongly, while in the region of $0.0 < \gamma < 2.0$ the variation of λ is almost constant. As the field strength γ is larger than 7 the variational parameter λ becomes negative. This indicates that our approach breaks down for magnetic field strength larger than 7.0 (which is about 10^{10} G for atoms) because in this case the wave function in Eq. (7) is no longer the solution of Eq. (3).

IV. SUMMARY

In summary, we have proposed a simple but efficient method to investigate the level structure of the hydrogenlike atom under a uniform high magnetic field. Our calculated results show that our approach is superior at least for moderate high magnetic fields up to 2.0×10^{10} G even though our method is very simple in the numerical treatments. Moreover, by using simple onedimensional hydrogenlike wave functions and two dimensional harmonic-oscillator wave functions, the physical picture is very strongly manifested and the expressions of the binding energy and transition probability calculations are easily extended to higher-order states. Finally, this algorithm is expected to be very useful for solving problems in which the Hamiltonian can be reasonably separated with an unperturbed Hamiltonian part which has exact eigenfunctions to follow.

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- [1] H.C. Praddaude, Phys. Rev. A 6, 1321 (1972).
- [2] J.M. Peek and J. Katriel, Phys. Rev. A 21, 413 (1980).
- [3] M.S. Kaschiev, S.I. Vinitsky, and F.R. Vukajlović, Phys. Rev. A 22, 557 (1980).
- [4] H. Friedrich, Phys. Rev. A 26, 1827 (1982).
- [5] S. Feneuille, Phys. Rev. A 26, 673 (1982).
- [6] J.B. Delos, S.K. Knudson, and D.W. Noid, Phys. Rev. A 28, 7 (1983).
- [7] M.C. Chu and H. Friedrich, Phys. Rev. A 29, 675 (1984).
- [8] M. Robnik and E. Schrüfer, J. Phys. A 18, L853 (1985).

- [9] Y. Chen, B. Gil, and H. Mathieu, Phys. Rev. B 34, 6912 (1986).
- [10] C.R. Liu and A.F. Starace, Phys. Rev. 35, 647 (1987).
- [11] S. Saini and D. Farrelly, Phys. Rev. A 36, 3556 (1987).
- [12] B.B. Kodomtsev and V.S. Kudryavtsev, Pis'ma Zh. Eksp. Teor. Fiz. 13, 15 (1971) [JETP Lett. 13, 9 (1971)].
- [13] E.R. Smith, R.J.W. Henry, G.L. Surmelian and R.F. O'Connell, Astrophys. J. 179, 659 (1973).
- [14] J.L. Greenstein and J.B. Oke, Astrophys. J. 252, 285 (1982).
- [15] G. Wunner, H. Ruder, and H. Herrold, Phys. Lett. **79A**, 159 (1980); Astrophys. J. **247**, 374 (1981).
- [16] H.S. Brandi, Phys. Rev. A 11, 1835 (1975).

- [17] C.M. Dai and D.S. Chuu, Physica B 172, 445 (1991).
- [18] Y.C. Lee, W.N. Mei, and K.C. Liu, J. Phys. C 15, L469 (1982).
- [19] Y. Chen and B. Gil, Phys. Status Solidi B 136, 629 (1986).
- [20] J.A.C. Gallas, J. Phys. B 18, 2199 (1985).
- [21] W. Rösner, G. Wunner, H. Herold, and H. Ruder, J. Phys. B 17, 29 (1984).
- [22] D. Cabib, E. Fabri, and G. Fiorio, Solid State Commun.9, 1517 (1971).
- [23] G.L. Surmelian and R.F. O'Connell, Astrophys. J. 204, 311(E) (1976).