Adiabatic representation for a hydrogen atom photoionization in an uniform magnetic field

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A new effective method of calculating wave functions of discrete and continuous spectra of a hydrogen atom in a strong magnetic field is developed based on 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 a 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 with long derivatives in a form appropriated for a generalization of **R**–matrix calculations following from a variational functional. The results are in good agreement with the photoionization calculations by other authors and have a true threshold behavior.

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1. INTRODUCTION

Recent Monte-Carlo estimations of the influence of the strong magnetic field on the spontaneous recombination of the antihydrogen in the cold positron–antiproton plasma conditions of the ATHENA [1, 2] and ALPHA [3] experiments (CERN) are shown that further quantum mechanical analysis is needed [4]. We can pay attention for a new enhancement mechanism of a laser-stimulated recombination of antihydrogen in cold antiproton-positron plasma in a laboratory magnetic field via quasistationary states embedded in the continuum that is reveled recently [5]. To realize such analysis in first stage the adiabatic representation known

in mathematics as a Kantorovich method is developed for solving: the problem of low-lying excited states of 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 the high magnetic quantum numbers in the magnetic traps [8]. It has been shown that the exhaust analysis of a complex behavior of the electron dynamics 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 the high magnetic numbers or dominating magnetic field [10]. So, using of the spherical coordinates is preferable when Coulomb and magnetic fields have comparable contributions in an average potential energy [11] but leads to non-true threshold behavior of photoionization cross section calculated by complex rotation variational method[12].

In this paper we develop the Kantorovich approach with a boundary condition of the third type in a form appropriated for the generalized **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]. 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 continues spectrum states is demonstrated by present calculations.

The paper is organized as follows. The 2D–eigenvalue problem for Schrödinger equation of the hydrogen atom in an axially symmetric magnetic field, written in spherical coordinates, is considered in section 2 together with the appropriate classification of states. The reduction of the 2D–eigenvalue problem to the 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 determine the solutions, and the reaction matrix, from the generalized **R**–matrix method, are presented in section 4. The method is applied to the calculation of ionization of the ground state to the different continues spectrum states in section 5. In conclusion, we point out at the perspectives for further applications of this approach.

2. STATEMENT OF THE PROBLEM

The Schrödinger equation for wave function $\hat{\Psi}(r,\theta,\varphi) = \Psi(\theta,r)\exp(\imath m\varphi)/\sqrt{2\pi}$ 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

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

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

$$U(r,\theta) = -\frac{2Z}{r} + V(r,\theta), \qquad V(r,\theta) = \frac{m^2}{r^2\sin^2\theta} + \gamma m + \frac{\gamma^2 r^2}{4}\sin^2\theta, \tag{2}$$

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 $|m\sigma>$ 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:

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

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

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

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

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

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

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

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

$$\mathbf{\Pi}(\Psi,\epsilon)=2\int\limits_0^{r_{\max}}\int\limits_0^{\pi/2}\sin\theta\left(r^2\left|\frac{\partial\Psi(r,\theta)}{\partial r}\right|^2+\left|\frac{\partial\Psi(r,\theta)}{\partial\theta}\right|^2+r^2(U(r,\theta)-\epsilon)|\Psi(r,\theta)|^2\right)d\theta dr.$$

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

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

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), (8)

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

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 the (1)–(5) with (6)/(8) corresponding to the eigenstate $|m\sigma i\rangle$ using the finite set of one–dimensional basis functions $\{\Phi_j^{m\sigma}(\theta;r)\}_{j=1}^{j_{\max}}$

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

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 $\mathbf{\Phi}(\theta;r)\equiv\mathbf{\Phi}^{m\sigma}(\theta;r)$, $(\mathbf{\Phi}(\theta;r))^T=(\Phi_1(\theta;r),\ldots,\Phi_{j_{\max}}(\theta;r))$ 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:

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

with the boundary conditions

$$\lim_{\theta\to 0}\sin\theta\frac{\partial\Phi_j(\theta;r)}{\partial\theta}=0,\ \text{for } m=0,\ \text{and } \Phi_j(0;r)=0,\ \text{for } m\neq 0, \tag{12}$$

$$\frac{\partial\Phi_j}{\partial\theta}\left(\frac{\pi}{2};r\right)=0,\ \text{for } \sigma=+1,\ \text{and } \Phi_j\left(\frac{\pi}{2};r\right)=0,\ \text{for } \sigma=-1. \tag{13}$$

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 $\mathbf{\Phi}(\theta;r)$ with respect to the angular variable θ in the interval $0<\theta<\pi$. Since the operator in the left–hand side of (11) is self–adjoint, its eigenfunctions are orthonormal

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

where δ_{ij} is the Kroneker symbol.

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

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

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 $\mathbf{\Phi}(\theta;r)$ at fixed $|m|$ and $\sigma=(-1)^{N_\theta}$ as a function of the parameter r is preserved, we get the 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:

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

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 $\mathbf{\Phi}(\theta;r)$ in the subinterval $0<\eta<1$ or $-1<\eta<0$, corresponding to the transversal variable $\rho=r\sin\theta$ on semi–axis, are expressed via the number of nodes N_θ of the solution $\mathbf{\Phi}(\theta;r)$: $N_\rho=1/2\cdot N_\theta$ 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.,

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

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 the uniform magnetic field or a helium atom.

After substituting the expansion (10) into variational problem (8), and using (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)

$$\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\mathbf{U}(r)}{r^2} + \mathbf{Q}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{d\,r^2\mathbf{Q}(r)}{dr}\right)\boldsymbol{\chi}^{(i)}(r) = \epsilon_i\,\mathbf{I}\boldsymbol{\chi}^{(i)}(r), \tag{18}$$

$$\lim_{r\to 0} r^2\left(\boldsymbol{D}_r\boldsymbol{\chi}^{(i)}(r)\right) \equiv \lim_{r\to 0} r^2\left(\frac{d\boldsymbol{\chi}^{(i)}(r)}{dr} - \mathbf{Q}(r)\boldsymbol{\chi}^{(i)}(r)\right) = 0.$$

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

$$U_{ij}(r) = \frac{E_i(r)+E_j(r)}{2}\delta_{ij} - 2Zr\delta_{ij} + r^2H_{ij}(r), \quad I_{ij} = \delta_{ij}, \tag{19}$$

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

The above matrix elements were calculated by means of the author combined computer algebra-numerical code MATRM implemented in both MAPLE 8 and FORTRAN [20].

The discrete spectrum solutions are obeyed the asymptotic boundary condition and orthonormal conditions

$$\lim_{r\to\infty} r^2\boldsymbol{\chi}^{(i)}(r) = 0 \quad \rightarrow \quad \boldsymbol{\chi}^{(i)}(r_{\max}) = 0, \qquad \int_0^{r_{\max}} r^2(\boldsymbol{\chi}^{(i)}(r))^T\boldsymbol{\chi}^{(j)}(r)dr = \delta_{ij}. \tag{20}$$

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

$$\left\langle \Phi_j(\theta;r)\,\middle|\,\frac{\partial\Psi_i^{Em\sigma}(r,\theta)}{\partial r} - \mu_i\,\Psi_i^{Em\sigma}(r,\theta)\right\rangle_\theta = 0, \quad r = r_{\max}, \tag{21}$$

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

$$\left(\mathbf{R} - \mathbf{Q}(r) - \mu_i\right)\boldsymbol{\chi}^{(i)}(r) = \left(\frac{d\boldsymbol{\chi}^{(i)}(r)}{dr}(\boldsymbol{\chi}^{(i)})^{-1}(r) - \mathbf{Q}(r) - \mu_i\right)\boldsymbol{\chi}^{(i)}(r) = 0. \tag{22}$$

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

$$\boldsymbol{D}_r\boldsymbol{\chi}(r) \equiv \frac{d\boldsymbol{\chi}(r)}{dr} - \mathbf{Q}(r)\boldsymbol{\chi}(r) = \boldsymbol{\chi}(r)\boldsymbol{\Lambda}, \tag{23}$$

that reformulates by averaging of variational problem (9) to the following one:

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

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

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

$$\boldsymbol{\Pi}\tilde{\boldsymbol{\chi}} = r^2_{\max}\tilde{\boldsymbol{\chi}}(r_{\max})\tilde{\boldsymbol{\Lambda}}, \quad r^2_{\max}\tilde{\boldsymbol{\chi}}^T(r_{\max})\tilde{\boldsymbol{\chi}}(r_{\max}) = \mathbf{I}. \tag{25}$$

The nonsymmetric $\mathbf{R}$ matrix is 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)

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

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

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

One can see that Eqs. (25) and (26) provide a generalization of the conventional $\mathbf{R}$–matrix calculations with a symmetric $\mathbf{R}$–matrix[24, 25], that originate from a conventional Galerkin expansion for which $\mathbf{Q}(r) \equiv 0$ and long derivatives are conventional ones $\boldsymbol{D}_r\boldsymbol{\chi}(r) \equiv \frac{d\boldsymbol{\chi}(r)}{dr}$.

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 semi–axis 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 $\mathbf{\Phi}(\theta;r)$ 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 the 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 $\sigma=\pm 1$, i.e., the number of nodes of the solution $\boldsymbol{\chi}(|z|)$ with respect to the longitudinal variable $z=r\cos\theta$ on semi–axis. 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 semi–axis, 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 asymptotics 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: $\mathcal{E}=(\epsilon^{th}_{m\sigma j}(\gamma)-\epsilon)/2$ (in $a.u.$), where $\epsilon^{th}_{m\sigma j}(\gamma)$ is the true threshold shift (16) or the reduced one $\epsilon^{th}_{m\sigma}(\gamma)=\gamma(|m|+m+1)$, respectively.

4. ASYMPTOTICS OF SOLUTION

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

$$\left(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{2Z}{r}-\epsilon+\frac{E_j(r)}{r^2}+H_{jj}(r)\right)\chi_{ji_o}(r) \tag{28}$$
$$=\sum_{j'=1,j'\neq j}^{j_{\max}}\left(-H_{jj'}(r)-Q_{jj'}(r)\frac{d}{dr}-\frac{1}{r^2}\frac{d\,r^2Q_{jj'}(r)}{dr}\right)\chi_{j'i_o}(r).$$

At large r asymptotics of matrix elements by inverse power of r (i.e., without exponential terms) is of the form (for details, see [20])

$$r^{-2}E_j(r)=E_j^{(0)}+\sum_{k=1}r^{-2k}E_j^{(2k)},\quad H_{jj'}(r)=\sum_{k=1}r^{-2k}H_{jj'}^{(2k)},$$
$$Q_{jj'}(r)=\sum_{k=1}r^{-2k+1}Q_{jj'}^{(2k-1)},\qquad r\gg\max(n_l,n_r)\gamma/2. \tag{29}$$

Here

$$\begin{aligned} E_j^{(0)} &= \gamma(2n+|m|+m+1), \\ E_j^{(2)} &= -2n^2-2n-1-2|m|n-|m|, \\ H_{jj'}^{(2)} &= (2n^2+2n+2|m|n+|m|+1)\delta_{|n_l-n_r|,0} \\ &\quad -\sqrt{n+1}\sqrt{n+|m|+1}\sqrt{n+2}\sqrt{n+|m|+2}\delta_{|n_l-n_r|,2}, \\ Q_{jj'}^{(1)} &= (n_r-n_l)\sqrt{n+1}\sqrt{n+|m|+1}\delta_{|n_l-n_r|,1}, \end{aligned} \tag{30}$$

In these formulas asymptotic quantum numbers n_l, n_r denote transversal quantum numbers N_ρ, N'_ρ, that connected with 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, $E_j^{(2)} + H_{jj}^{(2)} = 0$, 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 asymptotic of the Coulomb functions with zero angular momentum.

Let us consider asymptotic solution following paper [21]

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

where $R(p_{i_o}, r) = \imath\, F(p_{i_o}, r) + G(p_{i_o}, r)$; $F(p_{i_o}, r)$, $G(p_{i_o}, r)$ are the Coulomb regular, irregular functions and satisfy the differential equation

$$\frac{d^2R(p_{i_o}, r)}{dr^2} + \frac{2}{r}\frac{dR(p_{i_o}, r)}{dr} + \left(p_{i_o}^2 + \frac{2Z}{r}\right)R(p_{i_o}, r) = 0. \tag{32}$$

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

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

In result of substitution of expansions (33) to (31) and (28), using (32) and equating coefficients of expansion for the same powers of r, we arrive to the set of recurrence relations

with respect to unknown coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$:

$$\left(p_{i_o}^2 - 2E + E_j^{(0)}\right)\phi_{ji_o}^{(k)} - 2p_{i_o}^2(k-1)\psi_{ji_o}^{(k-1)} - (k-2)(k-3)\phi_{ji_o}^{(k-2)} - 2Z(2k-3)\psi_{ji_o}^{(k-2)}$$
$$+\sum_{k'=1}^{k}\left(E_j^{(k')} + H_{jj}^{(k')}\right)\phi_{ji_o}^{(k-k')} = \sum_{j'=1,j'\neq j}^{j_{\max}}\sum_{k'=1}^{k}\Bigg[\left((2k-k'-3)Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')}\right)\phi_{j'i_o}^{(k-k')}$$
$$+\left(2p_{i_o}^2 Q_{jj'}^{(k')} + 4ZQ_{jj'}^{(k'-1)}\right)\psi_{j'i_o}^{(k-k')}\Bigg], \tag{34}$$

$$(p_{i_o}^2 - 2E + E_j^{(0)})\psi_{ji_o}^{(k)} + 2(k-1)\phi_{ji_o}^{(k-1)} - k(k-1)\psi_{ji_o}^{(k-2)} + \sum_{k'=1}^{k}\left(E_j^{(k')} + H_{jj}^{(k')}\right)\psi_{ji_o}^{(k-k')}$$
$$= \sum_{j'=1,j'\neq j}^{j_{\max}}\sum_{k'=1}^{k}\Bigg[\left((2k-k'+1)Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')}\right)\psi_{j'i_o}^{(k-k')} - 2Q_{jj'}^{(k')}\phi_{j'i_o}^{(k-k')}\Bigg]. \tag{35}$$

From first four equations of set (34)–(35) for $\phi_{i_oi_o}^{(0)}$, $\phi_{j_0i_o}^{(0)}$, $\psi_{i_oi_o}^{(0)}$, $\psi_{j_0i_o}^{(0)}$, we have the leading terms of eigenfunction, eigenvalue and characteristic parameter, i.e., initial data for solving the recurrence sequence (34)–(35),

$$\phi_{j_0i_o}^{(0)} = \delta_{j_0i_o}, \quad \psi_{j_0i_o}^{(0)} = 0, \quad p_{i_o}^2 = 2E - E_{i_o}^{(0)}, \tag{36}$$

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

$$\begin{aligned}
\phi_{i_oi_o}^{(0)} &= 1, \qquad \psi_{i_oi_o}^{(0)} = 0,\\
\phi_{i_o-1i_o}^{(1)} &= 0, \qquad \psi_{i_o-1i_o}^{(1)} = \frac{\sqrt{n_o}\sqrt{n_o+|m|}}{\gamma},\\
\phi_{i_oi_o}^{(1)} &= 0, \qquad \psi_{i_oi_o}^{(1)} = -\frac{2n_o+|m|+1}{\gamma},\\
\phi_{i_o+1i_o}^{(1)} &= 0, \qquad \psi_{i_o+1i_o}^{(1)} = \frac{\sqrt{n_o+1}\sqrt{n_o+|m|+1}}{\gamma}.
\end{aligned}$$

Taking into account the region of convergence of matrix elements we find that the region of convergence of expansion (31) as follows from asymptotics of matrix elements which not depends on p_{i_o} is $r_{max} \gg n_{i_o}/(2\sqrt{\gamma})$ and $\hat{r}_{max} \gg \hat{Z}\gamma(2n_{i_o}+1)/p_{i_o}$.

5. THE SCATTERING STATES AND PHOTOIONIZATION CROSS SECTIONS

Solution of the scattering problem,

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

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 $\boldsymbol{\chi}^{s}(r) = 2\,\Im(\boldsymbol{\chi}(r))$, $\boldsymbol{\chi}^{c}(r) = 2\,\Re(\boldsymbol{\chi}(r))$ (corresponding 'regular', 'irregular' type) of Eqs. (28) and a reaction matrix $\mathbf{K} = \imath(\mathbf{I} + \mathbf{S})^{-1}(\mathbf{I} - \mathbf{S})$, where $\mathbf{S} = (\mathbf{I} + \imath\,\mathbf{K})(\mathbf{I} - \imath\,\mathbf{K})^{-1}$ is the scattering matrix.

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

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

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

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

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

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

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

and the Eq. (38) equivalent to

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

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

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

where

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

are the square matrices of dimension $N_o \times N_o$ and $\mathbf{X}(r_{\max})$ is should be a symmetric matrix 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 $\exp(2\imath\delta_i)$ and $\tan\delta_i$, respectively. Then

$$\mathbf{S}\,\mathbf{B} = \mathbf{B}\,\mathbf{exp(2\imath\boldsymbol{\delta})}, \quad \text{and} \quad \mathbf{K}\,\mathbf{B} = \mathbf{B}\,\mathbf{tan}\,\boldsymbol{\delta} \tag{43}$$

where $\mathbf{exp(2\imath\boldsymbol{\delta})}$, $\mathbf{tan}\,\boldsymbol{\delta}$, 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 denoted the eigenstate wave function of continuum $\Psi_i^{Em\sigma}(r,\theta)$ with energy $2E$ (of ejected electron) above the first threshold $\epsilon^{th}_{m\sigma 1}(\gamma) = \epsilon^{th}_{m\sigma}(\gamma) = \gamma(|m| + m + 1)$ by the following

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

where

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \boldsymbol{\chi}^{(ph)}(r)\mathbf{B} \quad \text{or} \quad \hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \boldsymbol{\chi}^{(p)}(r)\mathbf{B}\,\mathbf{cos}\,\boldsymbol{\delta}. \tag{46}$$

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

$$\begin{aligned}\left\langle \Psi_i^{Em\sigma}(r,\theta) \middle| \Psi_{i'}^{E'm'\sigma'}(r,\theta) \right\rangle &= \sum_{j=1}^{j_{\max}} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m\sigma)}(E,r)\right)^* \hat{\chi}_{ji'}^{(m'\sigma')}(E',r) \\ &= \delta(E-E')\delta_{mm'}\delta_{\sigma\sigma'}\delta_{ii'}. \end{aligned} \tag{47}$$

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

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

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 transversal moment, respectively

$$\begin{aligned}\hat{D}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) &= \delta_{|m-m'|0}\left\langle \Psi_i^{Em'-\sigma}(r,\theta) \middle| r\cos\theta \middle| \Psi^{m\sigma}_{N_{|z|},N_\rho}(r,\theta) \right\rangle \\ &= \sum_{j=1}^{N}\sum_{j'=1}^{N} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m'-\sigma)}(E,r)\right)^* D_{jj'}^{(m'm\sigma)}(r)\chi_{j'}^{(m\sigma)}(r), \end{aligned} \tag{49}$$

$$\begin{aligned}\hat{P}^{m'm\sigma}_{i,N_{|z|},N_\rho}(E) &= \delta_{|m-m'|1}\left\langle \Psi_i^{Em'\sigma}(r,\theta) \middle| \frac{r\sin\theta}{\sqrt{2}} \middle| \Psi^{m\sigma}_{N_{|z|},N_\rho}(r,\theta) \right\rangle \\ &= \sum_{j=1}^{N}\sum_{j'=1}^{N} \int_0^{r_{\max}} r^2 dr \left(\hat{\chi}_{ji}^{(m'\sigma)}(E,r)\right)^* P_{jj'}^{(m'm\sigma)}(r)\chi_{j'}^{(m\sigma)}(r). \end{aligned} \tag{50}$$

The longitudinal $\mathbf{D}^{(m\sigma)}(r)$ and transversal $\mathbf{P}^{(mm'\sigma)}(r)$ 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 $cm^{-1} = 4.55633 \times 10^{-6}\, a.u.$, Bohr radius $a_0 = 5.29177 \times 10^{-11} m$ and fine–structure constant $\alpha = 7.29735 \times 10^{-3}$ [22]. Fig. 1 displays the calculated photoionization cross-sections $\sigma^d(\omega)$ and $\sigma^p(\omega)$ from the ground state to the different continues spectrum states. On fig. 1a we use the energy interval from $E = 0.05\, a.u.$ to $E = 0.25\, a.u.$ for the final state with $\sigma = -1$, $m = 0$. Number of the open channels are equal from 1 to 2. One can see that behavior of the photoionization cross-section versus energy between first and second thresholds is an agreement in a qualitative sense with behavior of a short-range elastic scattering cross-section of the opposite charge particles with short-range potential[25]. On fig. 1b we used the energy interval from $E = 0.075\, a.u.$ to $E = 0.525\, a.u.$ for the final state with $\sigma = +1$, $m = 1$. The final state energy E is measured relative to the zero-field ionization threshold. Number of the open channels are equal from 1 to 9. Calculated photoionization cross section is in good agreement with [12] between the thresholds, but not near them. Here we show one of the goal of the elaborated approach to provide the stable and economy calculations of photoionization cross section having the true threshold behavior coincided with [15].

6. CONCLUSIONS

A new effective method of calculating wave functions of a hydrogen atom in a strong magnetic field is developed based on 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 a 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 yields a good tool for calculations of threshold phenomena in formation and ionization of (anti)hydrogen like atoms and ions in magnetic traps. In further we will calculate also a manifold of the excited states in a lair with the principle quantum number $N = 3$ of a hydrogen atom at the magnetic field $2.35 \times 10^4\, T$ and $6.1\, T$ that may be interested from our viewpoint for a laser stimulated recombination in a trap [23].

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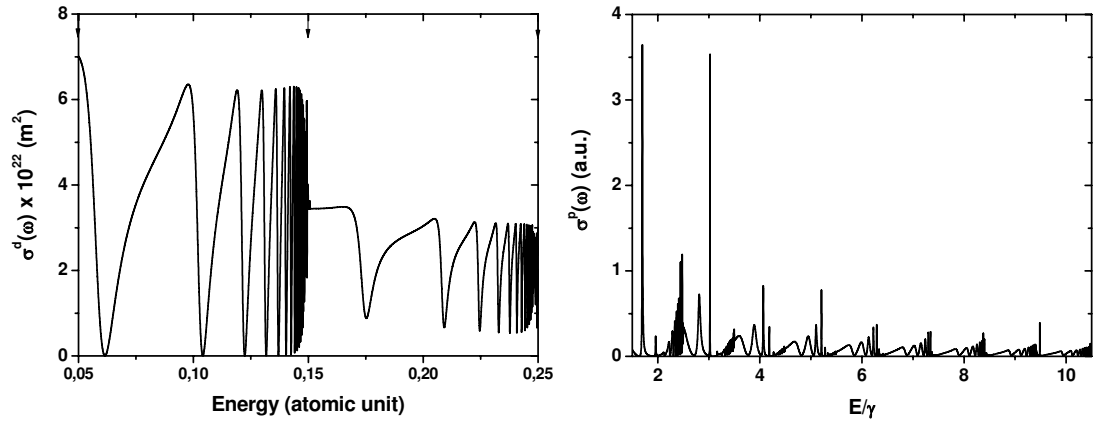

(a) (b)

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