Application of Kantorovich method for calculations of a hydrogen atom photoionization in a strong magnetic field

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ABSTRACT

A new efficient method of calculating the photoionization of a hydrogen atom in a strong magnetic field is developed basing on the Kantorovich approach to the parametric boundary problems in spherical coordinates. The progress as compared with our previous paper [SPIE Proc. **6165**, p. 66–82, (2006)] consists in computation of the wave functions of continuous spectrum, including the quasi-stationary states imbedded in the continuum. The photoionization cross sections for the ground and excited states are in good agreement with the calculations by other authors.

Keywords: Kantorovich approach, hydrogen atom, photoionization, strong magnetic field

1. INTRODUCTION

In recent decades the dynamics of transient processes in magnetic traps, such as excitation, de-excitation, ionization, recombination of ions and atoms, became a subject of intense experimental and theoretical studies.[1–3] Recently a new mechanism of formation of metastable positive-energy atoms via quasi-stationary states[4] due to the magnetic field was revealed. The most complicated case when the magnetic energy is comparable to that of Coulomb interaction requires really stable numerical schemes for the states of discrete and continuous spectra, including the quasi-stationary states, analogous to well-known doubly excited states of helium atom.[5–7]

In the present paper we develop the Kantorovich method (i.e. the reduction of the boundary problem for elliptical partial differential equation in a 2D domain to a regular boundary problem for a set of ordinary second-order differential equations with variable coefficients with the boundary conditions of the third kind) in the form, appropriate for **R**-matrix calculations of the continuous spectrum and photoionization of atomic hydrogen in a strong magnetic field.[8] The solution depending on the radial variable r and the angular variable $\eta = \cos\theta = z/r$ with fixed values of the magnetic quantum number m and z-parity σ is expanded using the basis set of oblate spheroidal functions, which is orthogonal at fixed values of the radial variable. A matter of principle in the implementation of Kantorovich method is how to calculate the matrix of the variable coefficients, expressed as angular integrals involving the derivatives of the angular functions with respect to a parameter, keeping the accuracy the same as for the angular functions themselves. This is achieved by calculating the mentioned derivatives as solutions of inhomogeneous boundary problem that results from differentiation of the ordinary second-order differential equation for the spheroidal functions with respect to the parameter and the corresponding algebraic eigenvalue problem, for which a stable symbolic-numerical algorithm is developed.[9] The stability of the computational scheme is achieved using the fact that at small r (in the vicinity of pair collision point) the angular functions turn into the associated Legendre polynomials, while at large r near $\eta = \pm 1$ they turn into the Laguerre functions. This makes it possible to construct asymptotic expansions in powers of r^{-2}, necessary for computer-accuracy calculation of the basis set of functions at all values of the parameter r. Substantial economy of computer resource in the numerical solution of the boundary problem for the set of radial equations is achieved by decreasing the integration interval $0 \le r \le r_{\max}$. In the present paper for large $r \ge r_{\max}$ new asymptotic expansions of the fundamental solutions of the radial equations are constructed in the basis of linear combinations of Coulomb regular and irregular functions and their derivatives. This is an important step forward compared with our previous work,[8] in which the basis included only the dominant asymptotic terms

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of the Coulomb regular and irregular functions. The capabilities of the computational scheme are demonstrated by the example of photoionization cross-section of a hydrogen atom in magnetic field.

The paper is organized as follows. In Section 2 the 2D-eigenvalue problem for the Schrödinger equation in cylindrical coordinates, describing a hydrogen atom in an axially symmetric magnetic field, is considered together with the appropriate classification of states. The reduction of the 2D-eigenvalue problem to a 1D-eigenvalue problem for a set of closed longitude equations via both the Kantorovich and Galerkin methods is described briefly. It is shown that Galerkin expansion follows from Kantorovich expansion at $z \to \infty$. In Section 2.3 the relation between the function with given parity and the function with physical scattering asymptotic form in cylindrical coordinates is established. In Section 3 the 2D-eigenvalue problem for the Schrödinger equation in spherical coordinates, describing a hydrogen atom in an axially symmetric magnetic field, is considered 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 3.1. Asymptotic expressions using regular and irregular Coulomb functions needed to determine the solutions and the reaction matrix by means of the **R**-matrix method, are presented in Section 4. The method is applied to the ionization of the low-lying states in Section 5. In Section 6 the numerical results obtained within the framework of the finite-element method are discussed. In Conclusion we outline the perspectives of further applications of this approach.

2. STATEMENT OF THE PROBLEM IN CYLINDRICAL COORDINATES

In cylindrical coordinates (ρ, z, φ) the wave function

$$\hat{\Psi}(\rho, z, \varphi) = \Psi(\rho, z)\frac{\exp(\imath m\varphi)}{\sqrt{2\pi}} \qquad (1)$$

of a hydrogen atom in an axially symmetric magnetic field $\vec{B} = (0, 0, B)$ satisfies the 2D Schrödinger equation

$$-\frac{\partial^2}{\partial z^2}\Psi(\rho, z) + \left(\hat{A}_c - \frac{2Z}{\sqrt{\rho^2 + z^2}}\right)\Psi(\rho, z) = \epsilon\Psi(\rho, z), \qquad (2)$$

$$\hat{A}_c = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{m^2}{\rho^2} + m\gamma + \frac{\gamma^2\rho^2}{4}, \qquad (3)$$

in the region Ω_c: $0 < \rho < \infty$ and $-\infty < z < \infty$. Here $m = 0, \pm 1, \ldots$ 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. We use the atomic units $(a.u.)$ $\hbar = m_e = e = 1$ and assume the mass of the nucleus to be infinite. In these expressions $\epsilon = 2E$, E is the energy (expressed in Rydbergs, $1\, Ry = (1/2)\, a.u.$) of the bound state $|m\sigma\rangle$ with fixed values of m and z-parity $\sigma = \pm 1$, and $\Psi(\rho, z) \equiv \Psi^{m\sigma}(\rho, z) = \sigma\Psi^{m\sigma}(\rho, -z)$ is the corresponding wave function. The boundary conditions in each $m\sigma$ subspace of the full Hilbert space have the form

$$\lim_{\rho\to 0} \rho\frac{\partial\Psi(\rho, z)}{\partial\rho} = 0, \quad \text{for} \quad m = 0, \quad \text{and} \quad \Psi(0, z) = 0, \quad \text{for} \quad m \neq 0, \qquad (4)$$

$$\lim_{\rho\to\infty} \Psi(\rho, z) = 0. \qquad (5)$$

The wave function of the discrete spectrum obeys the asymptotic boundary condition. Approximately this condition is replaced by the boundary condition of the first type at large, but finite $z = z_{\max} \gg 1$, namely,

$$\lim_{z\to\pm\infty} \Psi(\rho, z) = 0 \quad \to \quad \Psi(\rho, \pm z_{\max}) = 0. \qquad (6)$$

These functions satisfy the additional normalization condition

$$\int_{-\infty}^{\infty}\int_0^{\infty} |\Psi(\rho, z)|^2 \rho d\rho dz = 1. \qquad (7)$$

The asymptotic boundary condition for the continuum wave function will be considered in the subsection 2.3.

2.1. Kantorovich expansion

Consider a formal expansion of the partial solution $\Psi_i^{Em\sigma}(\rho,z)$ of Eqs. (2)–(5), corresponding to the eigenstate $|m\sigma i\rangle$, expanded in the finite set of one-dimensional basis functions $\{\hat{\Phi}_j^m(\rho;z)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(\rho,z)=\sum_{j=1}^{j_{\max}}\hat{\Phi}_j^m(\rho;z)\hat{\chi}_j^{(m\sigma i)}(E,z). \tag{8}$$

In Eq. (8) the functions $\hat{\boldsymbol{\chi}}^{(i)}(z)\equiv\hat{\boldsymbol{\chi}}^{(m\sigma i)}(E,z)$, $(\hat{\boldsymbol{\chi}}^{(i)}(z))^T=(\hat{\chi}_1^{(i)}(z),\ldots,\hat{\chi}_{j_{\max}}^{(i)}(z))$ are unknown, and the surface functions $\hat{\boldsymbol{\Phi}}(\rho;z)\equiv\hat{\boldsymbol{\Phi}}^m(\rho;z)=\hat{\boldsymbol{\Phi}}^m(\rho;-z)$, $(\hat{\boldsymbol{\Phi}}(\rho;z))^T=(\hat{\Phi}_1(\rho;z),\ldots,\hat{\Phi}_{j_{\max}}(\rho;z))$ form an orthonormal basis for each value of the variable z which is treated as a parameter.

In the Kantorovich approach the wave functions $\hat{\Phi}_j(\rho;z)$ and the potential curves $\hat{E}_j(z)$ (in Ry) are determined as the solutions of the following one-dimensional parametric eigenvalue problem

$$\left(\hat{A}_c-\frac{2Z}{\sqrt{\rho^2+z^2}}\right)\hat{\Phi}_j(\rho;z)=\hat{E}_j(z)\hat{\Phi}_j(\rho;z), \tag{9}$$

with the boundary conditions

$$\lim_{\rho\to0}\rho\frac{\partial\hat{\Phi}_j(\rho;z)}{\partial\rho}=0,\quad \text{for}\quad m=0,\quad \text{and}\quad \hat{\Phi}_j(0;z)=0,\quad \text{for}\quad m\neq0, \tag{10}$$

$$\lim_{\rho\to\infty}\hat{\Phi}_j(\rho;z)=0. \tag{11}$$

Since the operator in the left-hand side of Eq. (9) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle\hat{\Phi}_i(\rho;z)\middle|\hat{\Phi}_j(\rho;z)\right\rangle_\rho=\int_0^\infty\hat{\Phi}_i(\rho;z)\hat{\Phi}_j(\rho;z)\rho d\rho=\delta_{ij}, \tag{12}$$

where δ_{ij} is the Kronecker δ-symbol. Therefore we transform the solution of the above problem into the solution of an eigenvalue problem for a set of $j_{\max}$ ordinary second-order differential equations that determines the energy ϵ and the coefficients $\hat{\boldsymbol{\chi}}^{(i)}(z)$ of the expansion (8)

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\hat{\mathbf{U}}(z)+\hat{\mathbf{Q}}(z)\frac{d}{dz}+\frac{d\hat{\mathbf{Q}}(z)}{dz}\right)\hat{\boldsymbol{\chi}}^{(i)}(z)=\epsilon_i\,\mathbf{I}\hat{\boldsymbol{\chi}}^{(i)}(z). \tag{13}$$

Here $\mathbf{I}$, $\hat{\mathbf{U}}(z)=\hat{\mathbf{U}}(-z)$ and $\hat{\mathbf{Q}}(z)=-\hat{\mathbf{Q}}(-z)$ are the $j_{\max}\times j_{\max}$ matrices whose elements are expressed as

$$\begin{aligned}\hat{U}_{ij}(z)&=\frac{\hat{E}_i(z)+\hat{E}_j(z)}{2}\delta_{ij}+\hat{H}_{ij}(z),\quad I_{ij}=\delta_{ij},\\ \hat{H}_{ij}(z)&=\hat{H}_{ji}(z)=\int_0^\infty\frac{\partial\hat{\Phi}_i(\rho;z)}{\partial z}\frac{\partial\hat{\Phi}_j(\rho;z)}{\partial z}\rho d\rho,\\ \hat{Q}_{ij}(z)&=-\hat{Q}_{ji}(z)=-\int_0^\infty\hat{\Phi}_i(\rho;z)\frac{\partial\hat{\Phi}_j(\rho;z)}{\partial z}\rho d\rho.\end{aligned} \tag{14}$$

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

$$\lim_{z\to\pm\infty}\hat{\boldsymbol{\chi}}^{(i)}(z)=0\quad\to\quad\hat{\boldsymbol{\chi}}^{(i)}(\pm z_{\max})=0,\quad\int_{-z_{\max}}^{z_{\max}}\left(\hat{\boldsymbol{\chi}}^{(i)}(z)\right)^T\hat{\boldsymbol{\chi}}^{(j)}(z)dz=\delta_{ij}. \tag{15}$$

2.2. Galerkin expansion

Consider a formal expansion of the partial solution $\Psi_i^{Em\sigma}(\rho, z)$ of Eqs. (2)–(5) corresponding to the eigenstate $|m\sigma i\rangle$, in terms of the finite set of one-dimensional basis functions $\{\tilde{\Phi}_j^m(\rho)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(\rho, z) = \sum_{j=1}^{j_{\max}} \tilde{\Phi}_j^m(\rho)\tilde{\chi}_j^{(m\sigma i)}(E, z). \tag{16}$$

In the Galerkin approach the wave functions $\tilde{\Phi}_j(\rho) = \tilde{\Phi}_j^m(\rho)$ and the potential curves $\tilde{E}_j$ (in Ry) are determined as the solutions of the following one-dimensional eigenvalue problem

$$\hat{A}_c\tilde{\Phi}_j(\rho) = \tilde{E}_j\tilde{\Phi}_j(\rho), \tag{17}$$

with the boundary conditions

$$\lim_{\rho\to 0} \rho\frac{d\tilde{\Phi}_j(\rho)}{d\rho} = 0, \quad \text{for} \quad m = 0, \quad \text{and} \quad \tilde{\Phi}_j(0) = 0, \quad \text{for} \quad m \neq 0, \tag{18}$$

$$\lim_{\rho\to\infty} \tilde{\Phi}_j(\rho) = 0. \tag{19}$$

The above eigenvalue problem has the exact solution at fixed m

$$\tilde{\Phi}_j(\rho) = \sqrt{\frac{\gamma N_\rho!}{(N_\rho + |m|)!}} \exp\left(-\frac{\gamma\rho^2}{4}\right)\left(\frac{\gamma\rho^2}{2}\right)^{\frac{|m|}{2}} L_{N_\rho}^{|m|}\left(\frac{\gamma\rho^2}{2}\right), \quad \tilde{E}_j = \gamma(2N_\rho + |m| + m + 1), \tag{20}$$

where $N_\rho = j - 1$ is the transversal quantum number and $L_{N_\rho}^{|m|}(x)$ is the associated Laguerre polynomial. Note, that Galerkin expansion follows from Kantorovich expansion at $z \to \infty$, i.e.,

$$\tilde{\Phi}_j(\rho) = \lim_{r\to\infty, \eta\sim\pm 1} r^{-1}\,\Phi_j(\eta; r), \quad \lim_{r\to\infty} r^{-2}E_j(r) = \epsilon_{m\sigma j}^{th}(\gamma) = \gamma(2N_\rho + |m| + m + 1). \tag{21}$$

Therefore we transform the solution of the above problem into the solution of an eigenvalue problem for a set of $j_{\max}$ ordinary second-order differential equations that determines the energy ϵ and the coefficients $\tilde{\boldsymbol{\chi}}^{(i)}(z)$ of the expansion (16)

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \tilde{\mathbf{U}}(z)\right)\tilde{\boldsymbol{\chi}}^{(i)}(z) = \epsilon_i\,\mathbf{I}\tilde{\boldsymbol{\chi}}^{(i)}(z), \tag{22}$$

and the matrix $\tilde{\mathbf{U}}(z) = \tilde{\mathbf{U}}(-z)$ is expressed as

$$\tilde{U}_{ij}(z) = \frac{\tilde{E}_i + \tilde{E}_j}{2}\delta_{ij} + \tilde{H}_{ij}(z), \quad \tilde{H}_{ij}(z) = \tilde{H}_{ji}(z) = -\int_0^\infty \tilde{\Phi}_i(\rho)\frac{2Z}{\sqrt{\rho^2 + z^2}}\tilde{\Phi}_j(\rho)\rho d\rho. \tag{23}$$

The discrete spectrum solutions obey the asymptotic boundary condition and the orthonormality condition

$$\lim_{z\to\pm\infty} \tilde{\boldsymbol{\chi}}^{(i)}(z) = 0 \quad \to \quad \tilde{\boldsymbol{\chi}}^{(i)}(\pm z_{\max}) = 0, \quad \int_{-z_{\max}}^{z_{\max}} \left(\tilde{\boldsymbol{\chi}}^{(i)}(z)\right)^T \tilde{\boldsymbol{\chi}}^{(j)}(z)dz = \delta_{ij}. \tag{24}$$

2.3. Relation between the parity functions and the functions having physical scattering asymptotic form in cylindrical coordinates

The asymptotic form of the coefficients $\tilde{\boldsymbol{\chi}}^{(n)}(z)$ of the expansion (16) (or $\hat{\boldsymbol{\chi}}^{(n)}(z)$ of the expansion (8)) with fixed m, σ and $\epsilon = 2E$ for n-th solution in open channels is

$$\chi_{Em\sigma n'n}(z \to \pm\infty) = \begin{cases} \frac{a_{+1n'n}}{\sqrt{p_{n'}}}\cos\left(p_{n'}z + \frac{Z}{p_{n'}}\frac{z}{|z|}\ln(2p_{n'}|z|) + \frac{z}{|z|}\delta_{+1n}\right), & \sigma = +1, \\ \frac{a_{-1n'n}}{\sqrt{p_{n'}}}\sin\left(p_{n'}z + \frac{Z}{p_{n'}}\frac{z}{|z|}\ln(2p_{n'}|z|) + \frac{z}{|z|}\delta_{-1n}\right), & \sigma = -1, \end{cases} \tag{25}$$

where $p_n = \sqrt{2E - \epsilon^{th}_{m\sigma n}} \geq 0$ and $n, n' = 1, \ldots, N_o$, $\delta_{\sigma n} = \delta^{\sigma}_n + \delta^c_n - (\sigma+1)\pi/4$ are the phase shifts, δ^{σ}_n and δ^c_n are the eigenchannel short-range and Coulomb phase shifts, $a_{\sigma n' n} = C^{\sigma}_{n'n}$ are the amplitudes or mixed parameters defined in section 5, and $N_o = \max_{2E \geq \epsilon^{th}_{m\sigma n}} n$ is the number of open channels. Eq. (25) is rewritten in the matrix form so that

$$\chi_{E\sigma}(z \to \pm\infty) = \begin{cases} \begin{cases} \frac{1}{2}\mathbf{X}^{(+)}(z)\mathbf{A}_{+1} + \frac{1}{2}\mathbf{X}^{(-)}(z)\mathbf{A}^*_{+1}, & \sigma = +1, \\ \frac{1}{2\imath}\mathbf{X}^{(+)}(z)\mathbf{A}_{-1} - \frac{1}{2\imath}\mathbf{X}^{(-)}(z)\mathbf{A}^*_{-1}, & \sigma = -1, \end{cases} , & z > 0, \\ \begin{cases} \frac{1}{2}\mathbf{X}^{(+)}(z)\mathbf{A}^*_{+1} + \frac{1}{2}\mathbf{X}^{(-)}(z)\mathbf{A}_{+1}, & \sigma = +1, \\ \frac{1}{2\imath}\mathbf{X}^{(+)}(z)\mathbf{A}^*_{-1} - \frac{1}{2\imath}\mathbf{X}^{(-)}(z)\mathbf{A}_{-1}, & \sigma = -1, \end{cases} , & z < 0, \end{cases} \tag{26}$$

where

$$X^{(\pm)}_{n'n}(z) = p^{-1/2}_{n'} \exp\left(\pm\imath p_{n'} z \pm \imath \frac{Z}{p_{n'}} \frac{z}{|z|} \ln(2p_{n'}|z|)\right) \delta_{n'n}, \quad A_{\sigma n' n} = a_{\sigma n' n} \exp(\imath \delta_{\sigma n}). \tag{27}$$

On the other hand, the function that describes the incidence of the particle and its scattering, having the asymptotic form "incident wave + waves going out from the center", is

$$\chi^{(+)}_{E\hat{v}}(z \to \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\hat{\mathbf{T}}, & z > 0, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\hat{\mathbf{R}}, & z < 0, \end{cases} , & \hat{v} = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\hat{\mathbf{R}}, & z > 0, \\ \mathbf{X}^{(-)}(z)\hat{\mathbf{T}}, & z < 0, \end{cases} , & \hat{v} = \leftarrow, \end{cases} \tag{28}$$

where $\hat{\mathbf{T}}$ and $\hat{\mathbf{R}}$ are the transmission and reflection matrices, $\hat{\mathbf{T}}^\dagger\hat{\mathbf{T}} + \hat{\mathbf{R}}^\dagger\hat{\mathbf{R}} = \mathbf{I_{oo}}$, $\hat{v}$ is marked the initial direction of the particle motion along the z axis, and $\mathbf{I}_{oo}$ is the unit $N_o \times N_o$ matrix. Note, that due to the symmetry of the scattering potential the transmission and reflection coefficients are independent of the direction of the incident wave vector.

This wave function may be presented as a linear combination of the solutions having positive and negative parity

$$\chi^{(+)}_{E\rightleftarrows}(z) = \chi_{E,+1}(z)\mathbf{B}_{+1} \pm \imath \chi_{E,-1}(z)\mathbf{B}_{-1}. \tag{29}$$

It is easy to show that $\mathbf{B}_\sigma = [\mathbf{A}^*_\sigma]^{-1}$, and

$$\hat{\mathbf{T}} = \frac{1}{2}(\mathbf{A}_{+1}\mathbf{B}_{+1} + \mathbf{A}_{-1}\mathbf{B}_{-1}) = \frac{1}{2}(-\check{\mathbf{S}}_{+1} + \check{\mathbf{S}}_{-1}), \quad \hat{\mathbf{R}} = \frac{1}{2}(\mathbf{A}_{+1}\mathbf{B}_{+1} - \mathbf{A}_{-1}\mathbf{B}_{-1}) = \frac{1}{2}(-\check{\mathbf{S}}_{+1} - \check{\mathbf{S}}_{-1}), \tag{30}$$

where $\check{\mathbf{S}}_\sigma$ is the scattering matrix at fixed σ. However, to calculate the ionization cross section it is necessary to use the function having the asymptotic form "waves going into the center + outgoing wave", that is

$$\chi^{(-)}_{E\rightleftarrows}(z) = \chi_{E,+1}(z)\mathbf{B}^*_{+1} \pm \imath \chi_{E,-1}(z)\mathbf{B}^*_{-1}. \tag{31}$$

Note, that $\left(\chi^{(-)}_{E\rightleftarrows}(z)\right)^* = \chi^{(+)}_{E\leftrightarrows}(z)$. The functions are normalized so that

$$\sum_{n''=1}^{j_{\max}} \int_{-\infty}^{\infty} \left(\chi^{(+)}_{E' m \hat{v}' n'' n'}(z)\right)^* \chi^{(+)}_{E m \hat{v} n'' n}(z) dz = 2\pi\delta(E' - E)\delta_{\hat{v}'\hat{v}}\delta_{n'n}. \tag{32}$$

The $\hat{\mathbf{S}}$-matrix may be composed of the transmission and reflection coefficients

$$\hat{\mathbf{S}} = \begin{pmatrix} \hat{\mathbf{T}} & \hat{\mathbf{R}} \\ \hat{\mathbf{R}} & \hat{\mathbf{T}} \end{pmatrix}. \tag{33}$$

This matrix is unitary, since $\hat{\mathbf{T}}^\dagger\hat{\mathbf{T}} + \hat{\mathbf{R}}^\dagger\hat{\mathbf{R}} = \mathbf{I}_{oo}$ and $\hat{\mathbf{R}}^\dagger\hat{\mathbf{T}} + \hat{\mathbf{T}}^\dagger\hat{\mathbf{R}} = \mathbf{0}$.

To calculate the ionization it is convenient to use the function renormalized to $\delta(E'-E)$, i.e., divided by $\sqrt{2\pi}$

$$|E\hat{v}mN_\rho\rangle = \frac{\exp(\imath m\varphi)}{2\pi}\sum_{n'=1}^{j_{\max}}\tilde{\Phi}_{n'}(\rho)\tilde{\chi}^{(-)}_{Em\hat{v}n'n}(z) \quad \text{or} \quad |E\hat{v}mN_\rho\rangle = \frac{\exp(\imath m\varphi)}{2\pi}\sum_{n'=1}^{j_{\max}}\hat{\Phi}_{n'}(\rho;z)\hat{\chi}^{(-)}_{Em\hat{v}n'n}(z), \tag{34}$$

where $N_\rho = n-1$. The expression for the cross section of ionization by the light linearly polarized along z is

$$\sigma^{ion} = 4\pi^2\alpha\omega\sum_{N_\rho=0}^{N_o-1}\sum_{\hat{v}}|\langle E\hat{v}mN_\rho|z|Nlm\rangle|^2 a_0^2. \tag{35}$$

In the above expressions $\omega = E - E_{Nlm}$ is the frequency of radiation, E_{Nlm} is the energy of the initial bound state $|Nlm\rangle$, α is the fine-structure constant, a_0 is the Bohr radius.

For the recombination the wave function should be renormalized to one particle per the unit of length in the incident wave

$$|vmN_\rho\rangle = \sqrt{p_n}\frac{\exp(\imath m\varphi)}{\sqrt{2\pi}}\sum_{n'=1}^{j_{\max}}\tilde{\Phi}_{n'}(\rho)\tilde{\chi}^{(+)}_{Em\hat{v}n'n}(z) \quad \text{or} \quad |vmN_\rho\rangle = \sqrt{p_n}\frac{\exp(\imath m\varphi)}{\sqrt{2\pi}}\sum_{n'=1}^{j_{\max}}\hat{\Phi}_{n'}(\rho;z)\hat{\chi}^{(+)}_{Em\hat{v}n'n}(z), \tag{36}$$

where $v = \hat{v}p_n$ and $N_\rho = n-1$. The expression for the rate of recombination induced by the light linearly polarized along z for the particle, initially moving in the channel N_ρ with the velocity v has the form

$$\lambda^{rec}_{N_\rho}(v) = 4\pi^2\alpha I\sum_{l=0}^{N-1}\sum_{m=-l}^{0}|\langle Nlm|z|vmN_\rho\rangle|^2\delta(E-E_{Nlm}-\omega)a_0^2, \tag{37}$$

I being the intensity of the incident light.

For the light circularly polarized in the plane xOy the above expressions read as

$$\sigma^{ion} = 4\pi^2\alpha\omega\sum_{N_\rho=0}^{N_o-1}\sum_{\hat{v}}|\langle E\hat{v}m\pm 1N_\rho|\vec{e}_\pm\vec{r}|Nlm\rangle|^2 a_0^2, \tag{38}$$

$$\lambda^{rec}_{N_\rho}(v) = 4\pi^2\alpha I\sum_{l=0}^{N-1}\sum_{m=-l}^{0}|\langle Nlm\pm 1|\vec{e}_\pm\vec{r}|vmN_\rho\rangle|^2\delta(E-E_{Nlm}-\omega)a_0^2, \tag{39}$$

where the complex unit vectors are $\vec{e}_\pm = \frac{1}{\sqrt{2}}\vec{i}\pm\frac{\imath}{\sqrt{2}}\vec{j}$.

3. STATEMENT OF THE PROBLEM IN SPHERICAL COORDINATES

In spherical coordinates (r,θ,ϕ) the Eq. (2) can be rewritten as follows

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2}\hat{A}(p)-\frac{2Z}{r}\right)\Psi(r,\eta) = \epsilon\Psi(r,\eta), \tag{40}$$

in the region Ω: $0<r<\infty$ and $-1<\eta=\cos\theta<1$. Here $\hat{A}(p)$ is the parametric Hamiltonian

$$\hat{A}(p) = -\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}+\frac{m^2}{1-\eta^2}+2pm+p^2(1-\eta^2), \tag{41}$$

and $p=\gamma r^2/2$, and $\Psi(r,\eta)\equiv\Psi^{m\sigma}(r,\eta)=\sigma\Psi^{m\sigma}(r,-\eta)$. The sign of z-parity, $\sigma=(-1)^{N_\eta}$, is defined by the number of nodes N_η of the solution $\Psi(r,\eta)$ with respect to the variable η. We will also use the scaled radial variable $\hat{r}=r\sqrt{\gamma}$, the effective charge $\hat{Z}=Z/\sqrt{\gamma}$, and the scaled energy $\hat{\epsilon}=\epsilon/\gamma$ or $\hat{E}=E/\gamma$. Practically it means replacing γ with 1 and multiplying Z by $1/\sqrt{\gamma}$ and ϵ or E by $1/\gamma$ in all equations above.

The boundary conditions in each $m\sigma$ subspace of the full Hilbert space have the form

$$\lim_{\eta\to\pm 1}(1-\eta^2)\frac{\partial\Psi(r,\eta)}{\partial\eta}=0, \quad \text{for} \quad m=0, \quad \text{and} \quad \Psi(r,\pm 1)=0, \quad \text{for} \quad m\neq 0, \tag{42}$$

$$\lim_{r\to 0} r^2\frac{\partial\Psi(r,\eta)}{\partial r}=0. \tag{43}$$

The wave function of the discrete spectrum obeys the asymptotic boundary condition. Approximately this condition is replaced by the boundary condition of the first type at large, but finite $r=r_{\max}$, namely,

$$\lim_{r\to\infty} r^2\Psi(r,\eta)=0 \quad \to \quad \Psi(r_{\max},\eta)=0. \tag{44}$$

In the Fano-Lee **R**-matrix theory[10, 11] the wave function of the continuum $\Psi(r,\eta)$ obeys the boundary condition of the third type at fixed values of the energy ϵ and the radial variable $r=r_{\max}$

$$\frac{\partial\Psi(r,\eta)}{\partial r}-\mu\,\Psi(r,\eta)=0. \tag{45}$$

Here the parameters $\mu\equiv\mu(r_{\max},\epsilon)$, determined by the variational principle, play the role of eigenvalues of the logarithmic normal derivative matrix of the solution of the boundary problem (40)–(43), (45).

3.1. Kantorovich expansion

Consider a formal expansion of the partial solution $\Psi_i^{Em\sigma}(r,\eta)$ of Eqs. (40)–(43) with the conditions (44), (45), corresponding to the eigenstate $|m\sigma i\rangle$, in terms of the finite set of one-dimensional basis functions $\{\Phi_j^{m\sigma}(\eta;r)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(r,\eta)=\sum_{j=1}^{j_{\max}}\Phi_j^{m\sigma}(\eta;r)\chi_j^{(m\sigma i)}(E,r). \tag{46}$$

In Eq. (46) 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 $\boldsymbol{\Phi}(\eta;r)\equiv\boldsymbol{\Phi}^{m\sigma}(\eta;r)=\sigma\boldsymbol{\Phi}^{m\sigma}(-\eta;r)$, $(\boldsymbol{\Phi}(\eta;r))^T=(\Phi_1(\eta;r),\ldots,\Phi_{j_{\max}}(\eta;r))$ form an orthonormal basis for each value of the radius r which is treated as a parameter.

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

$$\hat{A}(p)\Phi_j(\eta;r)=E_j(r)\Phi_j(\eta;r), \tag{47}$$

with the boundary conditions

$$\lim_{\eta\to\pm 1}(1-\eta^2)\frac{\partial\Phi_j(\eta;r)}{\partial\eta}=0, \quad \text{for} \quad m=0 \quad \text{and} \quad \Phi_j(\pm 1;r)=0, \quad \text{for} \quad m\neq 0. \tag{48}$$

Since the operator in the left-hand side of Eq. (47) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle \Phi_i(\eta;r)\middle|\Phi_j(\eta;r)\right\rangle_\eta=\int_{-1}^{1}\Phi_i(\eta;r)\Phi_j(\eta;r)d\eta=\delta_{ij}. \tag{49}$$

Note, that the solutions of this problem with shifted eigenvalues, $\check{E}_j(r)=E_j(r)-2pm$, correspond to the solutions of the eigenvalue problem for oblate angular spheroidal functions[12]

$$A(p)\Phi_j(\eta;r)=\check{E}_j(r)\Phi_j(\eta;r), \tag{50}$$

where $A(p)=\hat{A}(p)-2pm$. It means that for small p the asymptotic behavior of the eigenvalues $E_j(r)$, $j=1,2,\ldots$ at fixed values of m and σ is determined 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 the fact that the number of nodes N_η of the eigenfunction $\mathbf{\Phi}(\eta; r)$ at fixed m and $\sigma = (-1)^{N_\eta}$ does not depend on the parameter p, we get the one-to-one correspondence between these sets, i.e., $N_\eta = l - |m|$.

For large r the asymptotic behavior of the eigenfunctions $\Phi_j(\eta; r)$ and eigenvalues $E_j(r)$ at fixed values of m and σ is determined by the value of the transversal quantum number, $N_\rho = j - 1$ (see Eqs. (20) and (51))

$$\tilde{\Phi}_j(\rho) = \lim_{r\to\infty, \eta\sim\pm 1} r\, \Phi_j(\eta; r), \quad \lim_{r\to\infty} r^{-2} E_j(r) = \epsilon^{th}_{m\sigma j}(\gamma) = \gamma(2N_\rho + |m| + m + 1). \tag{51}$$

The transversal quantum number N_ρ, i.e., the number of nodes of the eigenfunction $\mathbf{\Phi}^{m\sigma}(\eta; r)$ in the subinterval $0 < \eta < 1$ or $-1 < \eta < 0$, can be expressed via N_η as follows: $N_\rho = N_\eta/2$ for the even z-parity states, $\sigma = +1$, and $N_\rho = (N_\eta - 1)/2$ for the odd z-parity states, $\sigma = -1$. It means that the eigenfunctions $\mathbf{\Phi}^{m\hat{v}}(\eta; r) = (\mathbf{\Phi}^{m\sigma=+1}(\eta; r) \pm \mathbf{\Phi}^{m\sigma=-1}(\eta; r))/\sqrt{2}$ labeled by $\hat{v} = \leftrightarrows$ localized at large r in vicinity of $\eta = \pm 1$ (i.e., at $z \to +\infty$ and $z \to -\infty$), respectively, and have N_ρ nodes in the subintervals $0 < \eta < 1$ and $-1 < \eta < 0$. Such asymptotic functions $\mathbf{\Phi}^{m\hat{v}}(\eta; r)$ corresponds to $\tilde{\mathbf{\Phi}}^m(\rho)$ from Eqs. (20) and (51).

From here we transform the solution of the problem (40) into the solution of an eigenvalue problem for a set of $j_{\max}$ ordinary second-order differential equations that determines the energy ϵ and the coefficients (radial wave functions) $\boldsymbol{\chi}^{(i)}(r)$ of the expansion (46)

$$\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\mathbf{U}(r)}{r^2} + \mathbf{Q}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{d\, r^2\mathbf{Q}(r)}{dr}\right)\boldsymbol{\chi}^{(i)}(r) = \epsilon_i\, \mathbf{I}\boldsymbol{\chi}^{(i)}(r), \tag{52}$$

$$\lim_{r\to 0} r^2\left(\frac{d\boldsymbol{\chi}^{(i)}(r)}{dr} - \mathbf{Q}(r)\boldsymbol{\chi}^{(i)}(r)\right) = 0. \tag{53}$$

Here $\mathbf{U}(r)$ and $\mathbf{Q}(r)$ are the $j_{\max} \times j_{\max}$ matrices whose elements are expressed as

$$\begin{aligned} U_{ij}(r) &= \frac{E_i(r) + E_j(r)}{2}\delta_{ij} - 2Zr\delta_{ij} + r^2 H_{ij}(r), \\ H_{ij}(r) = H_{ji}(r) &= \int_{-1}^{1} \frac{\partial\Phi_i(\eta; r)}{\partial r}\frac{\partial\Phi_j(\eta; r)}{\partial r} d\eta, \\ Q_{ij}(r) = -Q_{ji}(r) &= -\int_{-1}^{1} \Phi_i(\eta; r)\frac{\partial\Phi_j(\eta; r)}{\partial r} d\eta. \end{aligned} \tag{54}$$

The calculations of the above matrix elements and there asymptotic forms were performed using the combined codes EIGENF, MATRM and MATRA implemented in MAPLE 8 and FORTRAN.[13]

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

$$\lim_{r\to\infty} r^2\boldsymbol{\chi}^{(i)}(r) = 0 \quad \to \quad \boldsymbol{\chi}^{(i)}(r_{\max}) = 0, \quad \int_0^{r_{\max}} r^2 \left(\boldsymbol{\chi}^{(i)}(r)\right)^T \boldsymbol{\chi}^{(j)}(r) dr = \delta_{ij}. \tag{55}$$

The continuous spectrum solution $\boldsymbol{\chi}^{(i)}(r)$ satisfies the third-type boundary conditions

$$\frac{d\boldsymbol{\chi}(r)}{dr} = \mathbf{R}\boldsymbol{\chi}(r), \tag{56}$$

where the nonsymmetric matrix $\mathbf{R}$ is calculated using the method of.[8]

4. ASYMPTOTIC FORM OF THE SOLUTION

Let us write the set of differential equations (52) at fixed m, σ and $\epsilon = 2E$ in the explicit form for $\chi_{ji_o}(r) \equiv \chi_j^{(i_o)}(r)$, $j = 1, \ldots, j_{\max}$, $i_o = 1, \ldots, N_o$

$$\begin{aligned} &\left(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{2Z}{r} - \epsilon + \frac{E_j(r)}{r^2} + H_{jj}(r)\right)\chi_{ji_o}(r) \\ &= \sum_{j'=1, j'\neq j}^{j_{\max}} \left(-H_{jj'}(r) - Q_{jj'}(r)\frac{d}{dr} - \frac{1}{r^2}\frac{d\, r^2 Q_{jj'}(r)}{dr}\right)\chi_{j'i_o}(r). \end{aligned} \tag{57}$$

At large r the asymptotic form of the matrix elements is given by the relations

$$r^{-2}E_j(r) = E_j^{(0)} + \sum_{k=1} r^{-2k}E_j^{(2k)}, \quad H_{jj'}(r) = \sum_{k=1} r^{-2k}H_{jj'}^{(2k)},$$
$$Q_{jj'}(r) = \sum_{k=1} r^{-2k+1}Q_{jj'}^{(2k-1)}, \qquad r \gg \max(n_l, n_r)\gamma/2, \tag{58}$$
$$E_j^{(2k-1)} = H_{jj'}^{(2k-1)} = Q_{jj'}^{(2k)} = 0.$$

In these expressions the asymptotic quantum numbers n_l, n_r correspond to the transversal quantum numbers N_ρ, N'_ρ that are related to the unified numbers j, j' as $n_l = j-1$, $n_r = j'-1$ and $n = \min(n_l, n_r)$. Below we display the matrix elements with arbitrary m: $Q_{jj'}(r)$ is an antisymmetric matrix with the elements

$$\begin{aligned} Q_{jj'}^{(1)} &= (n_r - n_l)\sqrt{n\ +1}\sqrt{n+|m|+1}\delta_{|n_l-n_r|,1}, \\ Q_{jj'}^{(3)} &= (4\gamma)^{-1}(n_r - n_l)\sqrt{n\ +1}\sqrt{n+|m|+1}\Big(2(2n+|m|+2)\delta_{|n_l-n_r|,1} \\ &\quad +\sqrt{n\ +2}\sqrt{n+|m|+2}\delta_{|n_l-n_r|,2}\Big), \end{aligned} \tag{59}$$

$H_{jj'}(r)$ is a symmetric matrix with the elements

$$\begin{aligned} H_{jj'}^{(2)} &= (2n^2+2n+2|m|n+|m|+1)\delta_{|n_l-n_r|,0} \\ &\quad -\sqrt{n\ +1}\sqrt{n+|m|+1}\sqrt{n\ +2}\sqrt{n+|m|+2}\delta_{|n_l-n_r|,2}, \\ H_{jj'}^{(4)} &= \gamma^{-1}\Big((2n+|m|+1)(2n^2+2n+2|m|n+|m|+2)\delta_{|n_l-n_r|,0} \\ &\quad +\sqrt{n\ +1}\sqrt{n+|m|+1}(n^2+2n+|m|n+|m|+2)\delta_{|n_l-n_r|,1} \\ &\quad -\sqrt{n\ +1}\sqrt{n+|m|+1}\sqrt{n\ +2}\sqrt{n+|m|+2}(2n+|m|+3)\delta_{|n_l-n_r|,2} \\ &\quad -\sqrt{n\ +1}\sqrt{n+|m|+1}\sqrt{n\ +2}\sqrt{n+|m|+2}\sqrt{n\ +3}\sqrt{n+|m|+3}\delta_{|n_l-n_r|,3}\Big), \end{aligned} \tag{60}$$

$E_j(r)$ is a diagonal matrix of potential curves, i.e., eigenvalues of the parametric problem

$$\begin{aligned} E_j^{(0)} &= \gamma(2n+|m|+m+1), \\ E_j^{(2)} &= -2n^2-2n-1-2|m|n-|m|, \\ E_j^{(4)} &= (2\gamma)^{-1}(-4n^3-6n^2-4n-6|m|n^2-6|m|n-2m^2n-2|m|-m^2-1). \end{aligned} \tag{61}$$

Note, that $E_j^{(2)} + H_{jj}^{(2)} = 0$, i.e., at large r the centrifugal terms are eliminated from Eq. (57). It means that the leading terms of the radial solutions, $\chi_{ji_o}(r)$, have the asymptotic form of the Coulomb functions with zero angular momentum.

Now let us consider the asymptotic solution following[14]

$$\chi_{ji_o}(r) = R(p_{i_o}, r)\phi_{ji_o}(r) + \frac{dR(p_{i_o}, r)}{dr}\psi_{ji_o}(r), \tag{62}$$

where $R(p_{i_o}, r) = (\imath F(p_{i_o}, r) + G(p_{i_o}, r))/2$, $F(p_{i_o}, r)$ and $G(p_{i_o}, r)$ are the Coulomb regular and irregular functions, respectively. These functions satisfy the condition

$$r^2\left(G(p_{i_o}, r)\frac{dF(p_{i_o}, r)}{dr} - \frac{dG(p_{i_o}, r)}{dr}F(p_{i_o}, r)\right) = 1. \tag{63}$$

The function $R(p_{i_o}, r)$ satisfies the differential equation

$$\frac{d^2 R(p_{i_o}, r)}{dr^2} + \frac{2}{r}\frac{dR(p_{i_o}, r)}{dr} + \left(p_{i_o}^2 + \frac{2Z}{r}\right) R(p_{i_o}, r) = 0. \tag{64}$$

Substituting the function (62) into Eq. (52), using (64) and extracting the coefficients for the Coulomb function and its derivative, we arrive at two coupled differential equations with respect to the unknown functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$

$$\left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + p_{i_o}^2 + H_{jj}(r) - \epsilon + \frac{E_j(r)}{r^2}\right)\phi_{ji_o}(r) + \left(\left(2p_{i_o}^2 + \frac{4Z}{r}\right)\frac{d}{dr} - \frac{2Z}{r^2}\right)\psi_{ji_o}(r) \tag{65}$$

$$= -\sum_{j'=1, j'\neq j}^{j_{\max}} \left(H_{jj'}(r) + Q_{jj'}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{d\, r^2 Q_{jj'}(r)}{dr}\right)\phi_{j'i_o}(r) + \left(2p_{i_o}^2 + \frac{4Z}{r}\right)\sum_{j'=1, j'\neq j}^{j_{\max}} Q_{jj'}(r)\psi_{j'i_o}(r),$$

$$\left(-\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + p_{i_o}^2 + H_{jj}(r) - \epsilon + \frac{E_j(r) - 2}{r^2}\right)\psi_{ji_o}(r) - 2\frac{d\phi_{ji_o}(r)}{dr} \tag{66}$$

$$= -\sum_{j'=1, j'\neq j}^{j_{\max}} \left(H_{jj'}(r) + Q_{jj'}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{d\, r^2 Q_{jj'}(r)}{dr} - \frac{4Q_{jj'}(r)}{r}\right)\psi_{j'i_o}(r) - 2\sum_{j'=1, j'\neq j}^{j_{\max}} Q_{jj'}(r)\phi_{j'i_o}(r).$$

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

$$\phi_{ji_o}(r) = \sum_{k=0}^{k_{\max}} \phi_{ji_o}^{(k)} r^{-k}, \quad \psi_{ji_o}(r) = \sum_{k=0}^{k_{\max}} \psi_{ji_o}^{(k)} r^{-k}. \tag{67}$$

After substituting the expansions (67) into (65) and (66) and equating the coefficients at the same powers of r we arrive at the set of recurrence relations with respect to the unknown coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$

$$\left(p_{i_o}^2 - 2E + E_j^{(0)}\right)\phi_{ji_o}^{(k)} - 2p_{i_o}^2(k-1)\psi_{ji_o}^{(k-1)} - (k-2)(k-3)\phi_{ji_o}^{(k-2)}$$

$$-2Z(2k-3)\psi_{ji_o}^{(k-2)} + \sum_{k'=1}^{k}\left(E_j^{(k')} + H_{jj}^{(k')}\right)\phi_{ji_o}^{(k-k')} \tag{68}$$

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

$$(p_{i_o}^2 - 2E + E_j^{(0)})\psi_{ji_o}^{(k)} + 2(k-1)\phi_{ji_o}^{(k-1)} - k(k-1)\psi_{ji_o}^{(k-2)} + \sum_{k'=1}^{k}\left(E_j^{(k')} + H_{jj}^{(k')}\right)\psi_{ji_o}^{(k-k')} \tag{69}$$

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

The first six equations of the set (68), (69) have the form

$$\left(p_{i_o}^2 - 2E + E_{i_o}^{(0)}\right)\phi_{i_oi_o}^{(0)} = 0,$$
$$\left(p_{i_o}^2 - 2E + E_{i_o}^{(0)}\right)\psi_{i_oi_o}^{(0)} = 0,$$
$$\left(p_{i_o}^2 - 2E + E_{j_0}^{(0)}\right)\phi_{j_0i_o}^{(0)} = 0,$$
$$\left(p_{i_o}^2 - 2E + E_{j_0}^{(0)}\right)\psi_{j_0i_o}^{(0)} = 0,$$
$$\left(p_{i_o}^2 - 2E + E_{i_o}^{(0)}\right)\phi_{i_oi_o}^{(1)} = 2p_{i_o}^2 \sum_{j_0\neq i_o} Q_{i_oj_0}^{(1)}\psi_{j_0i_o}^{(0)},$$

$$
\begin{aligned}
&\left(p_{i_o}^2-2E+E_{i_o}^{(0)}\right)\psi_{i_oi_o}^{(1)}=-2\sum_{j_0\neq i_o}Q_{i_oj_0}^{(1)}\phi_{j_0i_o}^{(0)},\\
&\left(p_{i_o}^2-2E+E_{j_1}^{(0)}\right)\phi_{j_1i_o}^{(1)}=2p_{i_o}^2Q_{j_1i_o}^{(1)}\psi_{i_oi_o}^{(0)}+2p_{i_o}^2\sum_{j_0\neq i_o,j_0\neq j_1}Q_{j_1j_0}^{(1)}\psi_{j_0i_o}^{(0)},\\
&\left(p_{i_o}^2-2E+E_{j_1}^{(0)}\right)\psi_{j_1i_o}^{(1)}=-2Q_{j_1i_o}^{(1)}\phi_{i_oi_o}^{(0)}-2\sum_{j_0\neq i_o,j_0\neq j_1}Q_{j_1j_0}^{(1)}\phi_{j_0i_o}^{(0)},\\
&\left(p_{i_o}^2-2E+E_{i_o}^{(0)}\right)\phi_{i_oi_o}^{(2)}-2p_{i_o}^2\psi_{i_oi_o}^{(1)}-2Z\psi_{i_oi_o}^{(0)}\\
&\qquad=\sum_{j_1\neq i_o}\left[-\left(Q_{i_oj_1}^{(1)}+H_{i_oj_1}^{(2)}\right)\phi_{j_1i_o}^{(0)}+2p_{i_o}^2Q_{i_oj_1}^{(1)}\psi_{j_1i_o}^{(1)}+4ZQ_{i_oj_1}^{(1)}\psi_{j_1i_o}^{(0)}\right],\\
&\left(p_{i_o}^2-2E+E_{i_o}^{(0)}\right)\psi_{i_oi_o}^{(2)}+2\phi_{i_oi_o}^{(1)}-2\psi_{i_oi_o}^{(0)}\\
&\qquad=\sum_{j_1\neq i_o}\left[\left(3Q_{i_oj_1}^{(1)}-H_{i_oj_1}^{(2)}\right)\psi_{j_1i_o}^{(0)}-2Q_{i_oj_1}^{(1)}\phi_{j_1i_o}^{(1)}\right],\\
&\left(p_{i_o}^2-2E+E_{j_2}^{(0)}\right)\phi_{j_2i_o}^{(2)}-2p_{i_o}^2\psi_{j_2i_o}^{(1)}-2Z\psi_{j_2i_o}^{(0)}\\
&\qquad=-\left(Q_{j_2i_o}^{(1)}+H_{j_2i_o}^{(2)}\right)\phi_{i_oi_o}^{(0)}+2p_{i_o}^2Q_{j_2i_o}^{(1)}\psi_{i_oi_o}^{(1)}+4ZQ_{j_2i_o}^{(1)}\psi_{i_oi_o}^{(0)}\\
&\qquad+\sum_{j_1\neq i_o,j_1\neq j_2}\left[-\left(Q_{j_2j_1}^{(1)}+H_{j_2j_1}^{(2)}\right)\phi_{j_1i_o}^{(0)}+2p_{i_o}^2Q_{j_2j_1}^{(1)}\psi_{j_1i_o}^{(1)}+4ZQ_{j_2j_1}^{(1)}\psi_{j_1i_o}^{(0)}\right],\\
&\left(p_{i_o}^2-2E+E_{j_2}^{(0)}\right)\psi_{j_2i_o}^{(2)}+2\phi_{j_2i_o}^{(1)}-2\psi_{j_2i_o}^{(0)}\\
&\qquad=\left(3Q_{j_2i_o}^{(1)}-H_{j_2i_o}^{(2)}\right)\psi_{i_oi_o}^{(0)}-2Q_{j_2i_o}^{(1)}\phi_{i_oi_o}^{(1)}\\
&\qquad+\sum_{j_1\neq i_o,j_1\neq j_2}\left[\left(3Q_{j_2j_1}^{(1)}-H_{j_2j_1}^{(2)}\right)\psi_{j_1i_o}^{(0)}-2Q_{j_2j_1}^{(1)}\phi_{j_1i_o}^{(1)}\right],\\
&\dots
\end{aligned}
\tag{70}
$$

The summation indices j_k, $k=0,1,\ldots,k_{\max}$ possess integer values, except i_o and j_{k+1}, i.e., $j_k=1,2,\ldots,j_{\max}$, $j_k\neq i_o$, $j_k\neq j_{k+1}$. From the first four equations of the set (70) for $\phi_{i_oi_o}^{(0)}$, $\phi_{j_0i_o}^{(0)}$, $\psi_{i_oi_o}^{(0)}$, $\psi_{j_0i_o}^{(0)}$ we get the leading terms of the eigenfunction, the eigenvalue and the characteristic parameter, i.e., the initial data for solving the recurrence equations (68), (69),

$$
\phi_{j_0i_o}^{(0)}=\delta_{j_0i_o},\quad \psi_{j_0i_o}^{(0)}=0,\quad p_{i_o}^2=2E-E_{i_o}^{(0)}, \tag{71}
$$

that correspond to the leading term of $\chi_{ji_o}(r)$ satisfying the asymptotic expansion at large r (see[8])

$$
\chi_{ji_o}(r)=\frac{\exp(\imath\, p_{i_o}r+\imath\,\zeta\ln(2p_{i_o}r)+\imath\,\delta_{i_o}^c)}{2r\sqrt{p_{i_o}}}\delta_{ji_o},\quad \zeta=\frac{Z}{p_{i_o}},\quad \delta_{i_o}^c=\arg\Gamma(1-\imath\zeta), \tag{72}
$$

where ζ is the Sommerfeld parameter and $\delta_{i_o}^c$ is the Coulomb phase. Open channels have $p_{i_o}^2\geq 0$, and close channels have $p_{i_o}^2<0$. Lets there are $N_o\leq j_{\max}$ open channels, i.e., $p_{i_o}^2\geq 0$ for $i_o=1,\ldots N_o$ and $p_{i_o}^2<0$ for $i_o=N_o+1,\ldots j_{\max}$. Substituting these initial data into the sequent equations of the set (70), we get a step-by-step procedure for determining the coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$

$$
\begin{aligned}
&\phi_{j_1i_o}^{(1)}=0,\\
&\psi_{j_1i_o}^{(1)}=\frac{2Q_{j_1i_o}^{(1)}}{E_{i_o}^{(0)}-E_{j_1}^{(0)}},\\
&\phi_{i_oi_o}^{(1)}=0,
\end{aligned}
$$

$$
\begin{aligned}
\psi^{(1)}_{i_o i_o} &= -\sum_{j_0=\max(1,i_o-1),j_0\neq i_o}^{\min(j_{\max},i_o+1)} Q^{(1)}_{i_o j_0}\psi^{(1)}_{j_0 i_o},\\
\phi^{(2)}_{j_2 i_o} &= \frac{Q^{(1)}_{j_2 i_o}+H^{(2)}_{j_2 i_o}-2p^2_{i_o}\left(Q^{(1)}_{j_2 i_o}\psi^{(1)}_{i_o i_o}+\psi^{(1)}_{j_2 i_o}\right)}{E^{(0)}_{i_o}-E^{(0)}_{j_2}} - \frac{2\,p^2_{i_o}\sum\limits_{\substack{j_1=\max(1,j_2-1)\\ j_1\neq j_2, j_1\neq i_o}}^{\min(j_{\max},j_2+1)} Q^{(1)}_{j_2 j_1}\psi^{(1)}_{j_1 i_o}}{E^{(0)}_{i_o}-E^{(0)}_{j_2}}, \qquad (73)\\
\psi^{(2)}_{j_2 i_o} &= 0,\\
\phi^{(2)}_{i_o i_o} &= \frac{3\psi^{(1)}_{i_o i_o}}{2}+\frac{1}{4}\sum_{j_1=\max(1,i_o-1),j_1\neq i_o}^{\min(j_{\max},i_o+1)}\left[-2Q^{(1)}_{i_o j_1}\phi^{(2)}_{j_1 i_o}+\left(5Q^{(1)}_{i_o j_1}-H^{(2)}_{i_o j_1}\right)\psi^{(1)}_{j_1 i_o}\right],\\
\psi^{(2)}_{i_o i_o} &= -\frac{3Z\psi^{(1)}_{i_o i_o}}{2p^2_{i_o}}-\frac{1}{4p^2_{i_o}}\sum_{j_1=\max(1,i_o-1),j_1\neq i_o}^{\min(j_{\max},i_o+1)}\left[4ZQ^{(1)}_{i_o j_1}\psi^{(1)}_{j_1 i_o}+2p^2_{i_o}Q^{(1)}_{i_o j_1}\psi^{(2)}_{j_1 i_o}\right],\\
&\dots
\end{aligned}
$$

Substituting the explicit asymptotic expressions of the matrix elements (58) into Eq. (73), we get the explicit expression of the coefficients $\phi^{(k)}_{j i_o}$ and $\psi^{(k)}_{j i_o}$ in terms of the number of the state (or of the channel) $i_o = n_o + 1$ and the number of the current equation $j = 1, \dots, j_{\max}$. For example, at $j_{\max} \geq i_o + k$ and $k = 0, 1, 2$ such elements take the form

$$
\begin{aligned}
&\phi^{(0)}_{i_o i_o} = 1, \qquad \psi^{(0)}_{i_o i_o} = 0,\\
&\phi^{(1)}_{i_o-1 i_o} = 0, \qquad \psi^{(1)}_{i_o-1 i_o} = \frac{\sqrt{n_o}\sqrt{n_o+|m|}}{\gamma},\\
&\phi^{(1)}_{i_o i_o} = 0, \qquad \psi^{(1)}_{i_o i_o} = -\frac{2n_o+|m|+1}{\gamma},\\
&\phi^{(1)}_{i_o+1 i_o} = 0, \qquad \psi^{(1)}_{i_o+1 i_o} = \frac{\sqrt{n_o+1}\sqrt{n_o+|m|+1}}{\gamma},\\
&\phi^{(2)}_{i_o-2 i_o} = -\sqrt{n_o-1}\sqrt{n_o+|m|-1}\sqrt{n_o}\sqrt{n_o+|m|}\left(\frac{p^2_{i_o}}{2\gamma^2}+\frac{1}{4\gamma}\right), \qquad \psi^{(2)}_{i_o-2 i_o} = 0, \qquad (74)\\
&\phi^{(2)}_{i_o-1 i_o} = \sqrt{n_o}\sqrt{n_o+|m|}\left(\frac{p^2_{i_o}(2n_o+|m|)}{\gamma^2}+\frac{1}{2\gamma}\right), \qquad \psi^{(2)}_{i_o-1 i_o} = 0,\\
&\phi^{(2)}_{i_o i_o} = -\frac{p^2_{i_o}(6n_o{}^2+6n_o+2+|m|(6n_o+3)+|m|^2)}{2\gamma^2}-\frac{2n_o+|m|+1}{2\gamma}, \qquad \psi^{(2)}_{i_o i_o} = \frac{Z(2n_o+|m|+1)}{2p^2_{i_o}\gamma},\\
&\phi^{(2)}_{i_o+1 i_o} = \sqrt{n_o+1}\sqrt{n_o+|m|+1}\left(\frac{p^2_{i_o}(2n_o+|m|+2)}{\gamma^2}+\frac{1}{2\gamma}\right), \qquad \psi^{(2)}_{i_o+1 i_o} = 0,\\
&\phi^{(2)}_{i_o+2 i_o} = -\sqrt{n_o+1}\sqrt{n_o+|m|+1}\sqrt{n_o+2}\sqrt{n_o+|m|+2}\left(\frac{p^2_{i_o}}{2\gamma^2}-\frac{1}{4\gamma}\right), \qquad \psi^{(2)}_{i_o+2 i_o} = 0.
\end{aligned}
$$

It should be noted that at large r the linearly independent function (62) satisfy the Wronskian-type relation

$$
\mathbf{Wr}(\mathbf{Q}(r); \boldsymbol{\chi}^*(r), \boldsymbol{\chi}(r)) = \frac{\imath}{2}\mathbf{I}_{oo}, \qquad (75)
$$

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

$$
\mathbf{Wr}(\bullet; \boldsymbol{\chi}^*(r), \boldsymbol{\chi}(r)) = r^2\left[(\boldsymbol{\chi}^*(r))^T\left(\frac{d\boldsymbol{\chi}(r)}{dr}-\bullet\,\boldsymbol{\chi}(r)\right)-\left(\frac{d\boldsymbol{\chi}^*(r)}{dr}-\bullet\,\boldsymbol{\chi}^*(r)\right)^T\boldsymbol{\chi}(r)\right]. \qquad (76)
$$

These relations will be used to examine the desirable accuracy of the above expansion.

5. THE SCATTERING STATES AND THE PHOTOIONIZATION CROSS SECTIONS

We express the eigenfunction of the continuum $\Psi_i^{Em\sigma}(r,\eta)$ with the energy $\epsilon = 2E$ describing the ejected electron above the first threshold $\epsilon^{th}_{m\sigma 1}(\gamma) = \epsilon^{th}_{m\sigma}(\gamma) = \gamma(|m| + m + 1)$ as follows

$$\Psi_i^{Em\sigma}(r,\eta) = \sum_{j=1}^{j_{\max}} \Phi_j^{m\sigma}(\eta; r)\hat{\boldsymbol{\chi}}_{ji}^{(m\sigma)}(E,r), \quad i = 1,\ldots,N_o, \tag{77}$$

where solution $\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r)$ is the radial part of the "incoming" or eigenchannel wave function. In this case the eigenfunction $\Psi_i^{Em\sigma}(r,\eta)$ is normalized by the condition

$$\left\langle \Psi_i^{Em\sigma}(r,\eta) \middle| \Psi_{i'}^{E'm'\sigma'}(r,\eta) \right\rangle = \sum_{j=1}^{j_{\max}} \int_0^\infty r^2 dr \left(\hat{\chi}_{ji}^{(m\sigma)}(E,r)\right)^* \hat{\chi}_{ji'}^{(m'\sigma')}(E',r) = \delta(E-E')\delta_{mm'}\delta_{\sigma\sigma'}\delta_{ii'}. \tag{78}$$

The radial of the eigenchannel function $\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r)$ is calculated by formula

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}}\boldsymbol{\chi}^{(p)}(r)\mathbf{C}\,\mathbf{cos}\,\boldsymbol{\delta}. \tag{79}$$

Here a numerical solution $\boldsymbol{\chi}^{(p)}(r)$ of the (52) that satisfies the "standing" wave boundary conditions (56) and has the standard asymptotic form[15]

$$\boldsymbol{\chi}^{(p)}(r) = \boldsymbol{\chi}^s(r) + \boldsymbol{\chi}^c(r)\,\mathbf{K}, \quad \mathbf{K}\,\mathbf{C} = \mathbf{C}\,\mathbf{tan}\,\boldsymbol{\delta}, \quad \mathbf{C}\mathbf{C}^T = \mathbf{C}^T\mathbf{C} = \mathbf{I}_{oo}. \tag{80}$$

where $\boldsymbol{\chi}^s(r) = 2\,\Im(\boldsymbol{\chi}(r))$ and $\boldsymbol{\chi}^c(r) = 2\,\Re(\boldsymbol{\chi}(r))$, $\mathbf{K}$ is the numerical short-range reaction matrix, $\mathbf{tan}\,\boldsymbol{\delta}$ and $\mathbf{C}$ are the eigenvalue and the orthogonal matrix a set of the corresponded eigenvectors. In the latter case the regular and irregular functions satisfy the generalized Wronskian relation (76) at large r

$$\mathbf{Wr}(\mathbf{Q}(r); \boldsymbol{\chi}^c(r), \boldsymbol{\chi}^s(r)) = \mathbf{I}_{oo}. \tag{81}$$

Using $\mathbf{R}$-matrix calculation,[8] we obtain the equation for the reaction matrix $\mathbf{K}$ expressed via the matrix $\mathbf{R}$ at $r = r_{\max}$

$$\left(\mathbf{R}\boldsymbol{\chi}^c(r) - \frac{d\boldsymbol{\chi}^c(r)}{dr}\right)\mathbf{K} = \left(\frac{d\boldsymbol{\chi}^s(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^s(r)\right). \tag{82}$$

When some channels are closed, the matrices in Eq. (82) are rectangular. Therefore, we obtain the following expression for the reaction matrix $\mathbf{K}$

$$\mathbf{K} = -\mathbf{X}^{-1}(r_{\max})\mathbf{Y}(r_{\max}), \tag{83}$$

where

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

are the square matrices of dimension $N_o \times N_o$ depended on the open-open matrix (channels).

The radial part of the "incoming" wave function is expressed via the numerical "standing" wave function and short-range reaction matrix $\mathbf{K}$ by the relation

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}}\boldsymbol{\chi}^-(r) = \imath\sqrt{\frac{2}{\pi}}\boldsymbol{\chi}^{(p)}(r)(\mathbf{I}_{oo} + \imath\,\mathbf{K})^{-1} \tag{84}$$

and has the asymptotic form

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}}(\boldsymbol{\chi}(r) - \boldsymbol{\chi}^*(r)\mathbf{S}^\dagger), \tag{85}$$

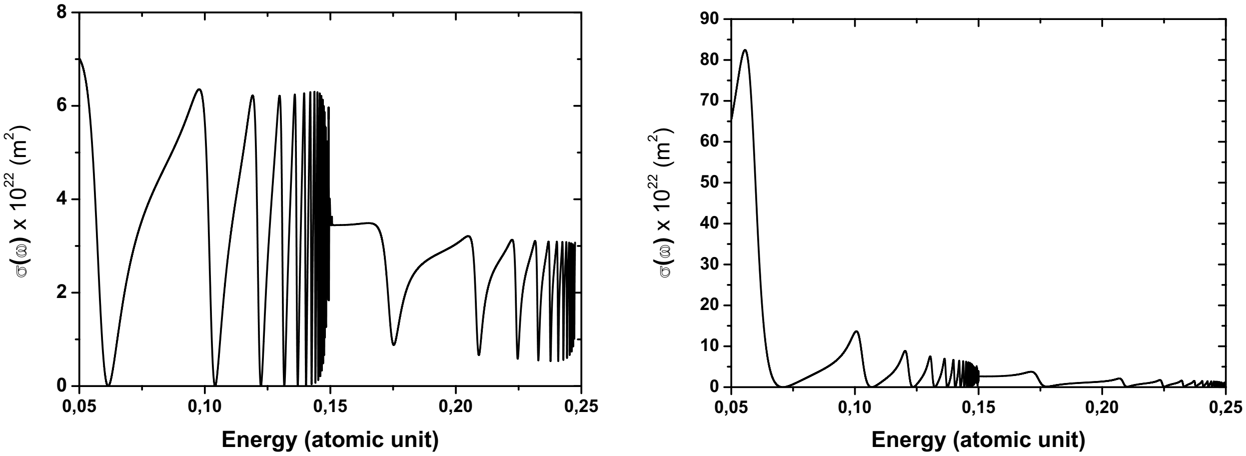

Figure 1. Cross sections of photoionization from the states $1s$ (left) and $3d$ (right) versus the energy for $B_0 = 2.35 \times 10^4\,T$ ($\gamma = 1 \times 10^{-1}$), and for the final state with $\sigma = -1$ $m = 0$

where $\mathbf{S}$ is the short-range scattering matrix, depends on the scattering matrix $\check{\mathbf{S}}_\sigma$ (30) and Coulomb phase shift $\boldsymbol{\delta}^c$, $\mathbf{S} = \exp(-\imath\boldsymbol{\delta}^c)\,\check{\mathbf{S}}_\sigma\,\exp(-\imath\boldsymbol{\delta}^c)$, and

$$\mathbf{S}^\dagger\mathbf{S} = \mathbf{S}\mathbf{S}^\dagger = \mathbf{I}_{oo}, \quad \mathbf{K} = \imath(\mathbf{I}_{oo} + \mathbf{S})^{-1}(\mathbf{I}_{oo} - \mathbf{S}), \quad \mathbf{S} = (\mathbf{I}_{oo} + \imath\,\mathbf{K})(\mathbf{I}_{oo} - \imath\,\mathbf{K})^{-1}. \tag{86}$$

In terms of the above definitions the photoionization cross section $\sigma(\omega)$ (35) is expressed as

$$\sigma(\omega) = 4\pi^2\alpha\omega\sum_{i=1}^{N_o}\left|D^{m\sigma\sigma'}_{i,N_{|z|},N_\rho}(E)\right|^2 a_0^2, \tag{87}$$

where $D^{m\sigma\sigma'}_{i,N_{|z|},N_\rho}(E)$ are the matrix elements of the dipole moment

$$D^{m\sigma\sigma'}_{i,N_{|z|},N_\rho}(E) = \left\langle \Psi_i^{Em\sigma=\mp1}(r,\eta)\middle| r\eta \middle| \Psi^{m\sigma'=\pm1}_{N_{|z|},N_\rho}(r,\eta)\right\rangle = \sum_{j=1}^{j_{\max}}\int_0^{r_{\max}} r^2 dr\,\hat{\chi}^{(m\sigma=\mp1)}_{ji}(E,r)\,d_j^{(m\sigma\sigma')}(r), \tag{88}$$

and $d_j^{(m\sigma\sigma')}(r)$ are the matrix elements of the partial dipole moments

$$d_j^{(m\sigma\sigma')}(r) = \sum_{j'=1}^{j_{\max}}\left\langle \Phi_j^{m\sigma=\mp1}(\eta;r)\middle| r\eta \middle| \Phi_{j'}^{m\sigma'=\pm1}(\eta;r)\right\rangle_\eta \chi_{j'}^{(m\sigma'=\pm1)}(r). \tag{89}$$

In the above expressions $\omega = E - E(N_{|z|}, N_\rho, \sigma', m)$ is the frequency of radiation, $E_{Nlm} \equiv E(N_{|z|}, N_\rho, \sigma', m)$ is the energy of the initial bound state $\Psi^{m\sigma'}_{N_{|z|},N_\rho}(r,\eta)$ and $N_{|z|} = N_r = N - l - 1$. The continuum spectrum solution $\boldsymbol{\chi}^{(p)}(r)$ having asymptotic of "standing" wave conditions and reaction matrix $\mathbf{K}$ required for calculating (79) or (85), and discrete spectrum solution $\boldsymbol{\chi}(r)$ and eigenvalue E can be calculated with help of the program KANTBP.[15] One can see that using (79) or (85) for calculation of absolute value in formula (87) yields the same result. Therefore, (79) is preferable for using real arithmetics.

6. NUMERICAL RESULTS

Fig. 1 displays the calculated photoionization cross section from the states $1s$ and $3d$ at $B_0 = 2.35 \times 10^4\,T$ ($\gamma = 1 \times 10^{-1}$) in the energy interval from $E = 0.05\,a.u.$ to $E = 0.25\,a.u.$ with the final state $\sigma = -1$, $m = 0$.

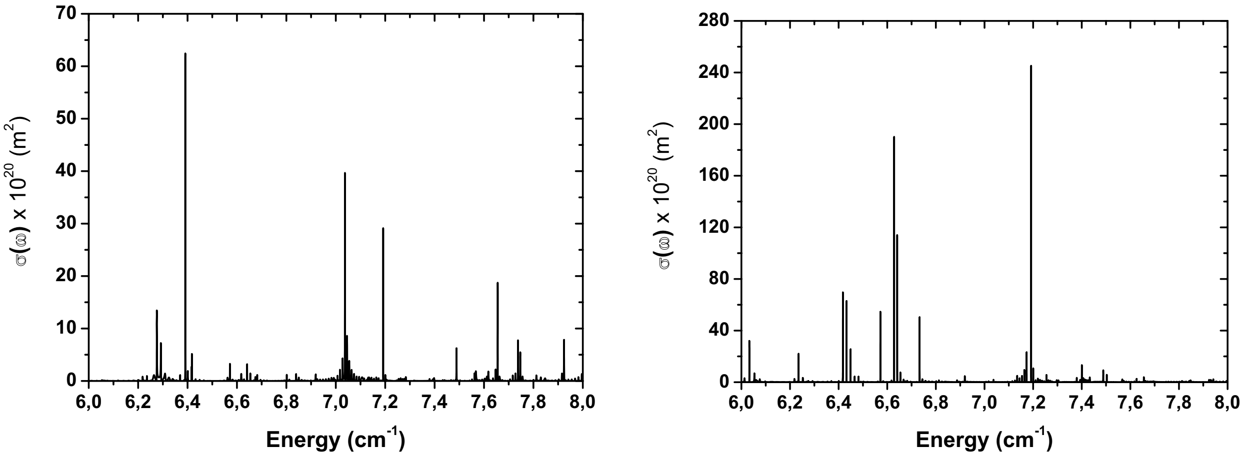

Figure 2. Photoionization cross section from the states $3s$ (left) and $3d$ (right) versus the energy for $B_0 = 6.10\,T$ ($\gamma = 2.595 \times 10^{-5}$) and for the final state with $\sigma = -1$, $m = 0$.

Table 1. The absolute maximum values, $\max_{j1}$, of the continuum wave functions $\hat{\chi}^{(01)}_{j1}(E, \hat{r})$ at $B_0 = 6.10\,T$ ($\gamma = 2.595 \times 10^{-5}$), $E = 6.0\,cm^{-1}$ and $j_{\max} = 35$. The numbers x in the parenthesis denote the factors 10^x.

j	$\max_{j1}$	j	$\max_{j1}$	j	$\max_{j1}$	j	$\max_{j1}$	j	$\max_{j1}$
1	2.309	8	0.109	15	0.080	22	0.038	29	2.974(-3)
2	0.637	9	0.234	16	0.088	23	0.075	30	1.088(-3)
3	1.859	10	0.317	17	0.084	24	0.056	31	2.677(-4)
4	1.064	11	0.171	18	0.061	25	0.058	32	5.998(-5)
5	0.510	12	0.089	19	0.087	26	0.131	33	1.689(-5)
6	0.271	13	0.055	20	0.055	27	0.071	34	3.781(-6)
7	0.183	14	0.098	21	0.051	28	0.014	35	1.043(-6)

For the initial state $1s$ in the whole energy interval the results are in good agreement with those of **R**-matrix calculations within the *multichannel quantum-defect theory*.[5] We also compared our results with those of the complex-rotation method combined with a basic set of the 10 000 complex spherical Sturmian-type expansion[16] and basic set of the 450 mixed Slater-Landau basis.[6] In this case the agreement is good between the thresholds, but not near them. So, the calculated photoionization cross section has threshold behavior coincided with.[5]

We used ten eigenfunctions ($j_{\max} = 10$) of the problem (47)–(49) which requires to solve ten equations of the system (52). The results coincide with those of the finite element method[7] to ten digits. The finite element grids of $\hat{r} = \sqrt{\gamma} r$ have been chosen as 0 (200) 3 (200) 20 (200) 100 for the discrete spectrum and 0 (200) 3 (200) 20 (200) 100 (1000) 1000 for the continuous one. The numbers in parentheses are the numbers of finite elements of the order $k = 4$ in each interval. The number of nodes in the grids is 2400 and 6401, so that the maximum number of unknowns in Eqs. (52) is 24000 and 64010, respectively.

Fig. 2 displays the cross section of photoionization from the states $3s$ (left) and $3d$ (right) at $B_0 = 6.10\,T$ ($\gamma = 2.595 \times 10^{-5}$) in the energy interval between $E = 6.0\,cm^{-1}$ and $E = 8.0\,cm^{-1}$. In this case we increased $j_{\max}$ up to 35, and the finite element grids were chosen as 0 (200) 0.03 (200) 0.2 (200) 1 and 0 (200) 0.03 (200) 0.2 (200) 1 (2000) 100 (4000) 1000. The number of nodes in these grids is 2400 and 26401, respectively. The corresponding maximum number of unknowns in Eqs. (52) is 84000 and 924035. Table 1 shows the absolute maximum values of the continuum spectrum wave functions $\hat{\chi}^{(01)}_{j1}(E, \hat{r})$ at $E = 6.0\,cm^{-1}$. We calculated the cross sections with the energy step $5 \times 10^{-4}\,cm^{-1}$ in all the region except the vicinity of peaks, where the step was $5 \times 10^{-6}\,cm^{-1}$.

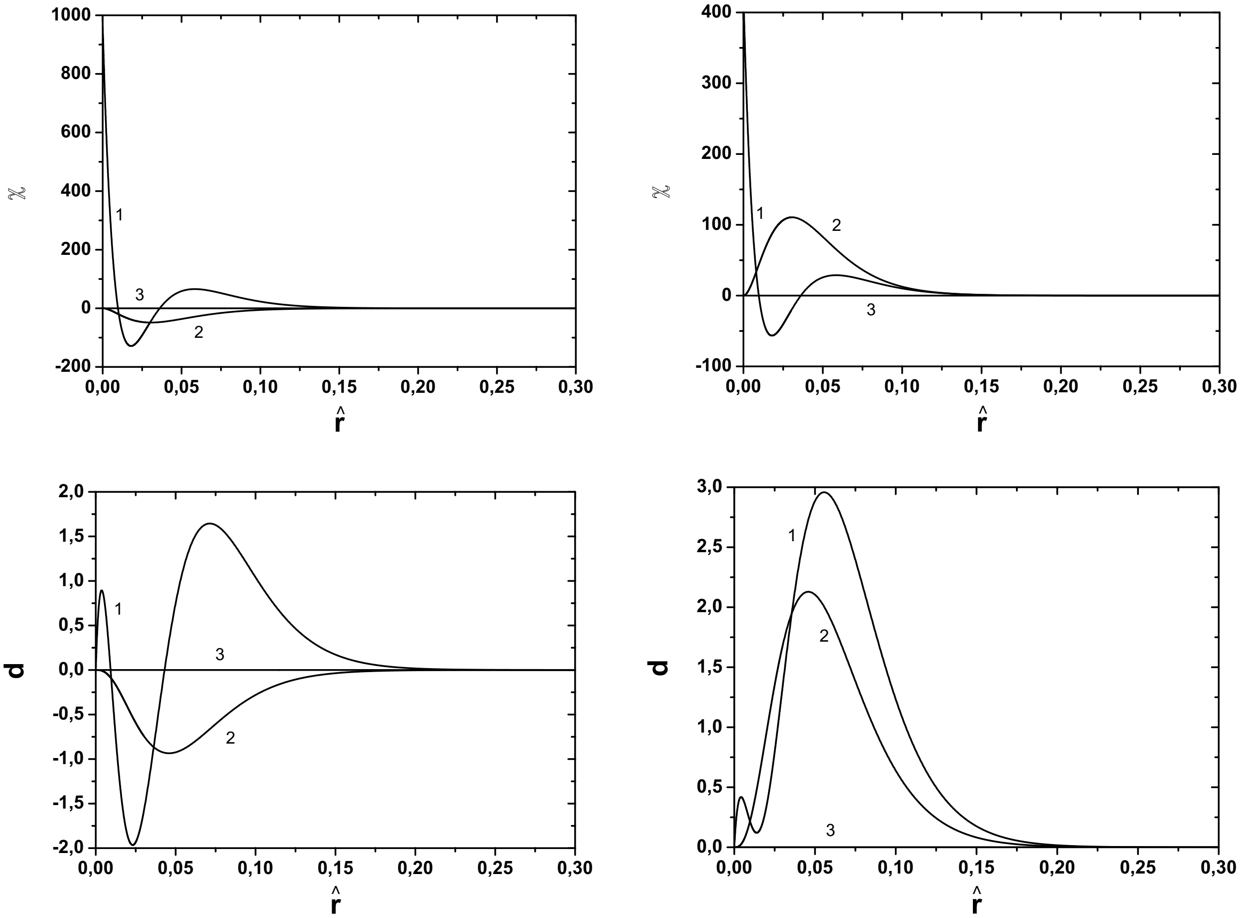

Figure 3. The first three components of the calculated wave functions, $\chi = \{\chi_j^{(m\sigma')}(\hat{r})\}$: 1 — $\chi_1^{(01)}(\hat{r})$, 2 — $\chi_2^{(01)}(\hat{r})$, 3 — $\chi_3^{(01)}(\hat{r})$ (upper), and the first three components of the calculated dipole moments, $d = \{d_j^{(m\sigma\sigma')}(\hat{r})\}$: 1 — $d_1^{(0-11)}(\hat{r})$, 2 — $d_2^{(0-11)}(\hat{r})$, 3 — $d_3^{(0-11)}(\hat{r})$ (lower) for the states $3s$ (left) and $3d$ (right) with $B_0 = 6.10\,T$ ($\gamma = 2.595 \times 10^{-5}$).

Note, that $3s$, $3p$ and $3d$ states are nearly degenerate and $E_{300} = -0.055\,555\,542\,37\,a.u.$, $E_{310} = -0.055\,555\,549\,49\,a.u.$, $E_{320} = -0.055\,555\,552\,07\,a.u.$, respectively. To calculate these energies we used three equations of the system (52) ($j_{\max} = 3$); increasing $j_{\max}$ keeps them stable. We also compared the energies with those calculated by means of the second-order algebraic perturbation theory.[17] The results agree to the 13-th digit. Fig. 3 displays the first three components of the wave functions (upper) of $3s$ and $3d$ states, and of the dipole moment (lower) from (89) versus $\hat{r}$. The probability density isolines for the Zeeman wave states $|NN_rm\rangle$ with even parity $\sigma = +1$ in a homogeneous magnetic field are shown in Fig. 4.

In the calculations we used the following values of the physical constants[18]: $1\,cm^{-1} = 4.55633 \times 10^{-6}\,a.u.$, the Bohr radius $a_0 = 5.29177 \times 10^{-11}m$ and the fine-structure constant $\alpha = 7.29735 \times 10^{-3}$.

7. CONCLUSIONS

A new efficient method of calculating both the discrete and the continuous spectrum wave functions of a hydrogen atom in a strong magnetic field is developed based on the Kantorovich approach to the parametric eigenvalue problems in spherical coordinates. The two-dimensional spectral problem for the Schrödinger equation with fixed magnetic quantum number and parity is reduced to a one-dimensional spectral parametric problem for the angular variable and a finite set of ordinary second-order differential equations for the radial variable. The rate

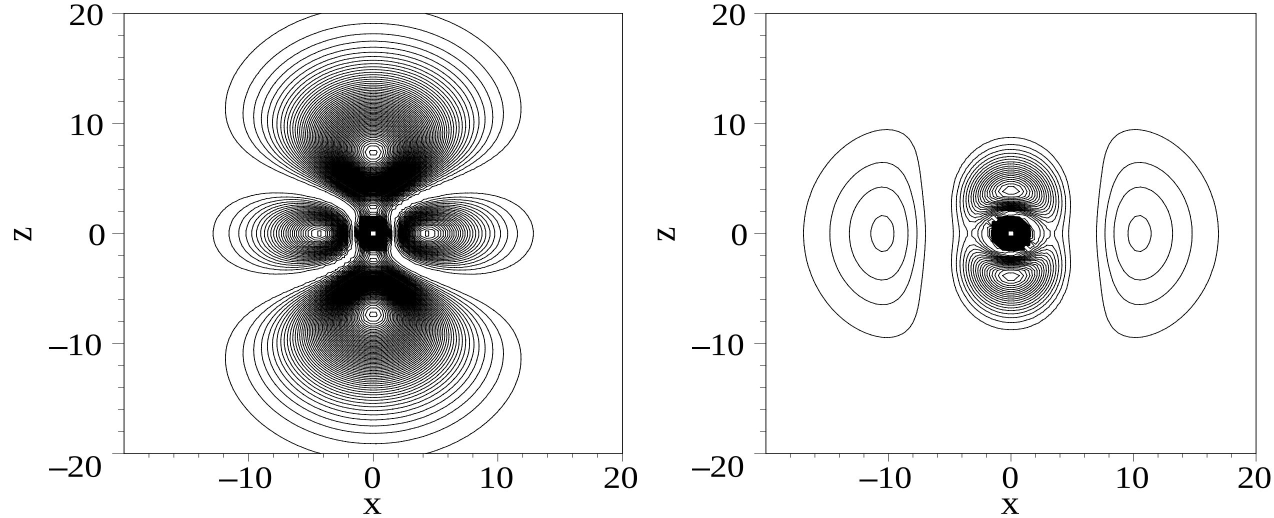

Figure 4. The probability density isolines for the Zeeman wave states $|N, N_r, m\rangle$ with even parity $\sigma = +1$ and $m = 0$ in the homogeneous magnetic field $\gamma = 2.595 \times 10^{-5}$: left — the state $|300\rangle$ with the minimal energy correction; right — the state $|320\rangle$ with the maximal energy correction.

of convergence is investigated numerically and is illustrated with a number of typical examples. The results are in good agreement with calculations of photoionization cross sections by other authors. The approach developed provides a useful tool for calculations of threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps.

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