ISSN 1063-7788, Physics of Atomic Nuclei, 2008, Vol. 71, No. 5, pp. 844–852. © Pleiades Publishing, Ltd., 2008.

ELEMENTARY PARTICLES AND FIELDS

Adiabatic Representation for a Hydrogen Atom Photoionization in a Uniform Magnetic Field*

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Received August 20, 2007

Abstract—A new effective method of calculating wave functions of discrete and continuous spectra of a hydrogen atom in a strong magnetic field is developed on the basis of the adiabatic approach to parametric eigenvalue problems in spherical coordinates. The two-dimensional spectral problem for the Schrödinger equation at a fixed magnetic quantum number and parity is reduced to a spectral parametric problem for a one-dimensional angular equation and a finite set of ordinary second-order radial differential equations. The results are in good agreement with the photoionization calculations by other authors and have a true threshold behavior.

PACS numbers: 31.15.Ja, 31.15.Pf, 34.50.-s, 34.50.Pi
DOI: 10.1134/S1063778808050128

1. INTRODUCTION

Recent Monte Carlo estimations of the influence of a strong magnetic field on the spontaneous recombination of the anti-hydrogen in the cold positron–antiproton plasma conditions of the ATHENA [1, 2] and ALPHA [3] experiments (CERN) have shown that further quantum mechanical analysis is needed [4]. We can draw attention to a new enhancement mechanism of a laser-stimulated recombination of anti-hydrogen in cold antiproton–positron plasma in a laboratory magnetic field via quasistationary states embedded in the continuum that has been revealed recently [5]. At the first stage of such an analysis, the adiabatic representation known in mathematics as a Kantorovich method is developed for solving the problem of low-lying excited states of the hydrogen atom in a magnetic field in spherical coordinates [6] and the benchmark three-body scattering problem on a line [7].

Indeed, the adiabatic representation in cylindrical coordinates was applied recently to revive the basic decay mechanisms of Rydberg states with high magnetic quantum numbers in the magnetic traps [8]. It has been shown that the exhaustive analysis of the complex dynamics of the electron with decreasing module of magnetic number is impossible without taking the nonadiabatic coupling into consideration [9]. However, high-accuracy calculations in cylindrical coordinates is a rather cumbersome problem except the cases of high magnetic numbers or a dominating magnetic field [10]. So, using spherical coordinates is preferable when Coulomb and magnetic fields have comparable contributions in the average potential energy [11] but leads to nontrue threshold behavior of the photoionization cross section calculated by the complex rotation–variational method [12].

In this paper, we develop the Kantorovich approach with a boundary condition of the third type in a form appropriate for the **R**-matrix calculations of atomic hydrogen photoionization in a strong magnetic field using a uniform orthogonal parametric basis of the angular oblate spheroidal functions [13] in spherical coordinates only, instead of the combined nonorthogonal basis of Landau and Sturmian functions in both cylindrical and spherical coordinates [14, 15]. The efficiency of the elaborated approach which provides true threshold behavior of photoionization cross sections of a hydrogen atom from the ground state to the different continuous-spectrum states is demonstrated.

The paper is organized as follows. The 2D eigenvalue problem for the Schrödinger equation for the hydrogen atom in an axially symmetric magnetic field,

*The text was submitted by the authors in English.

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written in spherical coordinates, is considered in Section 2 together with the appropriate classification of states. The reduction of the 2D eigenvalue problem to a 1D eigenvalue problem for a set of closed radial equations via four steps of the Kantorovich method is described briefly in Section 3. All the asymptotic expressions needed to find the solutions and the reaction matrix using the **R**-matrix method, are presented in Section 4. The method is applied to the calculation of ionization from the ground state to the different continuous-spectrum states in Section 5. In the Conclusions, we outline the prospects for further applications of this approach.

2. STATEMENT OF THE PROBLEM

The Schrödinger equation for the wave function $\hat{\Psi}(r,\theta,\varphi) = \Psi(\theta,r)\exp(im\varphi)/\sqrt{2\pi}$ in the spherical coordinates (r,θ,ϕ) of the hydrogen atom in an axially symmetric magnetic field $\vec{B} = (0,0,B)$ can be written as the 2D equation

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + U(r,\theta)\right)\Psi(r,\theta) = \epsilon\Psi(r,\theta), \quad (1)$$

in the region Ω: $0 < r < \infty$ and $0 < \theta < \pi$. The potential function $U(r,\theta)$ is given by

$$U(r,\theta) = -\frac{2Z}{r} + V(r,\theta), \quad (2)$$

$$V(r,\theta) = \frac{m^2}{r^2\sin^2\theta} + \gamma m + \frac{\gamma^2 r^2}{4}\sin^2\theta,$$

where $m = 0, \pm 1, \ldots$ is the magnetic quantum number, $\gamma = B/B_0$, $B_0 \cong 2.35\times 10^5$ T is a dimensionless parameter which determines the field strength B, and the atomic units (a.u.) $\hbar = m_e = e = 1$ are used under the assumption of infinite mass of the nucleus. In these expressions, $\epsilon = 2E$ is the doubled energy (in units of rydbergs, 1Ry = (1/2) a.u.) of the bound state $|m\sigma\rangle$ at fixed values of m and z parity; $\sigma = \pm 1$; $\Psi \equiv \Psi_{m\sigma}(r,\theta) = (\Psi_m(r,\theta) + \sigma\Psi_m(r,\pi-\theta))/\sqrt{2}$ is the corresponding wave function. Here, the sign of z parity $\sigma = (-1)^{N_\theta}$ is defined by the (even or odd) number of nodes N_θ in the solution Ψ with respect to the angular variable θ in the interval $0 < \theta < \pi$. The wave function satisfies the following boundary conditions in each $\mathbf{H}_{m\sigma}$ subspace of the full Hilbert space:

$$\lim_{\theta\to 0}\sin\theta\frac{\partial\Psi(r,\theta)}{\partial\theta} = 0, \quad \text{for} \quad m = 0, \quad (3)$$
$$\text{and} \quad \Psi(r,0) = 0, \quad \text{for} \quad m \neq 0,$$

$$\frac{\partial\Psi}{\partial\theta}\left(r,\frac{\pi}{2}\right) = 0, \quad \text{for} \quad \sigma = +1, \quad (4)$$
$$\text{and} \quad \Psi\left(r,\frac{\pi}{2}\right) = 0, \quad \text{for} \quad \sigma = -1,$$

$$\lim_{r\to 0} r^2\frac{\partial\Psi(r,\theta)}{\partial r} = 0. \quad (5)$$

The discrete-spectrum wave function obeys the asymptotic boundary condition approximated at large $r = r_{\max}$ by a boundary condition of the first type,

$$\lim_{r\to\infty} r^2\Psi(r,\theta) = 0 \quad \to \quad \Psi(r_{\max},\theta) = 0. \quad (6)$$

Here, the energy $\epsilon \equiv \epsilon(r_{\max})$ plays the role of eigenvalues of the boundary problem (1)–(6) determined by a variational principle with an additional normalization condition in a finite interval $0 \le r \le r_{\max}$,

$$\mathbf{\Pi}(\Psi,\epsilon) = 0, \quad (7)$$
$$2\int_0^{r_{\max}}\int_0^{\pi/2} r^2\sin\theta|\Psi(r,\theta)|^2 d\theta dr = 1,$$

where $\mathbf{\Pi}(\Psi,\epsilon)$ is a symmetric functional defined by

$$\mathbf{\Pi}(\Psi,\epsilon) = 2\int_0^{r_{\max}}\int_0^{\pi/2}\sin\theta\left(r^2\left|\frac{\partial\Psi(r,\theta)}{\partial r}\right|^2 + \left|\frac{\partial\Psi(r,\theta)}{\partial\theta}\right|^2 + r^2(U(r,\theta)-\epsilon)|\Psi(r,\theta)|^2\right)d\theta dr.$$

In the Fano–Lee **R**-matrix theory [16, 17], a continuum-spectrum wave function $\Psi(r,\theta)$ obeys the boundary condition of the third type at fixed values of energy ϵ and radial variable $r = r_{\max}$

$$\frac{\partial\Psi(r,\theta)}{\partial r} - \mu\Psi(r,\theta) = 0. \quad (8)$$

Here, the parameters, $\mu \equiv \mu(r_{\max},\epsilon)$, determined by a variational principle, play the role of eigenvalues of a logarithmic normal derivative matrix of the solution of the boundary problem (1)–(5) and (8)

$$\mathbf{\Pi}(\Psi,\epsilon) = 2\mu r_{\max}^2\int_0^{\pi/2}\sin\theta|\Psi(r_{\max},\theta)|^2 d\theta. \quad (9)$$

Standard theorems [18] ensure the existence of a function $\mu(r_{\max},\epsilon)$ such that Eq. (8) is satisfied (at any finite $r = r_{\max} < \infty$) [19].

3. REDUCTION OF THE 2D PROBLEM BY THE KANTOROVICH METHOD

Consider a formal expansion of the partial wave function $\Psi_i^{Em\sigma}(r,\theta)$ of (1)–(5) with (6)/(8) corresponding to the eigenstate $|m\sigma i\rangle$ using the finite set

of one-dimensional basis functions $\{\Phi_j^{m\sigma}(\theta;r)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(r,\theta)=\sum_{j=1}^{j_{\max}}\Phi_j^{m\sigma}(\theta;r)\chi_j^{(m\sigma i)}(E,r). \quad (10)$$

In Eq. (10), the functions $\boldsymbol{\chi}^{(i)}(r)\equiv\boldsymbol{\chi}^{(m\sigma i)}(E,r)$, $(\boldsymbol{\chi}^{(i)}(r))^T=(\chi_1^{(i)}(r),\ldots,\chi_{j_{\max}}^{(i)}(r))$ are unknown, and the surface functions $\boldsymbol{\Phi}(\theta;r)\equiv\boldsymbol{\Phi}^{m\sigma}(\theta;r)$, $(\boldsymbol{\Phi}(\theta;r))^T=(\Phi_1(\theta;r),\ldots,\Phi_{j_{\max}}(\theta;r))$ form an orthonormal basis for each value of the radius r, which is treated here as a parameter.

In the Kantorovich approach, the wave functions $\Phi_j(\theta;r)$ and potential curves $E_j(r)$ are determined as the solutions of the following one-dimensional parametric eigenvalue problem:

$$\left(-\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+r^2\sin\theta V(r,\theta)\right)\Phi_j(\theta;r) \quad (11)$$
$$=E_j(r)\sin\theta\Phi_j(\theta;r),$$

with the boundary conditions

$$\lim_{\theta\to0}\sin\theta\frac{\partial\Phi_j(\theta;r)}{\partial\theta}=0,\quad \text{for}\quad m=0, \quad (12)$$
$$\text{and}\quad \Phi_j(0;r)=0,\quad \text{for}\quad m\neq0,$$
$$\frac{\partial\Phi_j}{\partial\theta}\left(\frac{\pi}{2};r\right)=0,\quad \text{for}\quad \sigma=+1, \quad (13)$$
$$\text{and}\quad \Phi_j\left(\frac{\pi}{2};r\right)=0,\quad \text{for}\quad \sigma=-1.$$

Here, the sign of z parity, $\sigma=(-1)^{N_\theta}$, is defined by the (even or odd) number of nodes N_θ in the solution $\boldsymbol{\Phi}(\theta;r)$ with respect to the angular variable θ in the interval $0<\theta<\pi$. Since the operator on the left-hand side of (11) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle\Phi_i(\theta;r)\middle|\Phi_j(\theta;r)\right\rangle_\theta \quad (14)$$
$$=2\int_0^{\pi/2}\sin\theta\Phi_i(\theta;r)\Phi_j(\theta;r)d\theta=\delta_{ij},$$

where δ_{ij} is the Kronecker symbol.

Note that the solutions of this problem with shifted eigenvalues, $\tilde{E}_j(r,\gamma)=E_j(r,\gamma)-\gamma mr^2$, correspond to the solutions of the eigenvalue problem for oblate angular spheroidal functions [13] with respect to the variable $\eta=\cos\theta$:

$$\left(-\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}+\frac{m^2}{1-\eta^2}\right. \quad (15)$$
$$\left.+\left(\frac{\gamma r^2}{2}\right)^2(1-\eta^2)\right)\Phi_j(\eta;r)=\tilde{E}_j(r)\Phi_j(\eta;r).$$

It means that, for small r, the asymptotics of the eigenvalues $E_j(r)$, $j=1,2,\ldots$, at fixed values m and σ is defined by the values of the orbital quantum number, $l=s,p,d,f,\ldots$: $E_j(0)=l(l+1)$, $l=0,1,\ldots$, where j runs $j=(l-|m|)/2+1$ for even z-parity states, $\sigma=+1=(-1)^{l-|m|}$, and $j=(l-|m|+1)/2$ for odd z-parity states, $\sigma=-1=(-1)^{l-|m|}$. Taking into account that the number of nodes N_θ of the eigenfunction $\boldsymbol{\Phi}(\theta;r)$ at fixed $|m|$ and $\sigma=(-1)^{N_\theta}$ as a function of the parameter r is preserved, we get a one-to-one correspondence between these sets, i.e., $N_\theta=l-|m|$.

For large r, the asymptotics of eigenvalues $E_j(r)$, $j=1,2,\ldots$, at fixed values of m and σ is defined by the values of the transversal quantum number, N_ρ:

$$\lim_{r\to\infty}r^{-2}E_j(r,\gamma)=\epsilon_{m\sigma j}^{\text{th}}(\gamma) \quad (16)$$
$$=\gamma(2N_\rho+|m|+m+1),$$

where $N_\rho=0,1,\ldots,$ and j runs $j=N_\rho+1$. The values of the transversal quantum number N_ρ, i.e., the number of nodes of the eigenfunction $\boldsymbol{\Phi}(\theta;r)$ in the subinterval $0<\eta<1$ or $-1<\eta<0$, corresponding to the transversal variable $\rho=r\sin\theta$ on a semiaxis, are expressed via the number of nodes N_θ of the solution $\boldsymbol{\Phi}(\theta;r)$: $N_\rho=1/2\cdot N_\theta$ for the even z-parity states, $\sigma=+1=(-1)^{N_\theta}$, and $N_\rho=1/2\cdot(N_\theta-1)$ for the odd z-parity states, $\sigma=-1=(-1)^{N_\theta}$.

Such a transversal classification also reveals a violation of degeneracy of the states with azimuthal quantum numbers, $\pm m$, having the same module $|m|$ that holds for the angular oblate spheroidal functions, i.e.,

$$\lim_{r\to\infty}r^{-2}\tilde{E}_j(r,\gamma)=\gamma(2N_\rho+|m|+1). \quad (17)$$

Taking into account the above-mentioned correspondence rules between the quantum numbers $l-|m|$, N_θ, N_ρ and the number j at fixed values of m and σ, we use the *unified number* j without pointing out explicitly a concrete type of quantum numbers. These rules are similar to the conventional correlation diagrams for potential curves of a hydrogen atom in a uniform magnetic field or a helium atom.

After substituting the expansion (10) into the variational problem (7)/(9) and using Eqs. (11)–(14), the solution of the above problem is transformed into the solution of an eigenvalue problem for a system of $j_{\max}$ ordinary second-order differential equations for determining the energy ϵ and the coefficients (radial wave functions) $\boldsymbol{\chi}^{(i)}(r)$ of expansion (10),

$$\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{\mathbf{U}(r)}{r^2}+\mathbf{Q}(r)\frac{d}{dr}\right. \quad (18)$$

$$+\frac{1}{r^2}\frac{dr^2\mathbf{Q}(r)}{dr}\Big)\boldsymbol{\chi}^{(i)}(r)=\epsilon_i\mathbf{I}\boldsymbol{\chi}^{(i)}(r),$$

$$\lim_{r\to 0} r^2\left(\frac{\partial\boldsymbol{\chi}^{(i)}(r)}{\partial r}-\mathbf{Q}(r)\boldsymbol{\chi}^{(i)}(r)\right)=0.$$

Here, $\mathbf{I}, \mathbf{U}(r)$, and $\mathbf{Q}(r)$ are matrices of dimension $j_{\max}\times j_{\max}$ whose elements are given by the relations

$$U_{ij}(r)=\frac{E_i(r)+E_j(r)}{2}\delta_{ij}+2Zr\delta_{ij} \qquad (19)$$

$$+r^2H_{ij}(r),\quad I_{ij}=\delta_{ij},$$

$$H_{ij}(r)=2\int_0^{\pi/2}\sin\theta\frac{\partial\Phi_i(\theta;r)}{\partial r}\frac{\partial\Phi_j(\theta;r)}{\partial r}d\theta,$$

$$Q_{ij}(r)=-2\int_0^{\pi/2}\sin\theta\Phi_i(\theta;r)\frac{\partial\Phi_j(\theta;r)}{\partial r}d\theta.$$

The above matrix elements were calculated by means of the authors' combined symbolic–numerical code MATRM implemented in both MAPLE 8 and FORTRAN [20].

The discrete spectrum solutions obey the asymptotic boundary condition and orthonormal conditions

$$\lim_{r\to\infty} r^2\boldsymbol{\chi}^{(i)}(r)=0 \quad\to\quad \boldsymbol{\chi}^{(i)}(r_{\max})=0, \qquad (20)$$

$$\int_0^{r_{\max}} r^2(\boldsymbol{\chi}^{(i)}(r))^T\boldsymbol{\chi}^{(j)}(r)dr=\delta_{ij}.$$

For the continuum-spectrum solution $\boldsymbol{\chi}^{(i)}(r)$, we can alternatively require that projections of (8) onto all adiabatic functions hold,

$$\left\langle\Phi_j(\theta;r)\left|\frac{\partial\Psi_i^{Em\sigma}(r,\theta)}{\partial r}-\mu_i\Psi_i^{Em\sigma}(r,\theta)\right\rangle_\theta=0,\right. \qquad (21)$$

$$r=r_{\max},$$

which leads to the third-type boundary conditions at fixed values of energy $\epsilon>\epsilon^{\rm th}_{m\sigma 1}(\gamma)$ and radial variable $r=r_{\max}$

$$\Big(\mathbf{R}-\mathbf{Q}(r)-\mu_i\Big)\boldsymbol{\chi}^{(i)}(r) \qquad (22)$$

$$=\left(\frac{\partial\boldsymbol{\chi}^{(i)}(r)}{\partial r}(\boldsymbol{\chi}^{(i)})^{-1}(r)-\mathbf{Q}(r)-\mu_i\right)\boldsymbol{\chi}^{(i)}(r)=0.$$

From here, μ_i and $\boldsymbol{\chi}^{(i)}(r_{\max})$ should be a set of eigenvalues $\boldsymbol{\Lambda}=\{\delta_{ij}\mu_i\}_{ij=1}^{N_o}$ corresponding to a set of eigenvectors $\boldsymbol{\chi}(r)\equiv\{\boldsymbol{\chi}^{(i)}(r)\}_{i=1}^{N_o}$ of the following eigenvalue problem at $r=r_{\max}$

$$\frac{d\boldsymbol{\chi}(r)}{dr}-\mathbf{Q}(r)\boldsymbol{\chi}(r)=\boldsymbol{\chi}(r)\boldsymbol{\Lambda}, \qquad (23)$$

which is reformulated by averaging variational problem (9) to the following one:

$$\boldsymbol{\Pi}(\boldsymbol{\chi},\epsilon)-r_{\max}^2\boldsymbol{\chi}^T(r_{\max})\boldsymbol{\chi}(r_{\max})\boldsymbol{\Lambda}=0. \qquad (24)$$

Here N_o is the number of the open channels (i.e., the energy ϵ should belong to the interval $\epsilon^{\rm th}_{m\sigma N_o}(\gamma)<\epsilon<\epsilon^{\rm th}_{m\sigma N_o+1}(\gamma)$), and $j_{\max}>N_o$.

After discretization, Eq. (24) becomes the following algebraic eigenvalue problem

$$\boldsymbol{\Pi}\tilde{\boldsymbol{\chi}}=r_{\max}^2\tilde{\boldsymbol{\chi}}(r_{\max})\tilde{\boldsymbol{\Lambda}}, \qquad (25)$$

$$r_{\max}^2\tilde{\boldsymbol{\chi}}^T(r_{\max})\tilde{\boldsymbol{\chi}}(r_{\max})=\mathbf{I}.$$

The nonsymmetric $\mathbf{R}$ matrix obtained by the total set of eigenvalues $\tilde{\boldsymbol{\Lambda}}=\{\delta_{ij}\tilde{\mu}_i\}_{ij=1}^{j_{\max}}$ and eigenvectors $\tilde{\boldsymbol{\chi}}\equiv\{\tilde{\boldsymbol{\chi}}^{(i)}\}_{i=1}^{j_{\max}}$ of the eigenvalue problem (25) reads

$$\mathbf{R}=r_{\max}^2\tilde{\boldsymbol{\chi}}(r_{\max})\tilde{\boldsymbol{\Lambda}}\tilde{\boldsymbol{\chi}}^T(r_{\max})+\mathbf{Q}(r_{\max}) \qquad (26)$$

and gives the relation between $\boldsymbol{\chi}(r)$ and its derivative at $r=r_{\max}$

$$\frac{d\boldsymbol{\chi}(r)}{dr}=\mathbf{R}\boldsymbol{\chi}(r). \qquad (27)$$

Note that, in the diagonal approximation $i=j$ of the problem (18)–(20), the so-called adiabatic approximation, the number of nodes N_r of the solution $\boldsymbol{\chi}(r)$ with respect to the slow radial variable r on a semiaxis for small values of the parameter γ corresponds to the radial quantum number $N_r=N-l-1$ of a free hydrogen atom in the bound state characterized by a conventional set of quantum numbers $(N,l,m,\lambda=(-1)^l)$ and the binding energy $-\epsilon_j(\gamma=0)=-\epsilon_j^{(0)}=Z/N^2$ (in Ry).

Recalling that the number of nodes N_θ of the solution $\boldsymbol{\Phi}(\theta;r)$ with respect to the fast angular variable, θ, at fixed $|m|$ and $\sigma=(-1)^{N_\theta}$ as a function of the slow parameter, r, is conserved, i.e., $N_\theta=l-|m|$, we have a one-to-one correspondence between the quantum numbers (N,l) of the free atom at $\gamma=0$ and the adiabatic ones $\{N_r,N_\theta\}$ of the perturbed atom at $\gamma\neq 0$.

For large values of the parameter γ, the adiabatic radial number N_r corresponds to the longitudinal quantum number $N_{|z|}$ of a hydrogen atom in the strong magnetic field at fixed m and the sign of $\sigma=\pm1$, i.e., the number of nodes of the solution $\boldsymbol{\chi}(|z|)$ with respect to the longitudinal variable $z=r\cos\theta$ on a semiaxis. It means that the solution $\boldsymbol{\chi}(z)$ on

an axis is defined as follows: $\boldsymbol{\chi}_{m\sigma}(z) = (\boldsymbol{\chi}_m(\rho, z) + \sigma\boldsymbol{\chi}_m(\rho, -z))/\sqrt{2}$ or reduced to the solution $\boldsymbol{\chi}(|z|)$ of a conventional eigenvalue problem on a semiaxis, using the Neumann and Dirichlet boundary conditions at $z = 0$ for the even $\sigma = +1$ and odd $\sigma = -1$ solutions, respectively.

Taking into account the above correspondence rules with such an adiabatic set $[N_{|z|}N_\rho]$ and the asymptotic form of eigenvalues $E_j(r)$ at large r, we can express the binding energy $\mathcal{E}$ via the eigenvalues ϵ of the problem (18)–(20) as follows: $\mathcal{E} = (\epsilon^{\text{th}}_{m\sigma j}(\gamma) - \epsilon)/2$ (in a.u.), where $\epsilon^{\text{th}}_{m\sigma j}(\gamma)$ is the true threshold shift (16) or the reduced one $\epsilon^{\text{th}}_{m\sigma}(\gamma) = \gamma(|m| + m + 1)$, respectively.

4. ASYMPTOTIC FORM OF SOLUTION

We write system of differential equations (18) at fixed values m, σ and energy $\epsilon = 2E$ in the explicit form for $\chi_{ji_o}(r) \equiv \chi^{(i_o)}_j(r)$, $j = 1, \ldots, j_{\max}$, $i_o = 1, \ldots, N_o$,

$$\Big(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{2Z}{r} - \epsilon + \frac{E_j(r)}{r^2} \qquad (28)$$

$$+ H_{jj}(r)\Big)\chi_{ji_o}(r) = \sum_{j'=1, j'\neq j}^{j_{\max}} \Big(- H_{jj'}(r)$$

$$- Q_{jj'}(r)\frac{d}{dr} - \frac{1}{r^2}\frac{dr^2Q_{jj'}(r)}{dr}\Big)\chi_{j'i_o}(r).$$

At large r, the asymptotic form of matrix elements expanded in inverse powers of r (i.e., without exponential terms) has the form (for details, see [20])

$$r^{-2}E_j(r) = E^{(0)}_j + \sum_{k=1} r^{-2k}E^{(2k)}_j, \qquad (29)$$

$$H_{jj'}(r) = \sum_{k=1} r^{-2k}H^{(2k)}_{jj'},$$

$$Q_{jj'}(r) = \sum_{k=1} r^{-2k+1}Q^{(2k-1)}_{jj'},$$

$$r \gg \max(n_l, n_r)/(2\sqrt{\gamma}).$$

Here,

$$E^{(0)}_j = \gamma(2n + |m| + m + 1), \qquad (30)$$

$$E^{(2)}_j = -2n^2 - 2n - 1 - 2|m|n - |m|,$$

$$H^{(2)}_{jj'} = (2n^2 + 2n + 2|m|n + |m| + 1)\delta_{|n_l-n_r|,0}$$

$$- \sqrt{n+1}\sqrt{n+|m|+1}\sqrt{n+2}$$

$$\times \sqrt{n+|m|+2}\,\delta_{|n_l-n_r|,2},$$

$$Q^{(1)}_{jj'} = (n_r - n_l)\sqrt{n+1}\sqrt{n+|m|+1}\,\delta_{|n_l-n_r|,1}.$$

In these formulas, the asymptotic quantum numbers n_l, n_r denote transversal quantum numbers N_ρ and N'_ρ, related to the unified numbers j, j' by the above-mentioned formulas $n_l = j - 1$, $n_r = j' - 1$, and $n = \min(n_l, n_r)$.

Note that $E^{(2)}_j + H^{(2)}_{jj} = 0$; i.e., at large r, centrifugal terms are eliminated in Eq. (28). It means that the leading terms of radial solutions, $\chi_{ji_o}(r)$, have the asymptotic form of Coulomb functions with zero angular momentum.

Let us consider the asymptotic solution following [21]

$$\chi_{ji_o}(r) = R(p_{i_o}, r)\phi_{ji_o}(r) + \frac{dR(p_{i_o}, r)}{dr}\psi_{ji_o}(r), \qquad (31)$$

where $R(p_{i_o}, r) = iF(p_{i_o}, r) + G(p_{i_o}, r)$, [$F(p_{i_o}, r)$ and $G(p_{i_o}, r)$ are the Coulomb regular and irregular functions] and satisfies the differential equation

$$\frac{d^2R(p_{i_o}, r)}{dr^2} + \frac{2}{r}\frac{dR(p_{i_o}, r)}{dr} \qquad (32)$$

$$+ \left(p^2_{i_o} + \frac{2Z}{r}\right) R(p_{i_o}, r) = 0.$$

Then we can expand the functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$ in series in inverse powers of r

$$\phi_{ji_o}(r) = \sum_{k=0}^{k_{\max}} \phi^{(k)}_{ji_o} r^{-k}, \quad \psi_{ji_o}(r) = \sum_{k=0}^{k_{\max}} \psi^{(k)}_{ji_o} r^{-k}. \qquad (33)$$

As a result of substitution of expansions (33) into (31) and (28), using (32), and equating coefficients of expansion for the same powers of r, we arrive at the set of recurrence relations with respect to unknown coefficients $\phi^{(k)}_{ji_o}$ and $\psi^{(k)}_{ji_o}$:

$$\big(p^2_{i_o} - 2E + E^{(0)}_j\big)\phi^{(k)}_{ji_o} - 2p^2_{i_o}(k-1)\psi^{(k-1)}_{ji_o} \qquad (34)$$

$$- (k-2)(k-3)\phi^{(k-2)}_{ji_o} - 2Z(2k-3)\psi^{(k-2)}_{ji_o}$$

$$+ \sum_{k'=1}^{k} \big(E^{(k')}_j + H^{(k')}_{jj}\big)\phi^{(k-k')}_{ji_o}$$

$$= \sum_{j'=1, j'\neq j}^{j_{\max}} \sum_{k'=1}^{k} \Big[\big((2k-k'-3) Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')} \big) \phi_{j'i_o}^{(k-k')} + \big(2p_{i_o}^2 Q_{jj'}^{(k')} + 4Z Q_{jj'}^{(k'-1)} \big) \psi_{j'i_o}^{(k-k')} \Big],$$

$$(p_{i_o}^2 - 2E + E_j^{(0)}) \psi_{ji_o}^{(k)} + 2(k-1)\phi_{ji_o}^{(k-1)} - k(k-1)\psi_{ji_o}^{(k-2)} + \sum_{k'=1}^{k} \big(E_j^{(k')} + H_{jj}^{(k')} \big) \psi_{ji_o}^{(k-k')} \quad (35)$$

$$= \sum_{j'=1, j'\neq j}^{j_{\max}} \sum_{k'=1}^{k} \Big[\big((2k-k'+1) Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')} \big) \psi_{j'i_o}^{(k-k')} - 2 Q_{jj'}^{(k')} \phi_{j'i_o}^{(k-k')} \Big].$$

From the first four equations of the set in (34) and (35) for $\phi_{i_o i_o}^{(0)}$, $\phi_{j_0 i_o}^{(0)}$, $\psi_{i_o i_o}^{(0)}$, and $\psi_{j_0 i_o}^{(0)}$, we get the leading terms of the eigenfunction, the eigenvalue, and the characteristic parameter, i.e., initial data for solving the recurrent sequence (34) and (35),

$$\phi_{j_0 i_o}^{(0)} = \delta_{j_0 i_o}, \quad \psi_{j_0 i_o}^{(0)} = 0, \quad p_{i_o}^2 = 2E - E_{i_o}^{(0)}, \quad (36)$$

which corresponds to the leading term of $\chi_{ji_o}(r)$ satisfying the asymptotic expansion series (33) at large r. Substituting these initial data to the next equations of the set in (34) and (35), we get a step-by-step procedure for determining the series coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$. Using the explicit asymptotic matrix elements (29), we get an explicit expression of these coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$ via the values of the number of a state (or channel) $i_o = n_o + 1$ and the number of current equation $j = 1, \ldots, j_{\max}$. For example, at $k = 0, 1$, such elements take the form

$$\phi_{i_o i_o}^{(0)} = 1, \quad \psi_{i_o i_o}^{(0)} = 0,$$

$$\phi_{i_o - 1 i_o}^{(1)} = 0, \quad \psi_{i_o - 1 i_o}^{(1)} = \frac{\sqrt{n_o}\sqrt{n_o + |m|}}{\gamma},$$

$$\phi_{i_o i_o}^{(1)} = 0, \quad \psi_{i_o i_o}^{(1)} = -\frac{2n_o + |m| + 1}{\gamma},$$

$$\phi_{i_o + 1 i_o}^{(1)} = 0, \quad \psi_{i_o + 1 i_o}^{(1)} = \frac{\sqrt{n_o + 1}\sqrt{n_o + |m| + 1}}{\gamma}.$$

Taking into account the region of convergence of the matrix elements, we find that the region of convergence of expansion (31), as follows from asymptotic form of matrix elements which do not depend on p_{i_o}, is $r_{\max} \gg n_{i_o}/(2\sqrt{\gamma})$ and $r_{\max} \gg Z(2n_{i_o} + |m| + 1)/(p_{i_o}\sqrt{\gamma})$.

5. THE SCATTERING STATES AND PHOTOIONIZATION CROSS SECTIONS

The solution of the scattering problem,

$$\boldsymbol{\chi}^{(p)}(r) = i\boldsymbol{\chi}^{(ph)}(r)(\mathbf{I} - i\mathbf{K}) = \boldsymbol{\chi}^{s}(r) + \boldsymbol{\chi}^{c}(r)\mathbf{K}, \quad (37)$$

with N_o open channels for $p_{i_o}^2 \geq 0$ at $i_o = 1, \ldots, N_o$, is defined by means of the two independent fundamental asymptotic solutions $\boldsymbol{\chi}^{s}(r) = 2\Im(\boldsymbol{\chi}(r))$ and $\boldsymbol{\chi}^{c}(r) = 2\Re(\boldsymbol{\chi}(r))$ (corresponding to "regular" and "irregular" type) of Eqs. (28) and a reaction matrix $\mathbf{K} = i(\mathbf{I} + \mathbf{S})^{-1}(\mathbf{I} - \mathbf{S})$, where $\mathbf{S} = (\mathbf{I} + i\mathbf{K})(\mathbf{I} - i\mathbf{K})^{-1}$ is the scattering matrix.

In this case, the regular and irregular functions satisfy the generalized Wronskian relation at large r

$$\mathbf{Wr}(\mathbf{Q}(r); \boldsymbol{\chi}^{c}(r), \boldsymbol{\chi}^{s}(r)) = \frac{2}{\pi}\mathbf{I}_{oo}, \quad (38)$$

where $\mathbf{Wr}(\bullet; \boldsymbol{\chi}^{c}(r), \boldsymbol{\chi}^{s}(r))$ is a generalized Wronskian with a long derivative defined by

$$\mathbf{Wr}(\bullet; \boldsymbol{\chi}^{c}(r), \boldsymbol{\chi}^{s}(r)) = r^2 \left[(\boldsymbol{\chi}^{c}(r))^T \left(\frac{d\boldsymbol{\chi}^{s}(r)}{dr} - \bullet \boldsymbol{\chi}^{s}(r) \right) - \left(\frac{d\boldsymbol{\chi}^{c}(r)}{dr} - \bullet \boldsymbol{\chi}^{c}(r) \right)^T \boldsymbol{\chi}^{s}(r) \right], \quad (39)$$

which will be used to control a desirable accuracy of the above expansion. Here, $\mathbf{I}_{oo}$ is the unit matrix of dimension $N_o \times N_o$.

Using Eq. (27), we obtain the equation for the reaction matrix $\mathbf{K}$ via $\mathbf{R}$ matrix at $r = r_{\max}$

$$\left(\mathbf{R}\boldsymbol{\chi}^{c}(r) - \frac{d\boldsymbol{\chi}^{c}(r)}{dr} \right) \mathbf{K} = \left(\frac{d\boldsymbol{\chi}^{s}(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^{s}(r) \right), \quad (40)$$

and Eq. (38) is equivalent to

$$\mathbf{Wr}(\mathbf{Q}(r_{\max}); \boldsymbol{\chi}^{s}(r_{\max}), \boldsymbol{\chi}^{c}(r_{\max})) = \mathbf{Wr}(\mathbf{R}; \boldsymbol{\chi}^{s}(r_{\max}), \boldsymbol{\chi}^{c}(r_{\max})). \quad (41)$$

Note that, when some channels are closed, the left and right matrices of (40) are rectangular matrices. Therefore, multiplying (40) on the left by the matrix $(\boldsymbol{\chi}^{c}(\rho))^T$, we obtain the following formula for the reaction matrix $\mathbf{K}$:

$$\mathbf{K} = -\mathbf{X}^{-1}(r_{\max})\mathbf{Y}(r_{\max}), \quad (42)$$

where

$$\mathbf{X}(r) = (\boldsymbol{\chi}^c(r))^T \left(\frac{d\boldsymbol{\chi}^c(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^c(r) \right),$$

$$\mathbf{Y}(r) = (\boldsymbol{\chi}^c(r))^T \left(\frac{d\boldsymbol{\chi}^s(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^s(r) \right)$$

are square matrices of dimension $N_o \times N_o$ and $\mathbf{X}(r_{\max})$ should be a symmetric matrix, which follows from the condition $\mathbf{Wr}(\mathbf{R}; \boldsymbol{\chi}^c(r_{\max}), \boldsymbol{\chi}^c(r_{\max})) = 0$.

Let the matrices $\mathbf{S}$ and $\mathbf{K}$ have eigenvalues $\exp(2i\delta_i)$ and $\tan\delta_i$, respectively. Then

$$\mathbf{SB} = \mathbf{B}\exp(\mathbf{2i}\boldsymbol{\delta}), \quad \mathbf{KB} = \mathbf{B}\tan\boldsymbol{\delta}, \tag{43}$$

where $\exp(\mathbf{2i}\boldsymbol{\delta})$ and $\tan\boldsymbol{\delta}$ are diagonal matrices and $\mathbf{B}$ can be taken to be real and normalized to

$$\mathbf{B}^T\mathbf{B} = \mathbf{I}_{oo}. \tag{44}$$

We denote the eigenstate wave function of continuum $\Psi_i^{Em\sigma}(r,\theta)$ with energy $2E$ (of ejected electron) above the first threshold $\epsilon^{\text{th}}_{m\sigma 1}(\gamma) = \epsilon^{\text{th}}_{m\sigma}(\gamma) = \gamma(|m| + m + 1)$ by the following:

$$\Psi_i^{Em\sigma}(r,\theta) = \sum_{j=1}^{j_{\max}} \Phi_j^{m\sigma}(\theta; r)\hat{\chi}_{ji}^{(m\sigma)}(E,r), \tag{45}$$

where

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \boldsymbol{\chi}^{(ph)}(r)\mathbf{B} \tag{46}$$

$$\text{or} \quad \hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \boldsymbol{\chi}^{(p)}(r)\mathbf{B}\cos\boldsymbol{\delta}.$$

In this case, the eigenstate wave function $\Psi_i^{Em\sigma}(r,\theta)$ is normalized to

$$\left\langle \Psi_i^{Em\sigma}(r,\theta) \middle| \Psi_{i'}^{E'm'\sigma'}(r,\theta) \right\rangle \tag{47}$$

$$= \sum_{j=1}^{j_{\max}} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m\sigma)}(E,r) \right)^* \hat{\chi}_{ji'}^{(m'\sigma')}(E',r)$$

$$= \delta(E - E')\delta_{mm'}\delta_{\sigma\sigma'}\delta_{ii'}.$$

In terms of the above definitions, the photoionization cross sections $\sigma^d(\omega)$ and $\sigma^p(\omega)$ (for light polarized along the z axis and in the XOY plane, respectively) are expressed as

$$\sigma^d(\omega) = 4\pi^2\alpha\omega \sum_{i=1}^{N_o} \left| \hat{D}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) \right|^2 a_0^2, \tag{48}$$

$$\sigma^p(\omega) = 4\pi^2\alpha\omega \sum_{i=1}^{N_o} \left| \hat{P}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) \right|^2 a_0^2,$$

where $\hat{D}^{m\sigma}_{i,N_{|z|},N_\rho}(E)$ and $\hat{P}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E)$ are the matrix elements of the longitudinal and transverse moments, respectively,

$$\hat{D}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) \tag{49}$$

$$= \delta_{|m-m'|0} \left\langle \Psi_i^{Em'-\sigma}(r,\theta) \middle| r\cos\theta \middle| \Psi^{m\sigma}_{N_{|z|},N_\rho}(r,\theta) \right\rangle$$

$$= \sum_{j=1}^{N}\sum_{j'=1}^{N} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m'-\sigma)}(E,r) \right)^* \times D_{jj'}^{(m'm\sigma)}(r)\chi_{j'}^{(m\sigma)}(r),$$

$$\hat{P}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) \tag{50}$$

$$= \delta_{|m-m'|1} \left\langle \Psi_i^{Em'\sigma}(r,\theta) \middle| \frac{r\sin\theta}{\sqrt{2}} \middle| \Psi^{m\sigma}_{N_{|z|},N_\rho}(r,\theta) \right\rangle$$

$$= \sum_{j=1}^{N}\sum_{j'=1}^{N} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m'\sigma)}(E,r) \right)^* \times P_{jj'}^{(m'm\sigma)}(r)\chi_{j'}^{(m\sigma)}(r).$$

The longitudinal $D^{(m\sigma)}(r)$ and transversal $P^{(mm'\sigma)}(r)$ matrix elements are expressed as

$$D_{jj'}^{(m'm\sigma)}(r)$$

$$= \delta_{|m-m'|0} \left\langle \Phi_j^{m'-\sigma}(\theta; r) \middle| r\cos\theta \middle| \Phi_{j'}^{m\sigma}(\theta; r) \right\rangle_\theta,$$

$$P_{jj'}^{(m'm\sigma)}(r)$$

$$= \delta_{|m-m'|1} \left\langle \Phi_j^{m'\sigma}(\theta; r) \middle| \frac{r\sin\theta}{\sqrt{2}} \middle| \Phi_{j'}^{m\sigma}(\theta; r) \right\rangle_\theta.$$

In the above expressions, $\omega = E - E(N_{|z|}, N_\rho, \sigma, m)$ is the frequency of radiation, $E(N_{|z|}, N_\rho, \sigma, m)$ is the energy of the initial bound state $\Psi^{m\sigma}_{N_{|z|},N_\rho}(r,\eta)$, E is the energy of the final continuum state $\Psi_i^{Em\sigma}(r,\eta)$ such that N_o is the number of the open channels, α is the fine-structure constant, a_0 is the Bohr radius.

In our calculations, we used the following physical constants: inverse centimeter–Hartree relationship $\text{cm}^{-1} = 4.55633 \times 10^{-6}$ a.u., Bohr radius $a_0 = 5.29177 \times 10^{-11}$ m, and fine-structure constant $\alpha = 7.29735 \times 10^{-3}$ [22]. Figure 1 displays the calculated photoionization cross sections $\sigma^d(\omega)$ and $\sigma^p(\omega)$ from

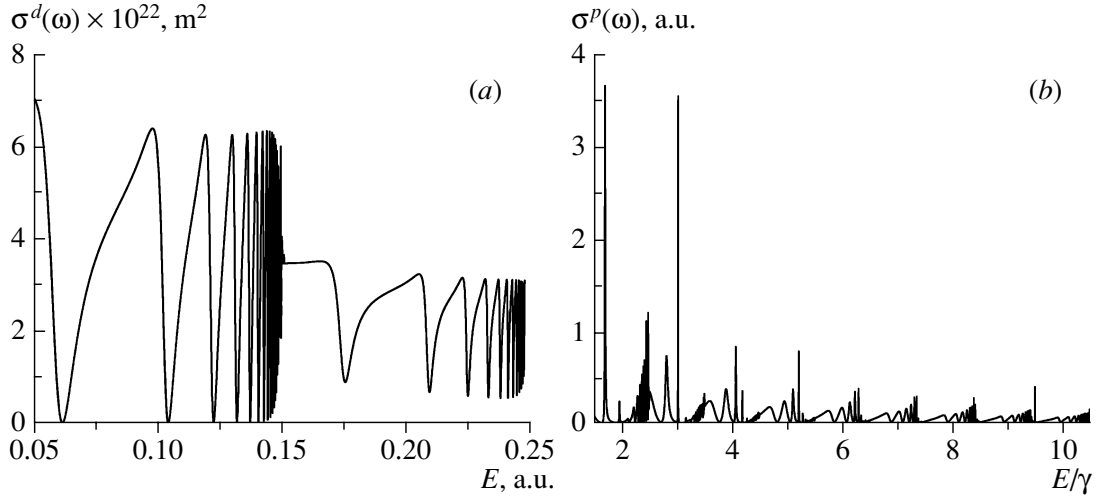

Fig. 1. Photoionization cross sections $\sigma^d(\omega)$ (a) and $\sigma^p(\omega)$ (b) from the ground state with $\gamma = 0.1$ to the final state with $\sigma = -1$ and $m = 0$ at $\gamma = 0.05$ to the final state with $\sigma = +1$ and $m = 1$, respectively.

the ground state to the different continuous spectrum states. In Fig. 1a, we use the energy interval from $E = 0.05$ to 0.25 a.u. for the final state with $\sigma = -1$ and $m = 0$. The number of open channels is equal to 1 to 2. In Fig. 1b, we used the energy interval from $E = 0.075$ to 0.525 a.u. for the final state with $\sigma = +1$ and $m = 1$. The final-state energy E is measured relative to the zero-field ionization threshold. The number of open channels varies from 1 to 9. The calculated photoionization cross section is in good agreement with [12] between the thresholds, but not near them. Here, we show one of the goals of the elaborated approach to provide stable and economical calculations of the photoionization cross section having the true threshold behavior coinciding with [15].

6. CONCLUSIONS

A new efficient method for calculating wave functions of a hydrogen atom in a strong magnetic field is developed on the basis of the Kantorovich approach to parametric eigenvalue problems in spherical coordinates. The two-dimensional spectral problem for the Schrödinger equation at a fixed magnetic quantum number and parity is reduced to a spectral parametric problem for a one-dimensional equation by the angular variable and a finite set of ordinary second-order differential equations by the radial variable. The results are in good agreement with calculations by other authors. The developed approach is a good tool for calculating threshold phenomena in formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps. In the future, we will also calculate a manifold of the excited states in a layer with the principle quantum number $N = 3$ of a hydrogen atom in the magnetic field 2.35×10^4 T and 6.1 T that may be interesting from our viewpoint for a laser-stimulated recombination in actually existing traps [23].

ACKNOWLEDGMENTS

This work was partly supported by grants of the Russian Foundation for Basic Research (nos. 07-01-00660 and 08-01-00604-a), by CRDF BRHE grant REC-006 SR-006-X1/B75M06 Y3-P-06-08, by a grant of the President of the Bulgarian State Agency for Atomic Energy (2004), by grant no. I-1402/2004 of the Bulgarian Fund for Scientific Investigations, and by grant NFSAT-CRDF ARP1-3228-YE-04.

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