Three-dimensional hydrogen atom in crossed magnetic and electric fields

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We give a solution of the three-dimensional Schrödinger equation for the electron of a hydrogen atom in external electric and magnetic fields of arbitrary mutual orientation. The rearrangement of the energy spectrum due to changing in the mutual orientation of the fields is evaluated by using the $n=2$ multiplet as an example. The calculations agree with second-order perturbation formulas that exist for the special cases of mutually parallel and orthogonal fields. For another special two-dimensional case which is currently being extensively investigated, namely, the hydrogen atom in a strong magnetic field, our approach agrees with calculations by other authors and yields more accurate binding energies for certain low-lying excited states that have been considered.

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I. INTRODUCTION

One of the basic quantum-mechanical problems, namely, the hydrogen atom in electromagnetic fields, has been of great importance for the progress of quantum theory and is still of significant interest because of its numerous physical applications. A large number of publications deal with partial aspects of the problem. The present paper is devoted to the solving of the three-dimensional Schrödinger equation for the electron of the hydrogen atom in external magnetic **B** and electric **F** fields of arbitrary mutual orientation. Although the problem has a history as long as quantum mechanics itself, only a few quantitative results have been obtained here for special cases of weak fields in the framework of perturbation theory so far. Initially, the problem was studied within the old quantum theory by Epstein (cf. [1]) and its quantal treatment was given in [2]. In both papers, the first order of perturbation theory was considered for weak fields **B** and **F** of arbitrary mutual orientation. The second-order formula was obtained in [3] and an equation for an additional second-order correction, which may completely lift the residual degeneracy of hydrogen levels for the case $\mathbf{B}\perp\mathbf{F}$, was analyzed [4]. The higher-order corrections B^2F^2 and B^2F^4 to the ground state of the two examples $\mathbf{B}\|\mathbf{F}$ and $\mathbf{B}\perp\mathbf{F}$ were computed in [5]. We also have to mention a quasiclassical analysis of the problem for $\mathbf{B}\perp\mathbf{F}$ [6]; this work offers a qualitative investigation of an interesting possibility where within the hydrogen atom the electron may be localized separately of the nucleus at a certain distance from the center of the Coulomb well, which gives rise to a large dipole moment of the ground state of the system.

In the general case of arbitrary mutual orientation of the fields the separation of variables is not possible. To solve this three-dimensional problem we use a method suggested by us in an earlier paper [7]. This approach has been applied to a number of two-dimensional examples, both for scattering and for the discrete spectrum of the Schrödinger equation. In particular, it has been demonstrated that the method converges quickly for the two-dimensional problem of a hydrogen atom in a homogeneous magnetic field [7]. An extension to a three-dimensional case, taking as an example a bound state of the helium atom, has been considered in [8].

In Sec. II, the formulation of the problem and the essence of the applied method are presented. In Sec. III, we consider a two-dimensional special case that is at present being investigated extensively, namely, the hydrogen atom in a strong magnetic field ($|\mathbf{B}|\geq 10^9$ G, $\mathbf{F}=\mathbf{0}$). Apart from the known applications in astrophysics, solid-state physics, and in chaotic studies (discussions of physical applications may be found in [9–11], and references therein), the problem has recently attracted attention as a convenient way of calibrating different approaches for solving the Schrödinger equation without separation of variables. By modifying the strength of the magnetic field $|\mathbf{B}|$, it is possible to change dramatically the wave function of the system from the Coulomb ($|\mathbf{B}|=0$) to the Landau ($|\mathbf{B}|=\infty$) limit. For solving the problem, variational methods ([12], and references therein), the adiabatic approach [13], the modified Hartree-Fock approach [14], finite-element methods [15,16], and Kato's method [17] have been applied recently. Only a few of the most successful analyses using different approaches are mentioned here. A complete list of publications devoted to this problem can be found in the papers cited above. The accuracy achieved by a recent, more refined method [12] for the ground state is better than 1 part in 10^7 for fields $|\mathbf{B}|\simeq 10^{19}$ G and better than 1 part in 10^{16} for $|\mathbf{B}|\leq 10^8$ G, which allows one to take into consideration relativistic corrections as well. We demonstrate that our approach is comparable in accuracy with the advanced variational finite-basis method [12] for the ground state of the problem and that it is more accurate for some of the low-lying states to be analyzed here.

An extension of the approach to the general three-dimensional case of nonzero fields **B** and **F** arbitrarily oriented to one another is given in Sec. IV, where the

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evolution of the electron state $n=2$ as a function of the angle $\alpha\in[0,\pi/2]$ between the fields and the relative strength $\eta=3n|\mathbf{F}|/|\mathbf{B}|$ of the fields is analyzed. For the limited cases $\alpha=0$ ($\mathbf{F}\|\mathbf{B}$) and $\alpha=\pi/2$ ($\mathbf{F}\perp\mathbf{B}$), the obtained results agree with perturbation theory [3,4]. The convergence of the method is demonstrated for these two mutual orientations and for different relative strengths ($\eta<1$, $\eta=1$, and $\eta>1$) of the fields. In Sec. V, possible applications of the obtained results and a possible extension of the usage of the method are discussed.

II. FORMULATION OF THE PROBLEM AND METHOD OF CALCULATION

The nonrelativistic Hamiltonian of a hydrogen electron in external electric field $\mathbf{F}$ and magnetic field $\mathbf{B}$ has a form:

$$H(R,\theta,\phi)=-\tfrac{1}{2}\Delta_{\mathbf{R}}-\frac{1}{R}+\tfrac{1}{2}(\mathbf{B}\cdot\mathbf{L})+\tfrac{1}{8}[\mathbf{B}\cdot\mathbf{R}]^2+(\mathbf{F}\cdot\mathbf{R}) , \tag{1}$$

where $\mathbf{R}=(R\sin\theta\cos\phi, R\sin\theta\sin\phi, R\cos\theta)$ is the radius vector of the electron and $\mathbf{L}$ is its orbital angular momentum. The Hamiltonian is written in atomic units, $\hbar=e=m_e=1$; the units of the electric and magnetic fields strengths are equal to $F_0=e^5m_e^2/\hbar^4\simeq 5.14\times10^9$ V/cm, $B_0=(e/\hbar)^3m_e^2c\simeq 2.35\times10^9$ G.

We introduce a coordinate frame in such a way that the vectors $\mathbf{B}$ and $\mathbf{F}$, which form an arbitrary angle α, determine the plane $y=0$ and the z axis coincides with the direction of the field $\mathbf{B}$:

$$\mathbf{B}=\beta\mathbf{n}_B, \quad \mathbf{F}=\gamma\mathbf{n}_F ,$$

where $\mathbf{n}_B=(0,0,1)$ and $\mathbf{n}_F=(\sin\alpha,0,\cos\alpha)$ are unit vectors and β and γ are the strengths of the magnetic and electric fields, respectively. In this case, the Hamiltonian is reduced to the form

$$H(R,\theta,\phi)=-\frac{1}{2R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R}+U(R,\theta,\phi)+\frac{1}{2R^2}L^2(\theta,\phi) , \tag{2}$$

where

$$L^2(\theta,\phi)=-\frac{1}{\sin\theta}\left[\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}\right] ,$$

$$U(R,\theta,\phi)=-\frac{1}{R}-i\frac{\beta}{2}\frac{\partial}{\partial\phi}+\frac{(\beta R)^2}{8}\sin^2\theta+\gamma R(\sin\theta\cos\phi\sin\alpha+\cos\theta\cos\alpha) .$$

An essential point of the method [7] for solving the Schrödinger equation with the Hamiltonian (2) is the reduction of the partial differential equation

$$\{H(X)-\varepsilon\}\psi(X)=0 \tag{3}$$

in the multidimensional space $X=\{R,\Omega\}$ to a system of differential difference equations in terms of one of the variables R. To make the procedure more efficient we have exploited the following idea (which has been developed in collocation [18,19] and pseudospectral methods [20,21]): to approximate the unknown wave function $\psi(X)$ that is to be calculated, we use a set of global basis functions on a difference grid Ω_k (and not a local pointwise basis as used in the standard discrete analysis of finite differences or finite elements). This idea has already been successfully applied in quantum chemistry to solve Schrödinger-type equations (the "discrete variable representation" of Light and co-workers [22–24]) and Hartree-Fock equations (the "pseudospectral method" of Friesner [25,26]), where hybrid computational schemes based on manipulating a basis set and a physical space grid have been developed to increase the efficiency of computations.

Below we give a brief account of our approach [7] with more detailed consideration of the peculiarities of problem (2). In space X subspace Ω is defined, and from the D-dimensional Hamiltonian (3) a $(D-1)$-dimensional Hamiltonian $h_0(\Omega)$ with an orthogonal set of eigenfunctions $\varphi_\mu(\Omega)$ is extracted:

$$H(X)=-\frac{1}{2R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R}+U(R,\Omega)+f(R)h_0(\Omega) . \tag{4}$$

In subspace Ω a difference grid Ω_k ($k=1,2,\ldots,N$) is introduced, in whose nodes the values of the wave function that is to be calculated are

$$\psi(R,\Omega)\Longrightarrow\psi(R,\Omega_k)=\frac{1}{R}\psi_k(R) . \tag{5}$$

Furthermore, a discrete index ν ($\nu=1,2,\ldots,\infty$) is introduced, which corresponds to the set $\{\mu\}$ of quantum numbers that characterize the system of basis functions $\varphi_\mu(\Omega)$. Now the set of the first N eigenfunctions $\varphi_\nu(\Omega)$ ($\nu=1,2,\ldots,N$) of the Hamiltonian $h_0(\Omega)$ at the nodal points Ω_k forms a square matrix $\varphi_{k\nu}=\{\varphi_\nu(\Omega_k)\}$ of dimension $N\times N$. Assuming the system $\varphi_\nu(\Omega)$ to be a Chebyshev set on Ω [27], we introduce the inverse matrix φ^{-1}_{kj} and represent the wave function $\psi(R,\Omega)$ we want to calculate as an expansion

$$\psi(R,\Omega)=\frac{1}{R}\sum_{j=1}^{N}\left[\sum_{\nu=1}^{N}\varphi_\nu(\Omega)\varphi^{-1}_{\nu j}\right]\psi_j(R) \tag{6}$$

in terms of the basis functions $\varphi_\nu(\Omega)$.

For this expansion relation (5) is fulfilled automatically, and the relations

$$(h_0(\Omega)\psi(R,\Omega))_{\Omega=\Omega_k}=\frac{1}{R}\sum_{j=1}^{N}\left[\sum_{\nu=1}^{N}\varphi_{k\nu}\epsilon_\nu\varphi^{-1}_{\nu j}\right]\psi_j(R) , \tag{7}$$

$$(U(R,\Omega)\psi(R,\Omega))_{\Omega=\Omega_k}=\frac{1}{R}\sum_{j=1}^{N}U(R,\Omega_k)\times\left[\sum_{\nu=1}^{N}\varphi_{k\nu}\varphi^{-1}_{\nu j}\right]\psi_j(R)=\frac{1}{R}U(R,\Omega_k)\psi_k(R) \tag{8}$$

are valid. Here ϵ_ν is the eigenvalue of the Hamiltonian h_0 that corresponds to the eigenfunction $\varphi_\nu(\Omega)$. By substituting expansion (6) into the Schrödinger equation (3) and using relations (7) and (8), we obtain a system of N differential difference equations:

$$F_1(z)=\sum_{j=1}^{N}\left[\delta_{kj}\frac{d^2}{dR^2}+2[\delta_{kj}\varepsilon-V_{kj}(R)]\right]\psi_j(R)=0\ , \tag{9}$$

where

$$V_{kj}(R)=U(R,\Omega_k)\delta_{kj}+\sum_{\nu=1}^{N}\varphi_{k\nu}\epsilon_\nu\varphi_{\nu j}^{-1}f(R)\ .$$

In [7] it was shown for the two-dimensional case how Eqs. (9) may be transformed to the equations of the discrete variable representation [22].

Following papers [28,29], we formulate the eigenvalue problem for the system of Eqs. (9) as a nonlinear equation $F(z)=0$ for an unknown eigenvalue ε and eigenfunctions $\psi_k(R)$, $z=\{\varepsilon,\psi_k(R)\}$, by adding to the equation $F_1(z)=0$ boundary conditions at $R=0$ and $R=R_m\to\infty$ and a normalization condition:

$$\begin{aligned}&F_2(z)=\psi_k(0)=0\ ,\quad F_3(z)=\psi_k(R_m)=0\ ,\\ &F_4(z)=\sum_{k,j}^{N}\int\psi_k(R)\psi_j(R)dR-1=0\ .\end{aligned} \tag{10}$$

In approach [29] both the eigenvalue and the scattering problem for the system of equations (9) are formulated as a functional equation $F(z)=0$, which is solved by Newton's method. So the same computing technique can be applied for calculating the bound states as well as the ionization of a hydrogen atom by the electric field.

Let us formulate problem (9) and (10) for a hydrogen atom in arbitrarily oriented magnetic and electric fields (2). For this case it is convenient to define subspace Ω as a rectangle $\Omega=\{x,\phi\}$, where $x=-\cos\theta\in[-1,1]$, $\phi\in[0,2\pi]$, and to choose the Hamiltonian $h_0(\Omega)$ as $L^2(x,\phi)$ with basis functions $\varphi_\nu(\Omega)$ defined by

$$\varphi_\nu(\Omega)=P_l^m(x)\times\begin{cases}\cos m\phi, & m\geq 0\\ \sin|m\phi|, & m<0\ ,\end{cases} \tag{11}$$

where $P_l^m(x)$ are the associated Legendre polynomials, $\nu=\{l,m\}$.

We will look for the wave function $\psi(R,\Omega)$ as an expansion

$$\psi(R,\Omega)=\frac{1}{R}\sum_{j=1}^{N}\left[\sum_{\nu=1}^{N}\varphi_\nu(\Omega)\varphi_{\nu j}^{-1}\right][\psi_j(R)+i\bar{\psi}_j(R)] \tag{12}$$

containing both real $\psi_j(R)$ and imaginary $\bar{\psi}_j(R)$ parts. By substituting this expansion into the Schrödinger equation (3) with Hamiltonian (2), we obtain a system of differential difference equations

$$F_1(z)=\begin{Bmatrix}\sum_{j=1}^{N}\left[\delta_{kj}\frac{d^2}{dR^2}+2[\delta_{kj}\varepsilon-V_{kj}(R)]\right]\psi_j(R)+\sum_{j=1}^{N}\bar{V}_{kj}(R)\bar{\psi}_j(R)\\ \sum_{j=1}^{N}\left[\delta_{kj}\frac{d^2}{dR^2}+2[\delta_{kj}\varepsilon-V_{kj}(R)]\right]\bar{\psi}_j(R)-\sum_{j=1}^{N}\bar{V}_{kj}(R)\psi_j(R)\end{Bmatrix}=0\ , \tag{13}$$

where

$$\begin{aligned}V_{kj}(R)&=\left[-\frac{1}{R}+\frac{(\beta R)^2}{8}(1-x_k^2)+\gamma R(\sqrt{1-x_k^2}\cos\phi_k\sin\alpha-x_k\cos\alpha)\right]\delta_{kj}+\frac{1}{2R^2}\sum_{\nu=\{l,m\}=1}^{N}l(l+1)\varphi_{k\nu}\varphi_{\nu j}^{-1}\ ,\\ \bar{V}_{kj}(R)&=\beta\sum_{\nu=1}^{N}\frac{\partial\varphi_\nu(\Omega)}{\partial\phi}\bigg|_{\Omega=\Omega_k}\varphi_{\nu j}^{-1}\ .\end{aligned} \tag{14}$$

In those equations the summation indices take the following values:

$$\begin{aligned}&k=\{k_\theta,k_\phi\}\ ,\quad k_\theta=1,\ldots,N_\theta\ ,\quad k_\phi=1,\ldots,N_\phi\ ,\\ &j=\{j_\theta,j_\phi\}\ ,\quad j_\theta=1,\ldots,N_\theta\ ,\quad j_\phi=1,\ldots,N_\phi\ ,\\ &\nu=\{l,m\}\ ,\quad l=0,1,\ldots,N_\theta-1\ ,\quad m=-(N_\phi-1),\ldots,(N_\phi-1)\ ,\\ &N_\theta=N_\phi\ ,\quad N=N_\theta N_\phi\ .\end{aligned}$$

III. HYDROGEN ATOM IN A STRONG MAGNETIC FIELD

We start the analysis of problem (13) and (14) from a special case $\beta\geq 1$, $\gamma=0$, i.e., a hydrogen atom in a strong magnetic field. Also, we do not include the term $-i(\beta/2)\partial/\partial\phi$, which is linear in the magnetic-field strength β, in the Hamiltonian (2) in order to have the possibility of direct comparison with the analyses of other authors. As in this instance the variable ϕ may be separated, the initial three-dimensional problem is reduced to the problem on the plane $X=\{R,x\}$, which al-

TABLE I. Binding energies E_v of the ground state $v=(1s_0/000)$ of the hydrogen atom in a magnetic field β.

Source \ β	1	2	20	200	2000
Ref. [13][a]		1.636 4		2.292 4	18.550 8
		2.120 0		2.477 4	18.620 4
Ref. [14][b]	1.662 338	2.044 428	4.430 797	9.453 1/50	18.608 96/986
Ref. [16][c]		2.044 426	4.430 786	9.454 16	18.609 28
Ref. [17][d]	1.662 337 793 2	2.044 427 816	4.430 792		
	1.662 337 794 6	2.044 427 820	4.431 826		
Ref. [12][e]	1.662 337 793 46	2.044 427 815 32	4.430 797 030	9.454 290 216	18.609 530 0
Present work	1.662 337 793 49	2.044 427 815 36	4.430 797 031	9.454 290 22	18.609 52

[a]Adiabatic approximation of Liu and Starace, giving both lower and upper limits for binding energies.
[b]Modified Hartree-Fock approach of Rösner *et al.* The value calculated with maximum number of expansion terms being used (n_c) is given before the slash; after the slash are the last figures of the value still changing if the two binding energies last computed are linearly extrapolated to $1/n_c \to 0$.
[c]Finite-element analysis of Shertzer.
[d]Lower and upper bounds obtained using Kato's method by Fonte *et al.*
[e]Variational finite-basis-set evaluation of Goldman and Chen.

lows one to use as the basis set $\varphi_\nu(\Omega)$ in expansion (12) the Legendre polynomials $P_l(x)$ instead of the two-dimensional basis functions (11). Also, as the Hamiltonian defined in such a way does not keep the terms that violate the wave-function symmetry relative to inversion ($x \to -x$), one may use either even or odd polynomials $P_l(x)$, depending on the z parity of the state one is seeking. Now the imaginary part of expansion (12) is equal to zero, and the effective potentials $V_{kj}(R)$ (14) of the system of Eqs. (13) are reduced to:

$$V_{kj}(R)=\left[-\frac{1}{R}+\frac{(\beta R)^2}{8}(1-x_k^2)\right]\delta_{kj} + \frac{1}{2R^2}\sum_{\nu=1}\nu(\nu-1)P_{\nu-1}(x_k)P_{kj}^{-1}, \quad (15)$$

where the summation index ν takes the values $\nu=1,3,\ldots,2N_x-1$ or $\nu=2,4,\ldots,2N_x$ for the respective states with positive or negative z parity, and the negative nodes of the $2N_x$-point Gauss quadrature on $[-1,1]$

TABLE II. Binding energies E_v of the low-lying excited states $v=(nl_m/n'm\nu)$ of the hydrogen atom in a magnetic field β.

State	Source \ β	1	2	20	200
$(2p_0/001)$	Ref. [13][a]	0.511 4	0.590 0		0.954 8
		0.524 4	0.598 2		0.955 0
	Ref. [14][b]	0.520 013 2	0.595 421 9	0.826 754 5/72	0.953 064 0/1
	Present work	0.520 013 779	0.595 422 153	0.826 756	0.953 0
$(2s_0/002)$	Ref. [13][a]	0.271 4	0.314 8		0.538 0
		0.318 8	0.348 8		0.540 0
	Ref. [14][b]	0.320 937 9	0.347 888 0	0.447 62/73	0.537 921/45
	Present work	0.320 938 144	0.347 889 41	0.447 678	0.537
$(3d_0/004)$	Ref. [14][b]	0.132 02/63	0.138 41/66	0.160 647/74	
	Present work	0.132 465 93	0.138 551 0	0.160 65	
$(3s_0/006)$	Ref. [14][b]	0.071 28/53	0.073 658/753		
	Present work	0.071 464 5	0.073 721 9		

[a]Adiabatic approximation of Liu and Starace.
[b]Modified Hartree-Fock approach of Rösner *et al.*

TABLE III. The convergence of the ground-state energy values E_v as a function of the number of terms, N_x, included in expansion (12) for various magnetic fields β.

N \ β	1	20	200	2000
8	1.662 337 793 449			
12		4.430 773 182		
16	1.662 337 793 593			
24	1.662 337 793 593	4.430 797 011		
32		4.430 797 012	9.454 276 938	
40			9.454 289 557	
48			9.454 290 139	
60			9.454 290 169	18.608 963
70			9.454 290 172	18.609 424
80				18.609 506
90				18.609 52

are used as N_x grid points $\Omega_k = x_k \in [-1,0]$. For solving problem (13) and (10) we use the computational scheme successfully applied to a number of various multichannel problems of muon-catalyzed fusion [30,31] and atomic physics [32–34]. Here we will not discuss the details of this scheme, which may be found in [7,29], but turn directly to the analysis of the obtained results.

In Tables I and II the evaluated quantities $E_v = -2(\varepsilon_v - \beta/2)$ are presented for the ground state and for several low-lying excited states of the problem together with more accurate results obtained recently by other authors using different approaches. We performed the calculations for several field strengths in the region $1 \le \beta \le 2\times 10^3$, which is usually tested. For numbering the states, the classification of [14] was used, $v = (nl_m/n'm\nu)$, with the set of asymptotic quantum numbers (nl_m) and $(n'm\nu)$ of the boundary cases $\beta = 0$ and $\beta = \infty$.

There are two sources of computational errors in our approach: $\Delta(N_x)$, caused by the truncation of expansion (12) and $\Delta(N_R)$, caused by numerical integration of system (13) over R, N_x and N_R being the numbers of grid points for x and R, respectively. Notice that the number N_x of grid points for x is equal to the number of terms in expansion (12). It has been shown in [7] that the accuracy of expansion (12) is of the order $\sim 1/N_x!$ for $N_x > \bar{N}_x$ (where $\bar{N}_x$ depends on β), and this estimate was proved by "numerical experiment" for fields $\beta \le 1$. It allows us to expect that expansion (12) will converge quite fast for stronger fields as well. The convergence of the method for $1 \le \beta \le 2\times 10^3$ with respect to N_x is demonstrated in Table III for the ground state and in Fig. 1 for two excited states. The calculations were performed on the quasiuniform grids $\{0 \cdots R_{i-1}(h_i)R_i \cdots R_m\}$ for R given in Table IV with finite-difference approximation of Eqs. (13) of the order $\sim h_i^4 \sim N_R^{-4}$. Estimating the accuracy $\Delta(N_R)$ of the approximation of problem (13) and (10) for variable R is quite standard procedure if the order of the approximation is known. The cutoff values R_m were selected by requiring that the error due to the truncation of infinite R should be at least one order of magnitude smaller then the errors $\Delta(N_x)$ and $\Delta(N_R)$. Some technical details con-

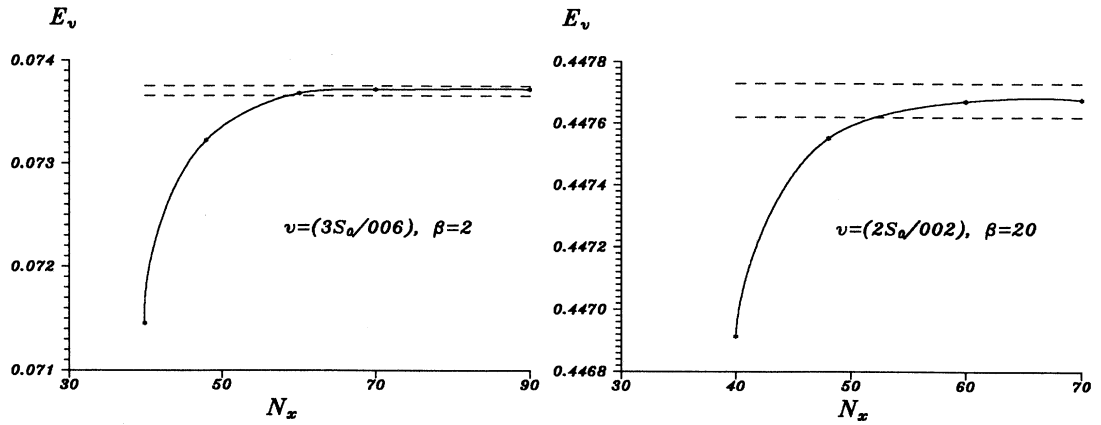

FIG. 1. Two examples illustrating the convergence behavior of energy values $E_v(N_x)$ of excited states v as $N_x \to \infty$. Here the dotted lines show the lower and upper bounds to $E_v(N_x)$ obtained in [14] by Rösner *et al.* Energies and magnetic-field strengths are given in atomic units.

cerning the integration of the problem over R for fixed N_x may be found in [7,29].

The error analysis of the computation is illustrated in Table V, which shows, as an example, the binding energy $E_v(N_x,N_R)$ of the ground state $v=(10_0/000)$ for a field $\beta=2$. An evaluation of the quantity $E_v(N_x,N_R)$ on a sequence of converging grids for both variables x ($N_x=8,12,24,32$) and R ($N_R=350,700,1400$) yields an estimate of the resulting computational error: $\Delta(N_x)+\Delta(N_R)$. Furthermore, since the computed quantities

$$\delta(N_R)|_{N_x=16}=E(\tfrac{1}{4}N_R)-E(\tfrac{1}{2}N_R)/E(\tfrac{1}{2}N_R)-E(N_R)\simeq 14$$

and

$$\delta(N_R)|_{N_x=24}\simeq 14\ ,$$

which characterize the order of the convergence over N_R, agree with the theoretical value $\delta_{\text{th}}=16$ for the h_i^4-order numerical integration, this allows one to suppress the error $\Delta(N_R=1400)$ at least on the order of magnitude by the extrapolation to $h_i\to 0$ ($N_R\to\infty$) (see last column in Table V):

$$E(N_R\to\infty)=E(N_R)-\tfrac{1}{15}[E(\tfrac{1}{2}N_R)-E(N_R)]\ .$$

Concerning the convergence of the results to $N_x\to\infty$, the following fact should be noted. It may be seen from Tables III and V that the quantity

$$\delta(N_x)=E(\tfrac{1}{4}N_x)-E(\tfrac{1}{2}N_x)/E(\tfrac{1}{2}N_x)-E(N_x)$$

is large enough and grows fast with increasing N_x, which shows quite high order of the convergence over N_x. However, for examining how the order of the convergence of expansion (12) for the fields $1\le\beta\le 2\times 10^3$ agrees with an estimation $\Delta(N_x)\sim 1/N_x!$ given in [7] for weak fields $\beta\le 1$ we would have to increase the accuracy of integration over R and to carry out the evaluation with more significant digits than we used here (all calculations were performed in double precision on a RISC/320h workstation computer).

In Tables I and II we give the calculated quantities E_v. For the ground states of the hydrogen atom in the fields $\beta<2\times 10^3$ the extrapolation to $N_R\to\infty$ has been performed to suppress the errors $\Delta(N_R)$. For the rest of the binding energies given in Tables I and II only the estimation of the errors $\Delta(N_R)$ has been done, and the grid points $\{0\cdots R_{i-1}(h_i)R_i\cdots R_m\}$ (see Table IV) were selected by requiring that the value $\Delta(N_R)$ should be the same order as the error $\Delta(N_x)$ due to the truncation of expansion (12). An analysis of the spread of computational errors allows us to guarantee the correctness of all digits given in the quantities E_v except for the last one, which may be subject to computational errors. This analysis and the comparison with advanced evaluations by other authors using different approaches, which are given in Tables I and II, allows us to come to the following conclusion: our approach agrees with very accurate variational calculations of the ground states [12] and yields more accurate binding energies for the low-lying excited states with different z parities, which are considered here for fields $\beta<2\times 10^2$.

It is also interesting to note that we have used the same expansion (12) over the whole range of field strengths

TABLE IV. Parameters of the method used for each calculation: quasiuniform grid $\{0\cdots R_{i-1}(h_i)R_i\cdots R_m\}$ over R with the total number of the points N_R and the maximum number N_x of the terms used in expansion (12). The steps of integration h_i are given in units h=0.000 625.

State	β	$0\cdots R_{i-1}(h_i)R_i\cdots R_m$	N_R	N_x
$(1s_0/000)$	1	0(h)0.125(2h)0.25(4h)0.5(8h)2(16h)6(32h)10(64h)14	1400	24
	2	0(h)0.125(2h)0.25(4h)0.5(8h)2(16h)6(32h)10(64h)14	1400	32
	20	0(h)0.125(2h)0.25(4h)0.5(8h)2(16h)6(32h)8	1200	32
	200	0(h)0.125(2h)0.25(4h)0.5(8h)2(16h)4	900	60
	2000	0(2h)0.25(8h)0.5(16h)1(32h)2	350	90
$(2p_0/001)$	1	0(h)0.125(2h)0.25(4h)2(8h)6(16h)10(32h)22	2800	24
	2	0(h)0.125(2h)0.25(4h)2(8h)6(16h)10(32h)22	2800	32
	20	0(2h)0.125(4h)0.25(8h)0.5(16h)2(32h)4(64h)16	750	60
	200	0(4h)0.125(8h)0.25(16h)0.5(32h)2(64h)6(128h)14	250	100
$(2s_0/002)$	1	0(h)0.125(2h)0.25(4h)0.5(8h)2(16h)6(32h)16(128h)28	1750	32
	2	0(32h)4(64h)8(128h)16(256h)32	500	40
	20	0(16h)1(32h)3(64h)5(128h)15	375	70
	200	0(32h)1(64h)3(128h)5(256h)9	150	120
$(3d_0/004)$	1	0(32h)4(64h)8(128h)30(256h)42	650	48
	2	0(32h)4(64h)8(128h)16(256h)32	500	60
	20	0(32h)1(64h)3(128h)5(256h)13(512h)37	250	120
$(3s_0/006)$	1	0(32h)4(64h)8(128h)30(256h)42	650	60
	2	0(32h)3(64h)6(128h)12(256h)32(512h)56	500	90

TABLE V. The convergence of the method over N_x and N_R for the example of the ground-state binding energy $E_v(N_x,N_R)$ for a magnetic field $\beta=2$.

N_x \ N_R	350	700	1400	$\to\infty$
8			2.044 427 793 139	
12	2.044 427 836 258	2.044 427 816 799	2.044 427 815 429	2.044 427 815 32
24	2.044 427 836 284	2.044 427 816 826	2.044 427 815 455	2.044 427 815 36
32			2.044 427 815 456	

$1\le\beta\le 2\times 10^3$ while other approaches normally use two separate expansions for the wave functions to be calculated and suppose either a spherical symmetry of the Coulomb states ($\beta=0$) for weak-to-moderate fields or a cylindrical symmetry of Landau states ($\beta=\infty$) for strong-to-very-strong fields. The exceptions are the finite-difference analysis of [16] with the local pointwise basis and the finite-basis method [12], where the basis set of trial functions contains both terms with spherical and cylindrical symmetry.

We have obtained a rather fast convergence of our approach over N_x and N_R, although the problem of finding the optimum distribution of grid points $\{x_k\}$ for given N_x has not been investigated. By carrying out such optimization and by using more accurate approximation formulae for R, the computational efficiency of the present method may be further increased.

IV. HYDROGEN ATOM IN ARBITRARILY ORIENTED MAGNETIC AND ELECTRIC FIELDS

Now, as an efficiency of our approach has been tested on a particularly well-investigated two-dimensional example, we turn to the general three-dimensional case of nonzero magnetic and electric fields of arbitrary mutual orientation: $\alpha\neq 0$, $\beta\neq 0$, $\gamma\neq 0$. To make the analysis clearer we consider a well-known example, the evolution of the $n=2$ multiplet in external fields, which is usually used in courses on quantum mechanics as an illustration of the development of the classical Stark (S) and Zeeman (Z) effects. Now we have the possibility of considering both effects simultaneously. We will analyze rather weak fields β and γ in order to separately investigate the states of the neighbor multiplets n and $n\mp 1$.

For the three-dimensional Schrödinger equation with Hamiltonian (2) the set of two-dimensional basis functions $\varphi_\nu(\Omega)$ in expansion (12) is defined by formula (11) on the rectangle $\Omega=\{x,\phi\}$, where $x\in[-1,1]$, $\phi\in[0,2\pi]$, and the index $\nu=\{l,m\}$ takes the values $l=0,1,\ldots,N_x-1$ and $m=-(N_\phi-1),\ldots,(N_\phi-1)$. Here the numbers $N_x=N_\phi$ have to be equal to the sums of the nodes in the N_x-point Gauss quadratures over the variables x and ϕ on the intervals $x\in[-1,1]$ and $\phi\in[0,2\pi]$. The total number of grid points Ω_k in the rectangle $\Omega=\{x,\phi\}$ is equal to $N=N_xN_\phi$ and the summation indices j and k in Eqs. (13) take the values $j=\{j_\theta,j_\phi\}=1,\ldots,N$ and $k=\{k_\theta,k_\phi\}=1,\ldots,N$. The x_{k_θ} and ϕ_{k_ϕ} coordinates of the grid points $\Omega_k=\{x_{k_\theta},\phi_{k_\phi}\}$ are determined as the nodes of the Gauss quadrature formulae over the variables x and ϕ. Notice that now the bound states of problem (13) and (10) do not have a definite symmetry relative to inversion ($z\to -z$) any more because in the Hamiltonian of the problem there are terms proportional to β and γ that violate the symmetry. Therefore in expansion (12) one has to keep both even and odd basis functions $P_l^m(x)$ (relative to inversion $x\to -x$), which are defined in the whole interval $x\in[-1,1]$, and the functions $\sin m\phi$ and $\cos m\phi$ as well. The abscissas ϕ_{k_ϕ} of the grid points Ω_k have been chosen as the nodes $\phi_{k_\phi}=(\pi/N_\phi)(2k_\phi-1)$ (with odd N_ϕ) of a quadrature on the whole interval $[0,2\pi]$ being two times larger than the standard intervals of the definition for orthogonal polynomials $\sin m\phi$ and $\cos m\phi$.

We start the analysis from the case of parallel fields ($\alpha=0$) where the problem still has cylindrical symmetry, which permits one to classify the bound states with parabolic quantum numbers ($\{n,n_1,n_2,m\}$, $n=n_1+n_2+|m|+1$). For small fields β and γ the second-order perturbation formulas are known [3]. According to these analyses the degeneracy of n multiplet is removed completely by the fields:

$$\varepsilon_n(\beta=\gamma=0)\Longrightarrow\varepsilon_{nQm}=\begin{cases}\varepsilon_n+\Delta\varepsilon^Z_{nQm}\ , & \beta\neq 0\ ,\ \gamma=0\\ \varepsilon_n+\Delta\varepsilon^S_{nQm}\ , & \beta=0\ ,\ \gamma\neq 0\\ \varepsilon_n+\Delta\varepsilon^{SZ}_{nQm}\ , & \beta\neq 0\ ,\ \gamma\neq 0\ .\end{cases}$$

Here $Q=n_1-n_2$, $\Delta\varepsilon^Z_{nQm}$ and $\Delta\varepsilon^S_{nQm}$ are the splittings of the Coulomb level n by magnetic and electric fields expressed as power series in β and γ, respectively. If both fields are applied to the system simultaneously, the splitting $\Delta\varepsilon^{SZ}_{nQm}$ is not equal to the sum of $\Delta\varepsilon^S_{nQm}$ and $\Delta\varepsilon^Z_{nQm}$:

$$\Delta\varepsilon^{SZ}_{nQm}=\Delta\varepsilon^S_{nQm}+\Delta\varepsilon^Z_{nQm}+\Delta E^{SZ}_{nQm}\ ,$$

where the additional shift ΔE^{SZ}_{nQm} contains cross terms of β and γ. However, the cross terms do not arise in the second-order perturbation theory yet [3]:

$$\varepsilon^{(2)}_{nQm}=\varepsilon_n+\Delta\varepsilon^{SZ(2)}_{nQm}=\varepsilon_n+\Delta\varepsilon^{S(1)}_{nQ}+\Delta\varepsilon^{S(2)}_{nQm}+\Delta\varepsilon^{Z(1)}_{nm}+\Delta\varepsilon^{Z(2)}_{nQm}\ . \tag{16}$$

The shifting ΔE^{SZ}_{nQm} has been analyzed only for the ground state $n=1$ in [5].

The results of our evaluation of the binding energies $-2\varepsilon_{nQm}$ of the (nQm) states of the multiplet $n=2$ are given in Table VI together with the quantities obtained with first- and second-order perturbation formulas [3]. We have performed calculations on a sequence of con-

verging grids $\{\Omega_k\}$ with $N=9(N_x=N_\phi=3)$, 25(5), and 49(7) grid points to examine the convergence of expansion (12). Note that the number of terms in the expansion is equal to the number of grid points $\{\Omega_k\}$, while the number of coupled equations in system (13) is twice as large because the expansion contains both real and imaginary parts. We have chosen a quasiuniform grid $\{0(0.04)4(0.08)8(0.16)28\}$ for R in such a way that the error of numerical integration over R would give a contribution in the last digit of the values given in Table VI. The evaluation has been done for three possible relative strengths of the fields, $\eta=3n\gamma/\beta<1$, $\eta=1$, and $\eta>1$, with respect to the critical point $\eta=1$, where the first-order perturbation corrections due to β and γ fields are identical. The magnetic field strength was fixed, $\beta=\frac{1}{2}\times10^{-2}$, and the strength of the electric field was varied, $\gamma=\frac{1}{6}\times10^{-3}$, $\frac{1}{12}\times10^{-2}$, and $\frac{1}{6}\times10^{-2}$ ($\eta=0.2$, 1, and 2).

The performed numerical analysis permits one to estimate the computational errors $\Delta\varepsilon(N_R,N)$ of the values $-2\varepsilon_{nQm}(N=49)$, given in Table VI, as $\Delta\varepsilon(N_R,N)\leq10^{-7}$ for $\eta=0.2$, and $\Delta\varepsilon(N_R,N)\leq10^{-5}$ for $\eta\geq1$. As in the investigated range of field strengths β and γ, our numerical evaluation of the binding energy ε_{nQm} is more accurate than the value $\varepsilon^{(2)}_{nQm}$ (16) given by second-order perturbation formulas [3], we have a possibility of estimating the main cross term in $\Delta E^{ZS}_{2Q0}=\varepsilon_{2Q0}-\varepsilon^{(2)}_{2Q0}$. From Fig. 2 one sees that the main term may be approximated as $\Delta E^{ZS}_{2Q0}\simeq A_{2Q0}\beta^2\gamma+\cdots$ in the limit $\gamma\to0$ with the coefficient A_{2Q0} estimated as $A_{2Q0}\simeq Q\times170$. For more accurate evaluation of this coefficient one can do the calculation with more significant digits and for smaller field strengths ($\gamma\sim0.0001$), where perturbation theory is applicable with a higher degree of accuracy.

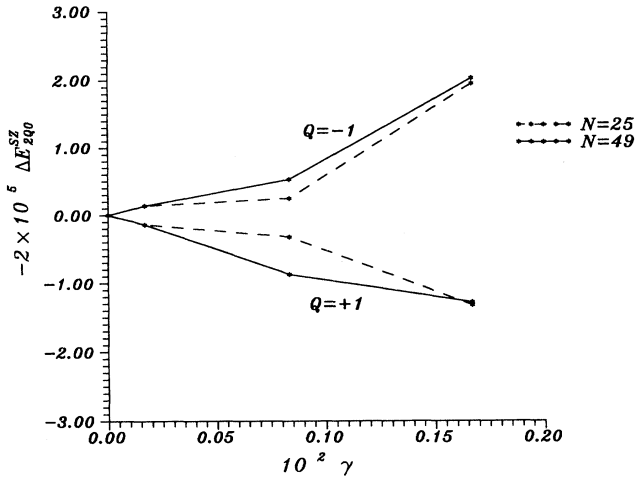

FIG. 2. Deviation ΔE^{SZ}_{2Q0} of the calculated binding energy ε_{2Q0} from the value $\varepsilon^{(2)}_{2Q0}$ given by the second-order perturbation formulae as a function of γ for fixed $\beta=\frac{1}{2}\times10^{-2}$ ($\mathbf{B}\|\mathbf{F}$ case). Energies and electric- and magnetic-field strengths are given in atomic units.

In Table VI the convergence of the method over N is analyzed for orthogonal fields ($\alpha=\pi/2$) too by analogy with the case of parallel fields ($\alpha=0$). For $\alpha=\pi/2$ the first- and second-order perturbation formulas [2,4] give the following:

TABLE VI. The convergence of the binding energies $-2\varepsilon_{2Qm}(\alpha=0)$ and $-2\varepsilon_{2q\lambda}(\alpha=\pi/2)$ over N for various relative strengths η of the fields β and γ: $\beta=10^{-2}/2$; $\gamma=10^{-3}/6$, $10^{-2}/12$, $10^{-2}/6$.

		Present work			Perturbation theory		(Q,m)
η	α	$N=9$	$N=25$	$N=49$	2nd order	1st order	$\{q\}$
0.2	0	0.245 152 9	0.244 853 9	0.244 854 5	0.244 854 3	0.245 000 0	(0,1)
		0.248 878 3	0.248 878 3	0.248 878 3	0.248 879 7	0.249 000 0	(1,0)
		0.250 881 1	0.250 881 1	0.250 881 1	0.250 879 7	0.251 000 0	(−1,0)
		0.255 153 1	0.254 853 9	0.254 854 4	0.254 854 4	0.255 000 0	(0,−1)
1	0	0.244 988 7	0.244 960	0.244 960	0.244 958 3		(0,1)
		0.245 989 4	0.244 988 5	0.244 988	0.244 991 7	0.245 000 0	(1,0)
		0.254 994 3	0.254 960	0.254 960	0.254 958 3	0.255 000 0	(0,−1)
		0.255 992 6	0.254 994 2	0.254 995	0.254 991 7		(−1,0)
2	0	0.240 326 3	0.240 328 5	0.240 328 9	0.240 341 7	0.240 000 0	(1,0)
		0.248 591 1	0.245 232 6	0.245 287 2	0.245 283 3	0.245 000 0	(0,1)
		0.258 563 8	0.255 231 8	0.255 287 2	0.255 283 3	0.255 000 0	(0,−1)
		0.260 358 6	0.260 361 2	0.260 362 0	0.260 341 7	0.260 000 0	(−1,0)
	$\frac{\pi}{2}$	0.238 326 6	0.239 123 9	0.239 130 7	0.239 136 4	0.238 819 7	{1}
		0.249 850 2	0.250 259 1	0.250 259 1	0.250 340 8	0.250 000 0	{0}
		0.250 335 3	0.250 259 0				
		0.260 319 9	0.261 499 9	0.261 507 8	0.261 497 0	0.261 180 3	{−1}

$$\varepsilon^{(2)}_{nq\lambda}=\varepsilon_n+\Delta\varepsilon^{(1)}_{nq}+\Delta\varepsilon^{(2)}_{nq\lambda}\ ,$$

$$\Delta\varepsilon^{(1)}_{nq}=\tfrac{1}{2}q\sqrt{(3n\gamma)^2+\beta^2}\ , \tag{17}$$

$$\Delta\varepsilon^{(2)}_{nq\lambda}=\frac{\beta^2n^2}{16}(3n^2+1-q^2+\lambda)+\frac{\gamma^2n^4}{16}\left[3q^2-17n^2-19-\frac{6}{1+\eta^2}(n^2-3q^2-1)\right].$$

Here the quantum number q takes the values $q=-(n-1),\ldots,(n-1)=-1,0,1$ and λ is the eigenvalue of the operator that removes $(n-q)$ degeneracy remained in the first-order correction $\Delta\varepsilon^{(1)}_{nq}$ [2]. The values $\varepsilon^{(2)}_{nq\lambda}=\varepsilon_n+\Delta\varepsilon^{(1)}_{nq}+\Delta\varepsilon^{(2)}_{nq\lambda}$ given in Table VI were evaluated with formulas (17) without contribution of terms $\sim\lambda$. The eigenvalue problem for λ (which does not allow an analytical solution) has been analyzed in [4] as a function of parameters β, γ, and η. According to this analysis the removal of the $(n-q)$ degeneracy for the states with $q=0$ does not take place for the fields considered here with the parameters $\beta=\frac{1}{2}\times10^{-2}$, $\gamma=\frac{1}{6}\times10^{-2}$ ($\eta=2$). But one may see an "artificial" removal of the $(n-q)$ degeneracy at $N=9$, which is, however, suppressed as the number of terms in expansion (12) is increased to $N=25$ and the approximation of the initial Hamiltonian is improved. The performed numerical analysis shows that the same accuracy of the method has been achieved for both considered cases, $\alpha=0$ and $\alpha=\pi/2$.

While analyzing the $n=2$ multiplet for the two limiting cases $\alpha=0$ and $\alpha=\pi/2$, we observed a total change in the structure of the spectrum due to changing in the mutual orientation of the fields **F** and **B**. The rearrangement of the spectrum of an electron in a hydrogen atom in crossed electric and magnetic fields as a function of their mutual orientation

$$\varepsilon_{nQm}(\alpha=0)\Longrightarrow\varepsilon_{nq\lambda}(\alpha=\pi/2)$$

is illustrated by the example of the $n=2$ multiplet shown in Fig. 3. The calculated curves are plotted as functions of α for fixed $\beta=\frac{1}{6}\times10^{-2}$ and γ varying over three possible relative strengths of the fields: $\eta=0.2$, 1, and 2 ($\gamma=\frac{1}{6}\times10^{-3}$, $\frac{1}{12}\times10^{-2}$, and $\frac{1}{6}\times10^{-2}$). The calculated binding energies $-2\varepsilon_{nQm}(\alpha)$ are also given for several values of α in Table VII. The calculations were performed with $N=25$. Computational errors may give a contribution to the last decimal digits of the values $-2\varepsilon_{nQm}(\alpha)$ presented in Table VII.

We also mention that, according to the analysis performed in [4] in the framework of perturbation theory, the $(n-q)$ degeneracy of the states with $q=0$ for $\alpha=\pi/2$ may be removed only in one of the cases being considered here, $\eta=1$, although the splitting of $\Delta\varepsilon^{(2)}_{nq\lambda}$ in the second-order of perturbation theory due to λ does not exceed by the order of magnitude the computational errors (see Table VII). To analyze a removal of the $(n-q)$ degeneracy due to the term λ one has to carry out the calculation with more significant digits and a higher value of N for various values of β and γ.

For classifying the states we used the quantum numbers (nQm) and $\{nq\lambda\}$ of the limiting cases of parallel ($\alpha=0$) and orthogonal ($\alpha=\pi/2$) fields but it is not clear if classification $\{nq\lambda\}$ is also useful for stronger fields where the application of perturbation theory becomes questionable. It seems that in the nonperturbative region only a classification by the well-defined quantum numbers of the **B**‖**F** case (for $\alpha\to0$) and by the number of nodal surfaces of the three-dimensional wave function, the form of the surfaces and the possible symmetry of the wave function with respect to the {**BF**} plane (for other α) would be meaningful.

It should be noted that the results presented in Tables VI and VII and in Figs. 2 and 3 do not depend on the space orientation of the {**BF**} plane. As the applied approach allows to carry out the calculations for different plane orientations, this yields an additional test of the consistency of the calculations.

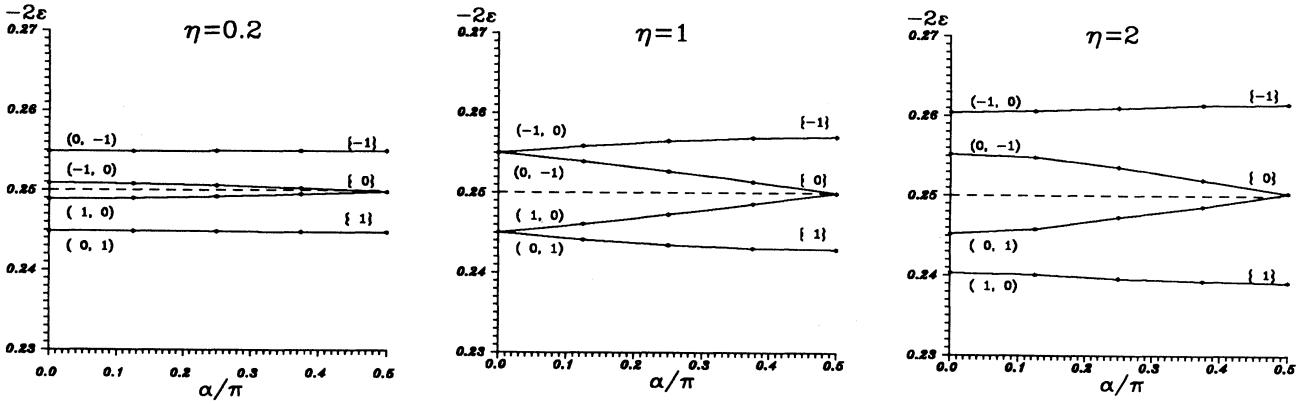

FIG. 3. The rearrangement $\varepsilon_{(Q,m)}(\alpha=0)\Longrightarrow\varepsilon_{\{q\}}(\alpha=\pi/2)$ of the structure of the $n=2$ multiplet due to changing of the angle α between fields **B** and **F** for three possible relative strengths $\eta=3n\gamma/\beta$ of the fields ($\beta=\frac{1}{2}\times10^{-2}$). Energies and electric- and magnetic-field strengths are given in atomic units.

TABLE VII. Evolution of the $n=2$ multiplet in crossed magnetic and electric fields as a function of the mutual orientation α for various relative strengths η of the fields β and γ: $\beta=10^{-2}/2$; $\gamma=10^{-3}/6$, $10^{-2}/12$, $10^{-2}/6$.

η	(Q,m)	$\alpha=0$	$\alpha=\frac{1}{8}\pi$	$\alpha=\frac{1}{4}\pi$	$\alpha=\frac{3}{8}\pi$	$\alpha=\frac{1}{2}\pi$	$\{q\}$
0.2	(0,1)	0.244 854	0.244 839	0.244 804	0.244 769	0.244 756	{1}
	(1,0)	0.248 878	0.248 957	0.249 178	0.249 500	0.249 830	{0}
	(−1,0)	0.250 881	0.250 802	0.250 582	0.250 259		
	(0,−1)	0.254 854	0.254 869	0.254 905	0.254 939	0.254 953	{−1}
1	(0,1)	0.244 96	0.244 09	0.243 44	0.243 03	0.242 90	{1}
	(1,0)	0.244 99	0.246 05	0.247 26	0.248 60	0.249 93	{0}
	(0,−1)	0.254 96	0.253 91	0.252 69	0.251 37		
	(−1,0)	0.255 00	0.255 85	0.256 50	0.256 90	0.257 04	{−1}
2	(1,0)	0.240 33	0.240 08	0.239 64	0.239 28	0.239 12	{1}
	(0,1)	0.245 23	0.245 76	0.247 00	0.248 57	0.250 26	{0}
	(0,−1)	0.255 23	0.254 80	0.253 62	0.252 04		
	(−1,0)	0.260 36	0.260 57	0.261 02	0.261 38	0.261 50	{−1}

V. CONCLUSION

Our interest in the problem considered here was aroused by two circumstances: we wanted to examine the efficiency of the method [7] in an application to a real three-dimensional physical problem whose solutions are known with high accuracy for certain special cases, and we tried to give an alternative point of view on the well-known classical problem usually analyzed with some additional conditions imposed upon its parameters (the conditions permitted the use of conventional methods of quantum theory such as separation of variables, perturbation theory, quasiclassical approximations, etc.).

In solving the Schrödinger equation for the electron of the hydrogen atom in external magnetic **B** and electric **F** fields as a three-dimensional problem without separation of variables we have calculated the rearrangement of the spectrum due to changing in the mutual orientations of the fields. As any interaction is introduced in addition to the Hamiltonian (2) and projected into the space $\{R,\theta,\phi\}$ is diagonal in our approach [see Eqs. (13) and (14)], this allows one to take into consideration in a natural way the effects of finite mass and finite size of nucleus, relativistic, and QED effects, etc., and yields a background for an experimental analysis of the rearrangement phenomena. The hydrogenlike atoms in external **B** and **F** fields have recently become feasible for experimental investigations [35,36].

Our approach may also be applied to analyzing the ionization of hydrogen atom which occurs when an electric field is added to the system [37], because Eqs. (9) and (10) have been formulated in [7] both for eigenvalue and the scattering problem.

It seems interesting to analyze the possibilities for the bounding of the electron away from the hydrogen nucleus, at a certain distance from the center of the Coulomb well and with another, deeper effective potential well, which gives rise to a large dipole moment of the ground state in the crossed fields [6]. So far the existing models for describing the effect are based on one-dimensional approximations [6,38–41], but an adequate theoretical consideration of the phenomenon demands direct analysis of the three-dimensional nature of the problem [42].

We would also like to mention a possible, quite unusual application of the problem of the hydrogen atom in crossed fields for describing the Coulomb interaction of a particle colliding with the hydrogen atom as an effective electromagnetic field in the rotating coordinate frame [3].

It is obvious that our approach may be applicable for investigating some particular aspects of the problem that are currently under study, such as the Stark effect in strong fields and the Zeeman effect in hydrogenlike atoms (or exitons in a magnetic field) with finite mass of the nucleus (it was shown [43] that the hydrogen Zeeman Hamiltonian with finite nuclear mass is unitary equivalent to the **B**⊥**F** Hamiltonian for hydrogen with infinitely heavy nucleus).

Concerning the efficiency of the method, the following should be noted. All computations were performed on a conventional RISC/320h workstation, which limited the number of terms in expansion (12) to $N\simeq 100$. However, for the special case of a hydrogen atom in a strong magnetic field, we obtained highly accurate binding energies for the low-lying excited states that were investigated, and for the ground state the results we obtained are in agreement with advanced variational calculations. This allows us to expect an important increase in the accuracy of the calculations when more powerful computers will be used. Possible optimization by an adequate distribution of the grid points Ω_k may give an additional increase in the efficiency of the calculations.

The rather good convergence of our method for the low-lying excited states we considered suggests that it might also be used for higher excitations, in the energy region where the application of quasiclassical analysis is still questionable. The high order of smoothness of the calculated wave function (12) allows one to expect highly accurate calculations for matrix elements with wave functions such as mean-square radii, multiple moments, oscillator strengths, etc.

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