Variational-integral perturbation corrections of some lower excited states for hydrogen atoms in magnetic fields*

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A variational-integral perturbation method (VIPM) is established by combining the variational perturbation with the integral perturbation. The first-order corrected wave functions are constructed, and the second-order energy corrections for the ground state and several lower excited states are calculated by applying the VIPM to the hydrogen atom in a strong uniform magnetic field. Our calculations demonstrated that the energy calculated by the VIPM only shows a negative value, which indicates that the VIPM method is more accurate than the other methods. Our study indicated that the VIPM can not only increase the accuracy of the results but also keep the convergence of the wave functions.

Keywords: variational-integral perturbation method, lower excited state, convergence

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1. Introduction

The Zeeman effect, which describes atoms in a constant magnetic field, was one of the earliest problems studied by quantum mechanics. The Zeeman effect plays a fundamental role in many fields, including astrophysics, solid state physics, and plasma physics.[1−4] Although a lot of research has been done in this field, some problems are still waiting to be solved. The behavior of hydrogen atom in a uniform magnetic field is one of the most fascinating unsolved problems in the nonrelativistic quantum mechanics. The nonseparability of the Schrödinger equation for an electron in combined Coulomb and magnetic fields makes the theoretical description of the problem quite difficult, especially when the strengths of the two fields are comparable. The hydrogen atom in a magnetic field has been tackled by many researchers with the aid of various approaches ranging from the perturbation theory for the weak-field regime[5] to the adiabatic approximation for the opposite limit of very strong magnetic fields.[6,7] There are many reports on the lower-order calculations, such as the straightforward integration of the perturbation differential equations in the spherical coordinates[8] and the use of matrix methods for the Hamiltonian in spherical[9,10] or parabolic coordinates.[11,12] Many techniques for the large-order calculations have recently been reported, such as the Lie algebraic methods,[13−15] the logarithmic-perturbation methods,[16−18] appropriate power-series expansions of the wave function,[19,20] and the moment method.[21−23] In addition, coherent population trapping (CPT) has been theoretically examined as a magnetic-field diagnostic tool for high-hydrogen plasma.[24]

Different methods have been used to investigate the energies of hydrogen atoms in magnetic fields, such as the first-order perturbation theory,[25,26] the combining variational calculation with the Laguerre polynomials in the cylindrical coordinates,[27] and the Zeeman Hamiltonian plus series method.[28] Machet and Vysotsky[29] obtained an analytical formula describing the dependence of the electric potential of a pointlike charge on the distance away from it in the

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direction of the external magnetic field. Efstathiou *et al.*[30] studied the perturbation to the hydrogen atom by small homogeneous static electric and magnetic fields in a specific mutual alignment with an angle approximately of $n/3$, which resulted in the 12 resonances of the linearized Keplerian n-shell approximation. For the field evolution of 13 excited states, Smith *et al.*[31] adopted an elaborate variation calculation by using an eigenfunction made of up to 12 Slater-type orbitals, while the same case was also investigated by Brandi[32] with ns, n'd, and n''p function ($1 \leq n \leq 6$, $2 \leq n'' \leq 7$, $3 \leq n' \leq 8$) and a hydrogen basis. At higher-field strengths, Peek and Katriel[33] numerically solved a pair of self-consistent equations (exact zero field) in the prolate spheroidal coordinates. Cohen and Herman[34] used the perturbation theory combined with the variational calculation. Gallas[35] used a simple basis for the hydrogen to obtain the evolution of the energy spectrum of atoms in strong and uniform magnetic fields. Gallas's results were in good agreement with the others'. However, the energy spectrum included positive energies, which indicates that the accuracy is expected to lost quickly.

It is known that the variational method and the quantum perturbation theory have their own advantages and disfigurements. Therefore, the calculation combining the variational method with the perturbation theory can result in the variational-perturbation method which takes advantages of these two methods and avoids the disfigurements. Thus, the variation-perturbation method is applied widely to various systems.[36−40] However, the divergence difficulty of the perturbed series solutions also exists in the standard quantum perturbation theory of the variational-perturbation method. In the previous works,[41−44] we have established an improved Rayleigh–Schrödinger perturbation method based on the integral equation for suppressing the divergences and numerical instabilities in the nonrelativistic quantum mechanics. The integral perturbation method fits for any physically interesting systems. Specifically, this method is valid for the degenerate or nearly degenerate system, and can be used to sutdy a lot of systems which usually cannot be treated with the standard quantum perturbation theories, such as the coupled Bose–Einstein condensates[45,46] and the Paul trap.[47−49]

In the present study, we combine the variational-perturbation method with the integral perturbation to construct an improved variational-integral perturbation method (VIPM). Applying the VIPM to the hydrogen atom in a strong uniform magnetic field, we construct the first-order corrected wave functions consisting of a few terms and calculate the second-order energy corrections for the ground state and some lower excited states. These values are compared with those of the elaborate calculations of Smith *et al.*[33] and the simple basis variational calculations of Gallas.[35] It is known that the energy of the atom is negative, but for the $2P_0$ upper state at higher-field strengths, the value appears positive in the simple basis variational method and the other methods,[28,31−35] which are then expected to lose accuracy quickly. However, the energies are negative in this study by using the VIPM. Our data clearly demonstrate that the results of the VIPM are more accurate than those of the others. The VIPM can not only increases the accuracy of the result but also keep the convergence of the wave function. So the VIPM can be widely applied to various systems.

2. Variational-integral perturbation method

With spin and relativistic effects being neglected, the Hamiltonian for a hydrogen atom in a uniform magnetic field characterized by a vector potential $\boldsymbol{A}$ is given in the form

$$H = \frac{1}{2m_{\rm e}}\Big[\boldsymbol{P} + \frac{e}{c}\boldsymbol{A}\Big] - \frac{{\rm e}^2}{r}. \tag{1}$$

By choosing the usual gauge $\boldsymbol{A} = \boldsymbol{B} \times \boldsymbol{r}/2$ in the spherical coordinates and the atomic units, such as $\hbar = e = m_{\rm e} = c = 1$, the Zeeman Hamiltonian is given as

$$H = -\frac{1}{2}\Delta - \frac{1}{r} + \frac{1}{2}\gamma L_z + \frac{\gamma^2}{8}r^2\sin^2\theta, \tag{2}$$

where L_z is the angular momentum in the z direction and takes to be along the magnetic field direction; and γ is a dimensionless coupling parameter describing the strength of the magnetic field, γ=1 corresponds to 2.3505×10^9 Gs (1 Gs = 10^{-4} T). We can choose a trial wave function in the form

$$\phi_{nlm}(\lambda, r, \theta, \varphi) = R_{nl}(\lambda, r)\,{\rm Y}_{lm}(\lambda, \theta, \varphi), \tag{3}$$

where λ is a variational parameter, and $\phi_{nlm}(\lambda, r, \theta, \varphi)$ are the usual normalized eigensolutions of the generating Hamiltonian

$$H_\lambda = -\frac{1}{2}\nabla_1^2 - \frac{\lambda}{r}. \tag{4}$$

The zeroth-order energy $E^{(0)}_{nlm}$ has the relations $H_\lambda|\phi(\lambda)\rangle = E^{(0)}_{nlm}|\phi(\lambda)\rangle$, $E^{(0)}_{nlm} = -(\lambda^2)/(2n^2)$. The original Hamiltonian is

$$\begin{aligned} H &= H_\lambda + H' \\ &= -\frac{1}{2}\nabla_1^2 - \frac{\lambda}{r} + \frac{\lambda-1}{r} + \frac{\gamma L_z}{2} + \frac{\gamma^2}{8}r^2\sin^2\theta. \end{aligned} \quad (5)$$

The perturbation Hamiltonian is

$$H' = \frac{\lambda-1}{r} + \frac{1}{2}\gamma L_z + \frac{\gamma^2}{8}r^2\sin^2\theta. \quad (6)$$

For $\phi_{nlm}(\lambda, r, \theta, \varphi)$, the average energy is

$$\begin{aligned} \bar{H} &= \int \phi^*_{nlm}(\lambda, r, \theta, \varphi) H \phi_{nlm}(\lambda, r, \theta, \varphi)\,\mathrm{d}\tau \\ &= -\frac{\lambda^2}{2n^2} + \frac{(\lambda-1)\lambda}{n^2} + \frac{m\gamma}{2} + \frac{\gamma^2 p(n,l,m)}{8\lambda^2} \end{aligned} \quad (7)$$

with $p(n,l,m) = n^2[5n^2 - 3l(l+1)+1][l(l+1)+m^2-1]/[4l(l+1)-3]$. Under the condition of minimal energy, $\partial\bar{H}/\partial\lambda = 0$, we establish the equation

$$\begin{aligned} &\lambda^4 - \lambda^3 - \frac{\gamma^2 n^2}{8}[5n^2 - 3l(l+1)+1] \\ &\quad\times \frac{[l(l+1)+m^2-1]}{4l(l+1)-3} = 0, \end{aligned} \quad (8)$$

where n is the main quantum number, l and m are the angular and the magnetic quantum numbers, respectively. We can obtain a nonzero and minimum real number value for variational parameter λ by solving Eq. (8). The first-order corrected energy is

$$\begin{aligned} E^{(1)}_{nlm} &= \int \phi^{(0)}_{nlm}(\lambda, r, \theta, \varphi)^* H' \phi^{(0)}_{nlm}(\lambda, r, \theta, \varphi)\,\mathrm{d}\tau \\ &= \frac{(\lambda-1)\lambda}{n^2} + \frac{m\gamma}{2} + \frac{\gamma^2 p(n,l,m)}{8\lambda^2}. \end{aligned} \quad (9)$$

Combining Eq. (7) with Eq. (9) and $E^{(0)}_{nlm}$, we obtain the total energy of the variational method

$$E_{nlm} = -\frac{\lambda^2}{2n^2} + \frac{(\lambda-1)\lambda}{n^2} + \frac{m\gamma}{2} + \frac{\gamma^2 p(n,l,m)}{8\lambda^2}. \quad (10)$$

It seems that the total energy is the sum of $E^{(0)}_{nlm}$ and $E^{(1)}_{nlm}$. We only consider the case with magnetic quantum number $m = 0$. Combining the variational-perturbation with the integral perturbation, we establish the VIPM. Applying the VIPM to the hydrogen atom in a strong uniform magnetic field, we investigate the corrected wave functions and the energy corrections. If $m = 0$, the perturbed Hamiltonian is

$$H'(\lambda, r, \theta) = \frac{\lambda-1}{r} + \frac{\gamma^2}{8}r^2\sin\theta^2. \quad (11)$$

It is independent of the variable φ. Therefore, we assume

$$\begin{aligned} \phi_{nl0}(\lambda, r, \theta, \varphi) &= r^{-1}\chi_{nl0}(\lambda, r, \theta, \varphi) \\ &= r^{-1}\chi_{nl}(\lambda, r, \theta)\phi^{(0)}_m(\varphi), \end{aligned} \quad (12)$$

$$\vartheta_{nl0}(\theta, \varphi) = \vartheta_{nl0}(\theta)\phi^{(0)}_m(\varphi), \quad (13)$$

$$\varepsilon_{nl0}(\theta, \varphi) = \varepsilon_{nl0}(\theta)\phi^{(0)}_m(\varphi). \quad (14)$$

Applying the Rayleigh–Schrödinger expansions

$$\begin{aligned} E_{nlm} &= E^{(0)}_{nlm} + \sum_{i=1}^{\infty} E^{(i)}_{nlm}, \\ \chi_{nlm}(\lambda, r, \theta) &= \sum_{i=1}^{\infty} \chi^{(i)}_{nlm}(\lambda, r, \theta), \end{aligned} \quad (15)$$

we can construct the i-th order corrected wave function and obtain the i-th order energy correction[41]

$$\begin{aligned} \vartheta^{(i)}_{nlm}(\lambda, \theta) &= \tilde{\vartheta}^{(0)}_{lm}\int_{C_i}^{\theta} \vartheta^{(0)}_{lm}(\theta)\varepsilon^{(i)}_{nlm}(\theta)\sin\theta\,\mathrm{d}\theta \\ &\quad - \vartheta^{(0)}_{lm}\int_{D_i}^{\theta} \tilde{\vartheta}^{(0)}_{lm}\varepsilon^{(i)}_{nlm}(\theta)\sin\theta\,\mathrm{d}\theta \\ &= \int_0^{\infty} R^{(0)}_{nl}(\lambda, r)\phi^{(i)}_{nlm}(\lambda, r, \theta)\,\mathrm{d}r, \end{aligned} \quad (16)$$

$$\begin{aligned} \varepsilon^{(i)}_{nlm}(\lambda, \theta) &= 2\int_0^{\infty} \Big[\sum_{j=1}^{i} E^{(j)}_{nlm}\phi^{(i-j)}_{nlm}(\lambda, r, \theta) \\ &\quad - H'(\lambda, r, \theta)\phi^{(i-1)}_{nlm}(\lambda, r, \theta)\Big] \\ &\quad \times R^{(0)}_{nl}(\lambda, r)r^2\,\mathrm{d}r, \end{aligned} \quad (17)$$

$$\begin{aligned} \bar{\varepsilon}^{(i)}_{nlm} &= -\int_0^{\pi} \vartheta^{(0)}_{lm}(\theta)\varepsilon^{(i)}_{nlm}(\lambda, \theta)\sin\theta\,\mathrm{d}\theta = 0, \\ &\quad \text{for } i = 1, 2, \ldots, \infty, \end{aligned} \quad (18)$$

$$\phi^{(i)}_{nlm} = \vartheta^{(i)}_{nlm}(\lambda, \theta)r^2 R^{(0)}_{nl}(\lambda, r), \quad (19)$$

where C_i and D_i are arbitrary constants. The corrected wave functions are given by Eqs. (16) and (17). Let us consider the nondegenerate case $i = 1$, $m = 0$. From Eqs. (17) and (18), we obtain

$$\begin{aligned} \varepsilon^{(1)}_{nl0}(\lambda, \theta) &= 2\int_0^{\infty} \Big[E^{(1)}_{nl0} - \frac{\lambda-1}{r} - \frac{\gamma^2}{8}r^2\sin\theta^2\Big] \\ &\quad \times \phi^{(0)}_{nl0}(\lambda, r, \theta)R^{(0)}_{nl}(\lambda, r)r^2\,\mathrm{d}r, \end{aligned} \quad (20)$$

$$\int_0^{\pi} \vartheta^{(0)}_{l0}(\theta)\varepsilon^{(1)}_{nl0}(\lambda, \theta)\sin\theta\,\mathrm{d}\theta = 0, \quad (21)$$

$$\begin{aligned} \vartheta^{(1)}_{nlm}(\lambda, \theta) &= \tilde{\vartheta}^{(0)}_{l0}\int_{C_i}^{\theta} \vartheta^{(0)}_{l0}(\theta)\varepsilon^{(1)}_{nl0}(\lambda, \theta)\sin\theta\,\mathrm{d}\theta \\ &\quad - \vartheta^{(0)}_{l0}\int_{D_i}^{\theta} \tilde{\vartheta}^{(0)}_{l0}\varepsilon^{(1)}_{nl0}(\lambda, \theta)\sin\theta\,\mathrm{d}\theta \\ &= \int_0^{\infty} R^{(0)}_{nl}(\lambda, r)\phi^{(1)}_{nl0}(\lambda, r, \theta)\,\mathrm{d}r. \end{aligned} \quad (22)$$

Combining Eq. (20) with Eq. (21), we can obtain the first-order corrected energy $E^{(1)}_{nlm}$. Inserting Eq. (22)

into Eq. (19), we can construct the first-order corrected wave function $\phi^{(1)}_{nlm}(\lambda, r, \theta)$. For $i = 2, 3, \ldots$, using Eqs. (16)–(19), we can obtain the second-order, the third-order, and the higher-order corrected energies and corrected wave functions.

3. Corrected wave functions and corrected energies

We only consider the nondegenerate cases of hydrogen atoms in a uniform magnetic field. For the simple case of $n = 1$, $l = 0$, $m = 0$ with the 1S states, the zeroth-order wave function $\phi^{(0)}_{100}(\lambda, r, \theta, \varphi)$ is

$$\phi^{(0)}_{100}(\lambda, r, \theta, \varphi) = \frac{2}{\sqrt{4\pi}}\lambda^{3/2}\,\mathrm{e}^{-\lambda r}, \tag{23}$$

$$\vartheta^{(0)}_{00} = \frac{1}{\sqrt{4\pi}}, \tag{24}$$

$$\begin{aligned}\tilde{\vartheta}^{(0)}_{00} &= -\vartheta^{(0)}_{00}\int \frac{\mathrm{d}\theta}{(\vartheta^{(0)}_{00})^2\sin\theta}\\ &= \sqrt{4\pi}(\ln(\sin\theta/2) - \ln(\cos\theta/2)).\end{aligned} \tag{25}$$

Inserting Eqs. (23) and (25) into Eqs. (16)–(19), we obtain the first-order corrected energy $E^{(1)}_{100}$ and the first-order corrected wave function $\phi^{(1)}_{100}$

$$E^{(1)}_{100} = \frac{\gamma^2 - 4(1-\lambda)\lambda^3}{4\lambda^2}, \tag{26}$$

$$\begin{aligned}\phi^{(1)}_{100} = {} & r^2\,\mathrm{e}^{-\lambda r}r^2\Big[\frac{\gamma^2\cos(\theta)^2}{8\sqrt{\pi}\lambda^{1/2}} + \frac{\gamma^2}{16\sqrt{\pi}\lambda^{1/2}}\\ & \times\Big[\cos(2\theta) + 4\cos(\theta)(-\ln\cos(\theta/2)\\ & + \ln\sin(\theta/2))\sin(\theta)^2\Big]\Big].\end{aligned} \tag{27}$$

Combining Eqs. (17), (18), (23), (26), and (27), we obtain the second-order corrected energy

$$E^{(2)}_{100} = \frac{(-9\gamma^4 - 4\gamma^2\lambda^3 + 4\gamma^2\lambda^4)}{128\lambda^6}. \tag{28}$$

For the 2S states, $n = 2$, $l = 0$, $m = 0$, the zeroth-order wave function $\phi^{(0)}_{200}(\lambda, r, \theta, \varphi)$ is

$$\phi^{(0)}_{200}(\lambda, r, \theta, \varphi) = \left(\frac{\lambda}{2}\right)^{3/2}(2-\lambda r)\,\mathrm{e}^{-\lambda r/2}\frac{1}{\sqrt{4\pi}}, \tag{29}$$

$$\vartheta^{(0)}_{00} = \frac{1}{\sqrt{4\pi}}, \tag{30}$$

$$\begin{aligned}\tilde{\vartheta}^{(0)}_{00} &= -\vartheta^{(0)}_{00}\int \frac{\mathrm{d}\theta}{(\vartheta^{(0)}_{00})^2\sin\theta}\\ &= \sqrt{4\pi}(\ln(\sin\theta/2) - \ln(\cos\theta/2)).\end{aligned} \tag{31}$$

By inserting Eqs. (29)–(31) into Eqs. (17)–(19), the first-order corrected energy $E^{(1)}_{200}$ and the first-order corrected wave function $\phi^{(1)}_{200}$ are obtained as

$$E^{(1)}_{200} = \frac{14\gamma^2 - (1-\lambda)\lambda^3}{4\lambda^2}, \tag{32}$$

$$\begin{aligned}\phi^{(1)}_{200} = {} & (2-\lambda r)r^2\,\mathrm{e}^{-\lambda r/2}\Big[\frac{7\gamma^2\cos(\theta)^2}{16\sqrt{2\pi\lambda}} + \frac{7\gamma^2}{32\sqrt{2\pi\lambda}}\\ & \times\Big[\cos(2\theta) + 4\cos(\theta)(-\ln\cos(\theta/2)\\ & + \ln\sin(\theta/2))\sin(\theta)^2\Big]\Big].\end{aligned} \tag{33}$$

By inserting Eqs. (29), (32), and (33) into Eqs. (17) and (18), the second-order corrected energy is given as

$$E^{(2)}_{200} = -\frac{7(254\gamma^4 - 3\gamma^2\lambda^3 + 3\gamma^2\lambda^4)}{16\lambda^6}. \tag{34}$$

For the $2P_0$ states, $n = 2$, $l = 1$, $m = 0$, the zeroth-order wave function $\phi^{(0)}_{210}(\lambda, r, \theta, \varphi)$ is

$$\begin{aligned}\phi^{(0)}_{210}(\lambda, r, \theta, \varphi) = {} & \left(\frac{\lambda}{2}\right)^{3/2}\\ & \times\left(\frac{\lambda r}{\sqrt{3}}\right)\mathrm{e}^{-\lambda r/2}\sqrt{3/4\pi}\cos(\theta),\end{aligned} \tag{35}$$

$$\vartheta^{(0)}_{10} = \sqrt{\frac{3}{4\pi}}\cos(\theta). \tag{36}$$

By inserting Eqs. (35) and (36) into Eqs. (17)–(19), the first-order corrected energy $E^{(1)}_{210}$ and the first-order corrected wave function $\phi^{(1)}_{210}$ are obtained as

$$E^{(1)}_{210} = \frac{6\gamma^2 - (1-\lambda)\lambda^3}{4\lambda^2}, \tag{37}$$

$$\begin{aligned}\phi^{(1)}_{210} = {} & r^3\,\mathrm{e}^{-\lambda r/2}\lambda^{1/2}\Big[\frac{3\gamma^2\cos(\theta)^3}{16\sqrt{2\pi}} - \frac{3\gamma^2\cos(\theta)}{64\sqrt{2\pi}}\\ & \times\Big[-2\cos(2\theta) + \cos(4\theta) + 8\cos(\theta)^3\\ & \times(\ln\cos(\theta/2) - \ln\sin(\theta/2))\sin(\theta)^2\Big]\Big].\end{aligned} \tag{38}$$

By inserting Eqs. (35), (37), and (38) into Eqs. (17) and (18), the second-order corrected energy is obtained as

$$E^{(2)}_{210} = \frac{(-174\gamma^4 + 155\gamma^2\lambda^3 - 155\gamma^2\lambda^4)}{160\lambda^6}. \tag{39}$$

For the 3S states, $n = 3$, $l = 0$, $m = 0$, the zeroth-order wave function $\phi^{(0)}_{300}(\lambda, r, \theta, \varphi)$ is

$$\begin{aligned}\phi^{(0)}_{300}(\lambda, r, \theta, \varphi) = {} & \frac{\lambda^{3/2}\,\mathrm{e}^{-\lambda r/3}}{4\sqrt{2\pi}}\\ & \times\left(2 - \frac{4\lambda r}{3} + \frac{4\lambda^2 r^2}{27}\right),\end{aligned} \tag{40}$$

$$\vartheta^{(0)}_{00} = \frac{1}{\sqrt{4\pi}}, \tag{41}$$

$$\begin{aligned}\tilde{\vartheta}^{(0)}_{00} &= -\vartheta^{(0)}_{00}\int \frac{\mathrm{d}\theta}{(\vartheta^{(0)}_{00})^2\sin\theta}\\ &= \sqrt{4\pi}(\ln(\sin(\theta/2)) - \ln(\cos(\theta/2)).\end{aligned} \tag{42}$$

By inserting Eqs. (40) and (42) into Eqs. (17)–(19), the first-order corrected energy $E^{(1)}_{300}$ and the first-order corrected wave function $\phi^{(1)}_{300}$ are obtained as

$$E^{(1)}_{300} = \frac{621\gamma^2 - 4(1-\lambda)\lambda^3}{36\lambda^2}, \tag{43}$$

$$\begin{aligned}\phi^{(1)}_{300} = {} & r^2\,\mathrm{e}^{-\lambda r/3}\left(1 - \frac{2\lambda r}{3} + \frac{2\lambda^2 r^2}{27}\right) \\ & \times \Big[\frac{1863\gamma^2\cos(\theta)^2}{256\sqrt{2\pi\lambda}} + \frac{1863\gamma^2}{512\sqrt{2\pi\lambda}} \\ & \times \Big[\cos(2\theta) + 4\cos(\theta)[-\ln\cos(\theta/2) \\ & + \ln\sin(\theta/2)]\sin(\theta)^2\Big]\Big].\end{aligned} \tag{44}$$

By inserting Eqs. (40), (43), and (44) into Eqs. (17) and (18), the second-order corrected energy is obtained as

$$E^{(2)}_{300} = \frac{-23(61425\gamma^4 + 76\gamma^2\lambda^3 - 76\gamma^2\lambda^4)}{128\lambda^6}. \tag{45}$$

For the $3P_0$ states, $n = 3$, $l = 1$, $m = 0$, the zeroth-order wave function $\phi^{(0)}_{310}(\lambda, r, \theta, \varphi)$ is

$$\begin{aligned}\phi^{(0)}_{310}(\lambda, r, \theta, \varphi) = {} & r\lambda^{5/2}\,\mathrm{e}^{-\lambda r/3} \\ & \times \left(\frac{4}{27\sqrt{2\pi}} - \frac{2\lambda r}{81\sqrt{2\pi}}\right)\cos\theta,\end{aligned} \tag{46}$$

$$\vartheta^{(0)}_{10} = \sqrt{\frac{3}{4\pi}}\cos(\theta). \tag{47}$$

By inserting Eqs. (46) and (47) into Eqs. (17)–(19), the first-order corrected energy $E^{(1)}_{310}$ and the first-order corrected wave function $\phi^{(1)}_{310}$ are obtained as

$$E^{(1)}_{310} = \frac{81\gamma^2 - \lambda^3 + \lambda^4}{9\lambda^2}, \tag{48}$$

$$\begin{aligned}\phi^{(1)}_{310} = {} & \left(\frac{2}{27} - \frac{\lambda r}{81}\right) r^3\lambda^{1/2}\,\mathrm{e}^{-\lambda r/3}\cos\theta \\ & \times \Big[\frac{9\gamma^2\cos(\theta)^3}{2\sqrt{2\pi}} - \frac{9\gamma^2\cos(\theta)}{8\sqrt{2\pi}} \\ & \times \Big[-2\cos(2\theta) + \cos 4\theta + 8\cos(\theta)^3 \\ & \times [\ln\cos(\theta/2) - \ln\sin(\theta/2)]\sin(\theta)^2\Big]\Big].\end{aligned} \tag{49}$$

By inserting Eqs. (46), (48), and (49) into Eqs. (17) and (18), the second order corrected energy is obtained as

$$E^{(2)}_{310} = \frac{-9(16929\gamma^4 - 310\gamma^2\lambda^3 + 310\gamma^2\lambda^4)}{160\lambda^6}. \tag{50}$$

For 1S, 2S, $2P_0, \ldots$ states, the total energies E and the second-order energy corrections $E^{(2)}_{nl0}$ are given in Tables 1, 2, and 3, they also include the results of the simple basis variational method, the perturbation method, the variation-perturbation method, and the elaborated variational calculation. Here, $E = E^{(0)}_{nl0} + E^{(1)}_{nl0} + E^{(2)}_{nl0}$, E_{VIPM} denotes the result of the total energy obtained by using the VIPM, E_{vp} is the result of the simple basis variation method, E_{fp} is the result of the perturbation method.

Table 1. Comparison of the results in the field of $B = 2.35 \times 10^8$ Gs ($\gamma = 0.1$).

State	λ	$E^{(0)}_{\mathrm{fp}}$	E_{vp}[35]	Killingbeak[38]	Praddaude[27]	$E^{(2)}_{nl0}$	E
1S	1.00493	−0.497500	−0.497512	−0.4975217	−0.497525	-5.3×10^{-6}	−0.497518
2S	1.17334	−0.090000	−0.095822	−0.0956530	−0.098085	−0.001777	−0.09760
$2P_0$	1.09212	−0.100000	−0.111363	−0.1117526	−0.112410	−0.0007492	−0.112112
3S	1.66849		0.0312354			−0.1063300	−0.079095
$3P_0$	1.48986		−0.001678			−0.00402	−0.04541

Table 2. Results for some different field strengths ($B = 1 \times 10^8$ Gs, $B = 5 \times 10^8$ Gs, $B = 1 \times 10^9$ Gs).

State	γ	λ	E_{vp}[35]	Peek[33]	Cohen[34]	$E^{(2)}_{nlm}$	E
1S	0.0425	1.0009	−0.499549	−0.498548		-1.77×10^{-7}	−0.499549
	0.2125	1.02124	−0.488930	−0.48905		−0.0000983	−0.489048
	0.425	1.07309	−0.458115	−0.45968		−0.0011685	−0.459283
2S	0.0425	1.0444	−0.118958	−0.1207	−0.11908	−0.0001166	−0.119074
	0.2125	1.43168	−0.024454	−0.05508	−0.03349	−0.0110000	−0.0356004
	0.425	1.82798	0.149886	0.06080	0.12216	−0.0638455	0.086040
$2P_0$	0.0425	1.0204	−0.122346	−0.12237	−0.12240	−0.0000367	−0.122383
	0.2125	1.26695	−0.073815	−0.07758	−0.07996	−0.0062913	−0.080169
	0.425	1.56523	0.025525	0.01018	0.00361	−0.0282045	−0.002680
$2P_1$	0.0425	1.03868	−0.098540	−0.09859	−0.09860	−0.00004354	−0.098584
	0.2125	1.39767	0.070596	0.06473	0.06392		
	0.425	1.77507	0.334568	0.3152	0.31336		
3S	0.0425	1.27231	−0.032188			−0.002967	−0.035155
	0.2125	2.24369	0.185400			−0.06179	0.123316
	0.425	3.02537	0.512756			−0.1641	0.38647

Table 3. Comparison of the energy spectra of the 13 excited states in a uniform magnetic field (in Rydberg units).

State	Authors	$\gamma = 0.005$	$\gamma = 0.02$	$\gamma = 0.05$	$\gamma = 0.1$	$\gamma = 0.2$
2S	Jason[35]	−0.2498	−0.2472	−0.2335	−0.1916	−0.06715
	Smith[31]	−0.2498	−0.2472	−0.2340		−0.09785
	$E_{\rm vp}$	−0.24982	−0.2472	−0.2335	−0.1916	−0.06715
	$E_{\rm VIPM}$	−0.24983	−0.2473	−0.2342	−0.1972	−0.09761
$2P_{-1}$	Jason	−0.2548	−0.2676	−0.2857	−0.2990	−0.2879
	Smith	−0.2549	−0.2676	−0.2861		−0.3007
	$E_{\rm vp}$	−0.2549	−0.2676	−0.2858	−0.2990	−0.2879
$2P_0$	Jason	−0.2499	−0.2488	−0.2427	−0.2227	−0.1575
	Smith	−0.2499	−0.2488	−0.2429		−0.1702
	$E_{\rm vp}$	−0.2499	−0.2488	−0.2427	−0.2227	−0.1576
	$E_{\rm VIPM}$	−0.24993	−0.24881	−0.2428	−0.2242	−0.1684
$2P_1$	Jason	−0.2448	−0.2276	−0.1857	−0.0990	0.1120
	Smith	−0.2448	−0.2276	−0.1861		
	$E_{\rm vp}$	−0.2449	−0.2276	−0.1858	−0.0992	0.1121
3S	Jason	−0.1102	−0.09860	−0.05025	0.06247	0.3339
	Smith	−0.1101	−0.09727	−0.04939		0.1778
	$E_{\rm vp}$	−0.1103	−0.09860	−0.05025	0.06247	0.3340
	$E_{\rm VIPM}$	−0.1103	−0.10287	−0.10207	−0.15019	−0.3367
$3P_0$	Jason	−0.1106	−0.1043	−0.07550	−0.0033	0.1782
	Smith	−0.1106	−0.1047	−0.08276		0.0521
	$E_{\rm vp}$	−0.1107	−0.1043	−0.07550	−0.00336	0.1782
	$E_{\rm VIPM}$	−0.1107	−0.1052	−0.08968	−0.07243	−0.0644
$3P_{-1}$	Jason	−0.1152	−0.1181	−0.09814	−0.03218	0.1464
	Smith	−0.1152	−0.1182	−0.1025		0.02174
	$E_{\rm vp}$	−0.1152	−0.1181	−0.09815	−0.03218	0.1464
$3P_1$	Jason	−0.1052	−0.07810	0.00186	0.1678	0.5464
	Smith	−0.1052	−0.08416			
	$E_{\rm VIPM}$	−0.1052	−0.07810	−0.000735	0.1573	0.5134
$3D_{-2}$	Jason	−0.1204	−0.1411	−0.1612	−0.1656	−0.1318
	Smith	−0.1204	−0.1414	−0.1635		−0.1606
	$E_{\rm vp}$	−0.1204	−0.1411	−0.1612	−0.1657	−0.1319
$3D_{-1}$	Jason	−0.1156	−0.1243	−0.1255	−0.1033	−0.02176
	Smith	−0.1156	−0.1245	−0.1282		−0.06225
	$E_{\rm vp}$	−0.1157	−0.1243	−0.1255	−0.1034	−0.02176
$3D_0$	Jason	−0.1107	−0.1053	−0.08063	−0.01727	0.1444
	Smith	−0.1108	−0.1072	−0.09096		0.05843
	$E_{\rm vp}$	−0.1107	−0.1054	−0.08063	−0.01727	0.1445
$3D_1$	Jason	−0.1056	−0.08431	−0.02550	0.09664	0.3782
	Smith	−0.1056	−0.08449			
	$E_{\rm vp}$	−0.1057	−0.08431	−0.02550	0.09664	0.3782
$3D_2$	Jason	−0.1004	−0.06114	0.03879	0.2343	0.6681
	Smith	−0.1004	−0.07821			
	$E_{\rm vp}$	−0.1004	−0.06114	0.03879	0.23435	0.6681

4. Discussion

A number of calculations have been proposed for studying the effect of a magnetic field on the spectrum of the hydrogen. We construct the first-order corrected wave functions consisting of a few terms and calculate the second-order energy corrections for the ground state and some lower excited states by applying the VIPM to the hydrogen atom in a strong uniform magnetic field. In general, it is quite hard to esti-

mate the error occurred in the calculation. Therefore, we try to assure the validity of the present calculation by a systematic comparison with the other methods.

Table 1 shows some energy values for $\gamma = 0.1$. The second column shows the variational parameter, the third column is the result of the first-order perturbation theory, the fourth column is the result obtained by using the simple parameter variational method,[35] and the last column is the result obtained by using the variational-integral perturbation method.

These values are compared with those obtained by Guth *et al.*[25,26] (using the first-order perturbation theory), Gallas[35] (using the simple basis variational method), Praddaude[27] (using the variational calculation with Laguerra polynomials in the cylindrical coordinates), and Killingbeck[28] (using the Zeeman Hamiltonian plus series method). We can clearly see the effect of the simple parameter variational method on the perturbation calculations. The results obtained by the VIPM are better than those by other methods.

Table 2 shows a similar comparison at higher field strengths for some states calculated by Peek and Katriel[33] and Cohen and Herman.[34] Peek and Katriel numerically solved a pair of self-consistent equations in the prolate spherical coordinates, Cohen and Herman used a combination method of the perturbation theory and the variational calculation, and Gallas[35] used the simple basis variational calculation. For the $2P_0$ state, the values obtained by the VIPM are all negative, while the results obtained by the other methods are positive, thus the other methods are expected to lose accuracy quickly. Table 2 shows that the results of the VIPM are more accurate than those of the other calculations.

Table 3 shows the field evolution of the 13 lowest excited states above the ground state. The results of Smith *et al.* and Gallas[31,35] also contain positive energies, while by using the VIPM, we only obtain negative energies for all states. Applying an elaborated variational calculation, Smith *et al.* used an eigenfunction made of up to 12 Slater-type orbits. The same states in the same field range were investigated by Gallas and Brandi. Brandi[32] used an hydrogen basis with ns, n'd, and n''p function ($1 \leq n \leq 6$, $2 \leq n'' \leq 7$ and $3 \leq n' \leq 8$). Gallas used a simple basis for the hydrogen atoms in magnetic fields, and his results were in good agreement with those from the elaborate calculation, but even better agreement with our VIPM results. Table 3 clearly reveals that the results of the VIPM are better than those of the other calculations.

5. Conclusion

In this paper, we combine the variational-perturbation method with the integral perturbation to construct the VIPM, which is then applied to construct the corrections of the wave functions and the corrected energies for a hydrogen atom in a uniform magnetic field. From Tables 1, 2, and 3, we can clearly see that the results obtained by the VIPM are more accurate than those of the other calculation methods. Therefore, the VIPM can be applied widely to various physical fields. The VIPM is valid not only for non-degenerate quantum systems but also for the degenerate or nearly degenerate systems which cannot be correctly treated by the standard quantum perturbation theory. Furthermore, the VIPM can also be extended to solve some time-dependent problems.

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