Hydrogen atom in a strong magnetic field. II. Relativistic corrections for low-lying excited states

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The highly accurate solution of the Schrödinger equation in the form of common Landau exponential factor multiplied by a power series in two variables, the sine of the cone angle and radial variable is completed by the first-order relativistic correction calculated within the framework of the relativistic direct perturbation theory (DPT). It is found that in contrast to behavior of relativistic corrections for the ground state and $2p_{-1}(m_s=-1/2)$ excited state, which change sign from negative to positive near $B\approx 10^{11}$ G and $B\approx 10^{10}$ G, respectively [Z. Chen and S. P. Goldman, Phys. Rev A **45**, 1722 (1992)], the relativistic corrections for $2s_0(m_s=-1/2)$ and $2p_0(m_s=-1/2)$ excited states are negative for the magnetic field varying in range $0<B<10^{13}$ G. If relativistic correction significantly mix nonrelativistic states the near-degenerate version of DPT is used. The avoided crossings of relativistic levels with $\mu=-1/2$ and $\pi=-1$, evolving from field-free states with principal quantum numbers $n=2,3,4$ are presented.

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I. INTRODUCTION

Hydrogen atom in a static and uniform magnetic field has been studied extensively in both the nonrelativistic and relativistic quantum mechanics for many physical reasons. For example, the measurement of the fine structure, the hyperfine structure, and the Lamb shifts require the use of a constant external magnetic field for their determination. To interpret these observation a precise understanding of the Zeeman effect for a week magnetic field is essential. Starting from the exactly solvable nonrelativistic problem of field-free atom and calculating the effects resulting from the Foldy-Wouthuysen reduction of single Dirac particle, Fermi-Breit interaction and additional radiative and recoil corrections in the framework of degenerate perturbation theory yields an extremely precise analysis of Zeeman splitting [1]. Such precise analysis is still unattainable for strong magnetic fields, which are of considerable interest in astrophysics and solid-state physics [2–6]. Owing to the mixture of spherical and cylindrical symmetries the Dirac or Schrödinger equations are not separable in any coordinate system.

In the framework of relativistic mechanics the behavior of the hydrogen atom in a uniform magnetic field can be considered in principle in two different manners. The more common approach is to solve the Dirac equation variationally (the most accurate lowest energy levels reported to date are obtained when in addition to the Slater-type basis functions [7], also Landau-type basis functions [8,9] have been used). Owing to the fact that the Dirac Hamiltonian is unbounded from below, the variational energy is not necessary an upper bound to the exact eigenvalue. The search for the optimal parameters in the basis is based in this case on the stationary properties of the eigenstates rather than the simple minimization procedure used in the nonrelativistic case.

Alternatively one may solve the Schrödinger equation and then account for relativity in a perturbative manner. The problem of accurate solving of the Schrödinger equation has been treated by several approaches including variational methods [7–9], eigenvalue analysis [10–12], and the finite-element methods [13]. Recently an exact Schrödinger solution in a sense that the energy and the wave function can be computed with any precision, was obtained in the form of common Landau exponential factor multiplied by a power series in the radial variable with the coefficients being polynomials in the sine of the polar angle [14–16]. Terms in the series are connected by explicit recurrent relations and a set of mathematical solutions is generated by starting from appropriate chosen starting values. The approximate physical solution in the form of linear combination of mathematical solutions is then determined by imposing on every radial function at a finite radius $r=R$ the boundary exponential decay [14,17]. Using such type of wave function we have calculated [18] the first-order relativistic correction in the framework of direct perturbation theory (DPT) [19,20]. The accuracy of the total energy matches or exceeds in some cases that of previous fully relativistic calculations [7–9,12].

The cancellation of a large number digits, caused by oscillating terms of power series, leads to the requirement for high computation precision. Both the number and amplitude of oscillating terms of power series increase rapidly with growing R. In consequence, the computational effort increases for excited states which are more radially extended than ground state.

In the previous paper [21] (hereafter referred to as I) the asymptotic behavior of the radial functions (more precise than simple exponential decay) was obtained. It was derived in the form of common exponential factor multiplied by a finite power of radius time a power series in the inverse of radius. A substantial advantage of the method using the inverse power expansion over the method using simple exponential decay as the boundary condition, resides in its high accuracy, which can be obtained at much smaller radius R and which do not require a high-precision arithmetic of hundreds decimal digits.

The aim of this paper is to provide a detailed analysis of the energy spectrum of a few low-lying excited states. Relativistic effects can significantly mix nonrelativistic near-degenerate states and relativistic energy $\mathcal{E}^{(1)}$ through the first

TABLE I. Nonrelativistic energies $E^{(0)}$ and first-order relativistic corrections $E^{(1)}$ for the states $2s_0(m_s=-1/2)$ and $2p_{-1}(m_s=-1/2)$ of hydrogen atom in a magnetic field B (in units of 2.35×10^9 G).

	$2s_0(m_s=-1/2)$		$2p_{-1}(m_s=-1/2)$	
B	$-E^{(0)}$ [a]	$E^{(1)}c^2$	$-E^{(0)}$	$E^{(1)}c^2$
10^{-4}	0.125049965000	−0.03905836	0.125099970000	−0.00780251
10^{-3}	0.125496500159	−0.03902343	0.125997000116	−0.00771379
10^{-2}	0.129651571359	−0.03889913	0.134701144177	−0.00693386
0.1	0.148089155790	−0.04850225	0.200845672373	−0.00421749
1	0.160468982634	−0.03922004	0.456597058424	−0.00334876
2	0.173944705973	−0.04384308	0.599612773602	−0.00285068
4	0.188846463700	−0.05451269	0.787825272030	−0.00118225
10	0.208951829045	−0.07667672	1.125422341839	0.00569476
20	0.223842126804	−0.09945889	1.465508545545	0.01885872
40	0.238199272863	−0.12751738	1.896082532426	0.04624607
100	0.256181570331	−0.17283760	2.634760665299	0.12612566
200	0.268968189189	−0.21338061	3.347145235707	0.24869176
400	0.281029709905	−0.25942407	4.215128283478	0.46680714
1000	0.295857474144	−0.32824668	5.638421079484	1.00898013
2000	0.306241266053	−0.38693856	6.951980031508	1.73564602
4000	0.315928273383	−0.45077194	8.493324580274	2.89266484

[a]For $B\geqslant10$ quoted from I.

order in c^{-2}, cannot be simply calculated as

$$\mathcal{E}^{(1)}=E^{(0)}+E^{(1)}. \tag{1}$$

For this reason the effective equation of the recently developed effective Schrödinger-like Hamiltonian equation (EHA) [22]

$$h_{eff}\varphi=\mathcal{E}s_{eff}\varphi \tag{2}$$

in a model space of near-degenerate nonrelativistic two-component spinors is taken into account. The eigenvectors of the effective equation are spin-mixed functions in a basis of nonrelativistic states, and the eigenvalues are the exact relativistic energies of the corresponding true states. Through the first order in c^{-2}, the effective operators are given by

$$h_{eff}^{(1)}=ph_sp+paVap/c^2, \tag{3}$$

$$s_{eff}^{(1)}=p+pa^2p/c^2, \tag{4}$$

where p stands for the projection onto model space, h_s is nonrelativistic Hamiltonian with electrostatic potential V, and

$$a=\boldsymbol{\sigma}\cdot(\mathbf{p}+\mathbf{A})/2. \tag{5}$$

The vector potential $\mathbf{A}$ can take the form $\mathbf{A}=\mathbf{B}\times\mathbf{r}/2$.

II. DETAILS OF CALCULATIONS

The nonrelativistic hydrogen atom in constant magnetic field $\mathbf{B}=(0,0,\gamma)$ has three good quantum numbers: the magnetic quantum numbers m, m_s, and the z parity ν. Substituting the nonrelativistic function in the general form

$$\Psi(r,\vartheta,\varphi)=e^{im\varphi}(r\sin\vartheta)^{|m|}(r\cos\vartheta)^{\nu}Y_{1/2,m_s}\times\exp\left(-\frac{1}{4}\gamma r^2\sin^2\vartheta\right)\sum_{k=0}^{l}(r\sin\vartheta)^{2k}g_{2k}(r), \tag{6}$$

where

$$g_{2k}(r)=\sum_{i=2k}^{I}A_{i,2k}r^{i-2k}, \tag{7}$$

to the Schrödinger equation for a nonrelativistic particle with spin

$$\left[\frac{1}{2}(\mathbf{p}+\mathbf{A})^2-\frac{Z}{r}+\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi=E\Psi, \tag{8}$$

we obtain a linear formula for generating the coefficients $A_{i,2k}$ [14]:

$$A_{i,2k}=\mathcal{L}(A_{i,2k+2},A_{i-2,2k-2},A_{i-2,2k},A_{i-1,2k}). \tag{9}$$

Following Ref. [14] we generate a set of particular solutions $\Psi^{(p)}$ $(p=0,1,2,\ldots,l)$ by starting from Ref. [18]:

$$A_{0,2k}^{(p)}=\delta_{p,k}, \tag{10}$$

$$A_{i,2k}^{(p)}\equiv0, \quad k>l. \tag{11}$$

For bound state the wave function Ψ tends to zero as r goes to infinity. The radial functions behave in the same way. The asymptotic behavior of g_{2k} was considered in paper I and is given by inverse power expansion of the form

TABLE II. Comparison of the nonrelativistic $E^{(0)}$ and relativistic perturbative $\mathcal{E}^{(1)}$ energies for the $2p_{3/2}(\mu=-3/2)$ excited state of hydrogen atom in an intense magnetic field B (in units of 2.35×10^9 G). The numbers in column 3, 4, and 6 give the previous most accurate nonrelativistic E_{NR} and relativistic E_r results.

B	$-E^{(0)}$	$-E_{NR}$ [a]	$-E_{NR}$ [b]	$-\mathcal{E}^{(1)}$	$-E_r$ [b]
0.1	0.200845672373	0.200845672373	0.20084567237333	0.20084589696	0.200845897
1	0.456597058424	0.456597058424	0.4565970584	0.45659723675	0.45659724
10	1.125422341839	1.125422341839	1.1254223418	1.12542203859	1.12542204
100	2.634760665299	2.634760665299	2.634760665	2.63475394894	2.63475395
200	3.347145235707	3.34714523		3.34713199253	
400	4.215128283478	4.21512828		4.21510342536	
1000	5.638421079484	5.63842108	5.63842105	5.63836734992	5.6383673
2000	6.951980031508			6.95188760599	
4000	8.493324580274			8.49317054193	

[a]Reference [14].
[b]Reference [9].

$$g_{2k}(r)=r^{\eta-\nu-k}p_{2k}(x)\exp(-\kappa r), \tag{12}$$

$$p_{2k}(x)=\sum_{i=0}^{\infty}B_{2k}^{(i)}x^i, \tag{13}$$

where

$$\kappa=\sqrt{2E_b}, \quad \eta=1/\kappa, \quad x=1/r, \tag{14}$$

and

$$E_b=(1+m+|m|+2m_s)B/2-E. \tag{15}$$

Following paper I we generate the set of coefficients $B_{2k}^{(j)}$ until $j=n$ by starting from arbitrary $B_0^{(0)}$ and using linear recurrent relations of the form

$$B_0^{(j)}=\mathcal{L}_0(B_0^{(j-1)},B_2^{(j-1)},B_2^{(j-2)},B_4^{(j-1)}), \tag{16}$$

and

$$B_{2k}^{(j)}=\mathcal{L}_{2k}(B_{2k-2}^{(j)},B_{2k-2}^{(j-1)},B_{2k}^{(j-1)},B_{2k+2}^{(j-1)},B_{2k}^{(j-2)}) \tag{17}$$

for $k>0$. Owing to the asymptotic convergence of expansion (13) the values of $B_{2k}^{(j)}$ disclose a more rapid increase than the geometric progression and the summation over j should be terminated at some value of $j=n$.

An approximate physical solution

$$\Psi=\sum_{p=0}^{l}c_p\Psi^{(p)} \tag{18}$$

is determined by imposing the condition

$$\frac{g'_{2k}(r)}{g_{2k}(r)}=f_{2k}(r)=-\kappa+x(\eta-\nu-k)-x^2\frac{p'_{2k}(x)}{p_{2k}(x)} \tag{19}$$

at finite radius $r=R$. Consequently, the boundary conditions

$$g'_{2k}(R)-f_{2k}(R)g_{2k}(R)=0 \tag{20}$$

can be reduced to a system of $l+1$ homogeneous linear equations for coefficients c_p. Here E_b can be found in the l, R, I, and n approximation from the condition of the linear dependence of this system.

Solving this system of linear equations and choosing the initial values of coefficients

$$A_{0,2k}=c_k, \tag{21}$$

we generate the physical solution Ψ. In the basis set of two component spinors (6) the matrix elements of effective Hamiltonian and effective metric [Eqs. (3) and (4)] can be expressed in terms of the integrals

$$K_{kk'}^{\mu\nu}=\int_0^{\infty}I(a,b,\gamma)r^c g_{2k}^{(\mu)}g_{2k'}^{(\nu)}dr,$$

where a,b, and c are integer numbers, superscripts μ and ν distinguish the states in the model space and $I(a,b,\gamma)$ stands for angular integral

$$\begin{aligned}I(a,b,\gamma)&=\int_0^{\pi}(\sin\vartheta)^{a+1}(\cos\vartheta)^b\exp\left(-\frac{1}{4}\gamma r^2\sin^2\vartheta\right)d\vartheta\\&=\frac{\Gamma\left(\frac{a+2}{2}\right)\Gamma\left(\frac{b+1}{2}\right)}{\Gamma\left(\frac{a+b+1}{2}\right)}\\&\quad\times F\left(\frac{a+2}{2},\frac{a+b+1}{2},-\frac{1}{2}\gamma r^2\right),\end{aligned} \tag{22}$$

where Γ is the gamma function and F is the confluent hypergeometric function which can be calculated by Kummer's formula or by an asymptotic expansion [23]. The radial integral from 0 to R is mapped to the integral from 0 to 1 and evaluated numerically by Gaussian quadrature. The integration from R to ∞ gives negligible impacts to the relativistic effects and for this reason the radial integrals from R to ∞ are neglected.

TABLE III. Nonrelativistic $E^{(0)}$ and relativistic perturbative $\mathcal{E}^{(1)}$ energies calculated in the standard nondegenerate and the effective Hamiltonian near-degenerate perturbation approach for the model space of two nonrelativistic states $2p_0(m_s=-1/2)$ and $2p_{-1}(m_s=1/2)$ of hydrogen atom in a magnetic field B (in units of 2.35×10^9 G).

	$2p_0$		$2p_{-1}$		EHA	
B	$-E^{(0)}$	$-\mathcal{E}^{(1)}$	$-E^{(0)}$	$-\mathcal{E}^{(1)}$	$-\mathcal{E}_1^{(1)}$	$-\mathcal{E}_2^{(1)}$
0	0.125000000000	0.125000970725	0.125000000000	0.125001525425	0.125002081244	0.125000416025
10^{-6}	0.125000499999	0.125001470720	0.124999999997	0.125001525420	0.125002282959	0.125000713181
10^{-5}	0.125004999850	0.125005970541	0.124999999700	0.125001525111	0.125006104738	0.125001390914
10^{-4}	0.125049985000	0.125050955392	0.124999970000	0.125001495292	0.125050967663	0.125001483022
10^{-3}	0.125498500042	0.125499467481	0.124997000116	0.124998524311	0.125499468548	0.124998523244
10^{-2}	0.129850415833	0.129851357419	0.124701144177	0.124702666403	0.129851357483	0.124702666338
0.1	0.162410078399	0.162410980720	0.100845672373	0.100847819138	0.162410980722	0.100847819137

III. NUMERICAL RESULTS AND DISCUSSION

In relativistic case 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. There is unique correspondence between the two nonrelativistic excited states $2s_0(m_s=-1/2)$ and $2p_{-1}(m_s=-1/2)$ and two relativistic states $2s_{1/2}(\mu=-1/2,\pi=+1)$ and $2p_{3/2}(\mu=-3/2,\pi=-1)$. Table I lists the nonrelativistic energies and first-order relativistic corrections obtained in the spirit of nondegenerate perturbation approach for well energetically isolated nonrelativistic states evolving from atomic states $2s_0$ and $2p_{-1}$ of same principal number $n=2$, projection of spin $m_s=-1/2$, and z parity $\nu=0$ but different m values. The maximal absolute error of each value displayed in Table I does not exceed ±1 in the last digit.

It should be observed that for the $2p_{3/2}(\mu=-3/2)$ excited state the relativistic correction changes sign near $B=5$ and then increases considerably with growing intensity of magnetic field. The absolute value of relativistic correction for $B=4000$ is two orders of magnitude greater than for field-free atom. This is in full agreement with previous results of generalized relativistic variational calculations [9] and very similar to the dependence of the relativistic correction for the ground state [7,18]. Quite different behavior disclose the relativistic corrections for the $2s_{1/2}(\mu=-1/2)$ excited state. It is negative for all values of magnetic field displayed in Table I. To our knowledge for this excited state there is no fully relativistic results for comparison in the literature. A comparison with previous results for the state evolving from $2p_{3/2}$ is made in Table II. The calculations have been performed with $c=137.035\,989\,5$ [24]. A 12-figure accuracy of the present nonrelativistic results exceeds for $B\geqslant200$ that of previous calculations. The accuracy of perturbation results through the first order in c^{-2} matches that of previous fully relativistic calculations.

Two others of lowest excited $(n=2)$ nonrelativistic states $2p_0(m_s=-1/2)$ and $2p_{-1}(m_s=1/2)$ have in magnetic field the same relativistic symmetry $(\mu=-1/2$ and $\pi=-1)$. Since for small intensities of magnetic field the relativistic perturbation and the magnetic interaction are comparable, the effective relativistic eigenfunctions in two-dimensional nonrelativistic model space are strongly mixed. The transformation matrix from nonrelativistic states $2p_0$ and $2p_{-1}$ to relativistic eigenfunctions $2p_{1/2}$ and $2p_{3/2}$ is given in the field-free limit by

TABLE IV. Nonrelativistic energies $E^{(0)}$, first-order relativistic corrections $E^{(1)}$ and relativistic perturbative energies $\mathcal{E}^{(1)}$ for the state $2p_0(m_s=-1/2)$ of hydrogen atom in a magnetic field B (in units of 2.35×10^9 G).

B	$-E^{(0)}$	$E^{(1)}c^2$	$-\mathcal{E}^{(1)}$
1	0.260006615944	−0.05108661	0.260009336375
2	0.297710972385	−0.08256629	0.297715369153
4	0.335695728671	−0.13473441	0.335702903462
10	0.382649848306	−0.25043170	0.382663184136
20	0.413377734222	−0.38443574	0.413398205949
40	0.438733801355	−0.56492728	0.438763884502
100	0.463617764477	−0.87516918	0.463664368427
200	0.476532014388	−1.15701265	0.476593626760
400	0.485363074873	−1.46926971	0.485441315486
1000	0.492495007408	−1.91188465	0.492596817870
2000	0.495594803690	−2.25912955	0.495715105416
4000	0.497463531134	−2.61114956	0.497602578405

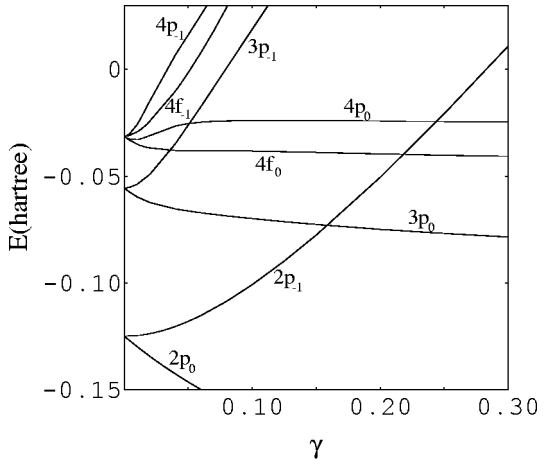

FIG. 1. Behavior of slightly excited nonrelativistic levels with $\mu=m+m_s=-1/2$ and $\pi=-1$, evolving from field-free states with principal quantum numbers $n=2$, 3, and 4.

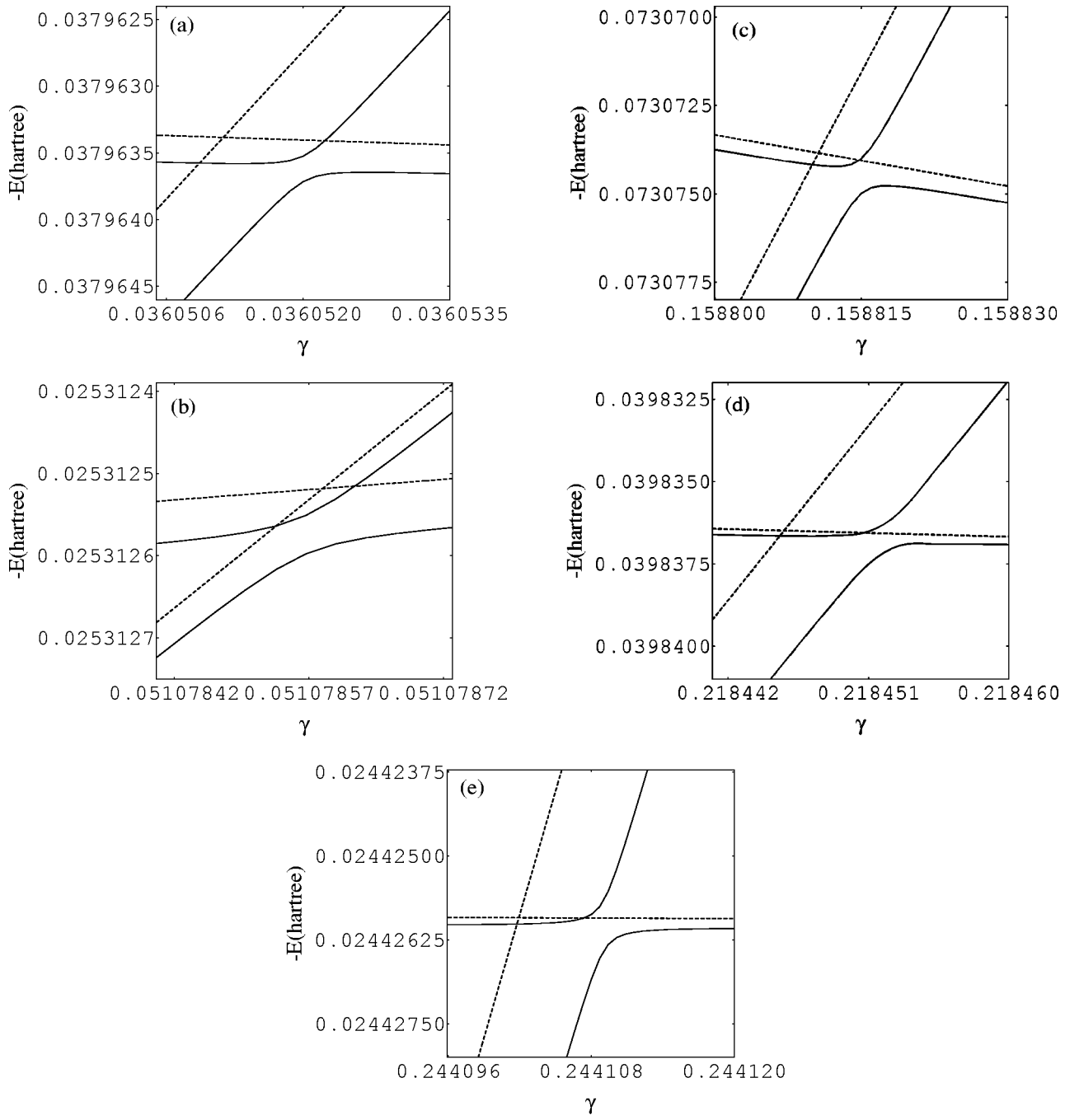

FIG. 2. Crossings (ordered according to increasing intensity of magnetic field) of nonrelativistic levels: (a) $3p_{-1}(m_s=+1/2)$ and $4f_0$ $(m_s=-1/2)$, (b) $3p_{-1}(m_s=+1/2)$ and $4p_0(m_s=-1/2)$, (c) $2p_{-1}(m_s=+1/2)$ and $3p_0(m_s=-1/2)$, (d) $2p_{-1}(m_s=+1/2)$ and $4f_0(m_s=-1/2)$, (e) $2p_{-1}(m_s=+1/2)$ and $4p_0(m_s=-1/2)$ (dashed lines), and avoided crossings between relativistic levels with $\mu=-1/2$ and $\pi=-1$ (solid lines).

$$\frac{1}{\sqrt{3}}\begin{pmatrix} 1 & \sqrt{2} \\ -\sqrt{2} & 1 \end{pmatrix}.$$

There is no unique correspondence between the two nonrelativistic and the two relativistic states. Nondegenerate DPT break down in such cases. The EHA-DPT recovers the relativistic splitting already at the first order, while nondegenerate DPT yields vanishing spin orbit coupling. As a numerical illustration of this case of near-degeneracy we display in Table III the zeroth-order nonrelativistic energies, the nondegenerate perturbative energies through the first order and the EHA energies in a model space spanned by two nonrelativistic orthogonal two-component reference states evolving from $2p_0(m_s=-1/2)$ and $2p_{-1}(m_s=1/2)$. One can see that with growing intensity of magnetic field the considered states become well energetically separated and for $B\geqslant 0.1$ the difference between nondegenerate DPT and EHA-DPT results are negligible. Table IV lists the nonrelativistic energy, first-order relativistic correction and total relativistic

energy up to first order of the state evolving from nonrelativistic state $2p_0(m_s=-1/2)$ for $1\leqslant B\leqslant 4000$. Relativistic correction is negative for all values of magnetic field and its magnitude increases considerably with growing intensity of magnetic field (much faster than for the $2s_0$ excited state displayed in Table I).

Energy of state $2p_{-1}(m_s=1/2)$ goes quickly up and near $B=0.3$ reaches zero [compare Table I; according to Eq. (18) $E(m_s=1/2)=E(m_s=-1/2)+B$]. Therefore there are many crossings of this state with other states in nonrelativistic case and many avoided crossings in the relativistic case. In similar way behave the next excited states with $m_s=1/2$ $(3p_{-1},4p_{-1},4f_{-1},\ldots)$. Figure 1 shows the general picture of levels with $\mu=m+m_s=-1/2$ and $\pi=-1$ evolving from field-free states with principal quantum numbers 2, 3, and 4. Figure 2 demonstrates that relativity causes lowering of the energy and avoided crossing due to breaking the symmetry.

We have shown in this paper that accurate first-order relativistic energy corrections for excited states of hydrogen atom in a magnetic field can be obtained in the framework of direct perturbation theory using a highly accurate series solution of the Schrödinger equation. The accuracy of the total energy matches or exceeds in some cases that of previous fully relativistic calculations. The main advantage of the perturbation approach is that like the nonrelativistic case [25], the relativistic energy corrections with $Z\neq 1$ can be calculated by a simple scaling relation [26]:

$$E^{(i)}(Z,B)=Z^{2(i+1)}E^{(i)}(1,B/Z^2) \tag{23}$$

and there is no necessity to perform separate calculations for different values of Z.

The problem of the hydrogen atom, placed in a uniform magnetic field has important applications in such different areas of physics as atomic spectroscopy, solid-state physics, and astrophysics. Our calculations indicate the necessity to include relativistic corrections given the current numerical accuracy of the nonrelativistic calculations. It is especially pronounced for excited states because for high intensities of magnetic field the first-order relativistic energy correction can be a few orders of magnitude greater than for field-free atom. Depending on the state considered and intensity of the field the relativistic energy corrections have different signs what gives considerable impact to the spectral lines. In astronomy, the knowledge of the spectrum of the atomic hydrogen in magnetic field will help in accurate measurements of stellar magnetic fields (about 10^6–10^9 G on white dwarfs [3] and 10^{11}–10^{13} G on neutron stars [4]).

The technique presented in the present work is effective and ensures a high accuracy of calculations. One may hope that this approach will find also its application in testing various approximate methods.

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