On an effective approximation of the Kantorovich method for calculations of a hydrogen atom in a strong magnetic field

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ABSTRACT

A new effective method of calculating the wave functions of discrete and continuous spectra 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 spectral parametric problem for a one-dimensional equation for the angular variable and a finite set of ordinary second-order differential equations for the radial variable. A canonical transformation is applied to approximate the finite set of radial equations by means of a new radial equation describing an open channel. The rate of convergence is examined numerically and illustrated with a set of typical examples. The results are in good agreement with calculations by other authors.

Keywords: Kantorovich approach, Hydrogen atom, strong magnetic field

1. INTRODUCTION

Recent Monte-Carlo estimations of the influence of the strong magnetic field on the spontaneous recombination of antihydrogen in the cold positron-antiproton plasma conditions of the ATHENA[1] and ALPHA[2] experiments (CERN) have shown that further quantum mechanical analysis is needed.[3] At the first stage of the implementation of this analysis we developed the Kantorovich method (known in physics as the adiabatic approach) and first applied it to the problem of low-lying excited states of a hydrogen atom in a magnetic field in spherical coordinates[4] and the benchmark three-body scattering problem on a line.[5,6]

Recently the adiabatic representation in cylindric coordinates was applied to reveal the basic decay mechanisms of Rydberg states with high magnetic quantum numbers in the magnetic traps.[7] It has been shown that the exhaustive analysis of the complex electron dynamics at smaller magnetic numbers is impossible without taking the non-adiabatic coupling into account.[8] However, high-accuracy calculations in cylindric coordinates is a rather cumbersome problem except the cases of high magnetic numbers or dominating magnetic field.[9] Hence, the use of spherical coordinates is preferable when the contributions of Coulomb and magnetic fields to the average potential energy are comparable..[10]

In the present paper we develop the Kantorovich approach with the boundary condition of the third type in the 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[11] in spherical coordinates only instead of the combined nonorthogonal basis of Landau and Sturmian functions in both cylindrical and spherical coordinates.[12] We also calculate a manifold of the excited states with the principle quantum number N=9 of a hydrogen atom in the magnetic field of 3 T that may be interesting for laser-stimulated recombination in a trap[13] .

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 a 1D eigenvalue

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problem for the set of closed radial equations via three steps of the Kantorovich method is described briefly in Section 3. These steps of the implementation of the Kantorovich method are considered in detail in Sections 4 and 5. The method is applied to the calculation of low-lying states in Section 6 where the rate of convergence is demonstrated explicitly for typical examples and the results are compared with the best of the known ones. In Section 7 the conclusions are made and the possible future applications of the method are discussed.

2. STATEMENT OF THE PROBLEM

The Schrödinger equation for the hydrogen atom in an axially symmetric magnetic field $\vec{B} = (0, 0, B)$ in the spherical coordinates (r, θ, ϕ) can be written as the 2D equation

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

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

$$V(r,\theta) = \frac{m^2}{r^2\sin^2\theta} + \gamma m + \frac{1}{4}\gamma^2 r^2\sin^2\theta,$$

where $m = 0, \pm 1, \dots$ is the magnetic quantum number, $\gamma = B/B_0$, $B_0 \cong 2.35\times 10^9 G$ is a dimensionless parameter which determines the field strength B, and the atomic units (a.u.) $\hbar = m_e = e = 1$ are used, assuming the mass of the nucleus to be infinite. In these expressions ϵ is twice the energy, $\epsilon = 2E$ (in Rydbergs, 1Ry=(1/2)a.u.), of the bound state $|m\sigma>$ at fixed values of m and z-parity, $\sigma = \pm 1$, and Ψ is the corresponding wave function, $\Psi \equiv \Psi_{m\sigma}(r,\theta) = (\Psi_m(r,\theta) + \sigma\Psi_m(r,\pi-\theta))/2$. Here the sign of z-parity, $\sigma = (-1)^{N_\theta}$, is determined by the number of nodes N_θ (even or odd) in the solution Ψ with respect to the angular variable θ in the interval $0 < \theta < \pi$. We will also use the units $\hbar = m_e = e = \gamma = 1$ and the corresponding scaled radial coordinate $\hat{r} = r/\sqrt{\gamma}$, the effective charge $\hat{Z} = Z/\sqrt{\gamma}$ and the scaled energy $\hat{\epsilon} = \epsilon/\gamma$.

The function Ψ satisfies the following boundary conditions in each $m\sigma$ subspace of the full Hilbert space:

$$\lim_{\theta\to 0}\sin\theta\frac{\partial\Psi}{\partial\theta} = 0, \quad \text{if} \quad m = 0, \quad \text{and} \quad \Psi(r,0) = 0, \quad \text{if} \quad m \neq 0, \tag{2}$$

$$\frac{\partial\Psi}{\partial\theta}(r,\frac{\pi}{2}) = 0, \quad 0 \le r < \infty, \quad \text{for the even parity state } (\sigma = +1), \tag{3}$$

$$\Psi(r,\frac{\pi}{2}) = 0, \quad 0 \le r < \infty, \quad \text{for the odd parity state } (\sigma = -1), \tag{4}$$

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

The discrete spectrum wave function obeys the asymptotic boundary condition which can be approximated by the boundary condition of the first type at large $r = r_{max}$

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

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

$$\mathbf{\Pi}(\Psi,\epsilon) = 0, \quad 4\pi\int_0^{r_{max}}\int_0^{\pi/2} r^2\sin\theta|\Psi(r,\theta)|^2 dr d\theta = 1, \tag{7}$$

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

$$\mathbf{\Pi} = 4\pi\int_0^{r_{\max}}\int_0^{\pi/2}\sin\theta\left(r^2\frac{\partial\Psi^*(r,\theta)}{\partial r}\frac{\partial\Psi(r,\theta)}{\partial r} + \frac{\partial\Psi^*(r,\theta)}{\partial\theta}\frac{\partial\Psi(r,\theta)}{\partial\theta} - (2Zr - V(r,\theta)r^2 + \epsilon r^2)|\Psi(r,\theta)|^2\right)drd\theta. \tag{8}$$

In the Fano-Lee reaction matrix $\mathbf{R}$ theory[14] the continuum wave function $\Psi(r,\theta)$ obeys the boundary condition of the third type at the fixed values of energy ϵ and radial variable $r = r_{\max}$

$$\frac{\partial \Psi(r,\theta)}{\partial r} - \lambda\,\Psi(r,\theta) = 0, \quad r = r_{\max}. \tag{9}$$

Here the parameters $\lambda \equiv \lambda(r_{\max},\epsilon)$, determined by the variational principle, play the role of eigenvalues of a logarithmic normal derivative matrix of the solution of the boundary problem (1)-(5), (9)

$$\mathbf{\Pi} \equiv \mathbf{\Pi}(\Psi,\epsilon) = 4\pi\lambda r_{\max}^2 \int_0^{\pi/2} \sin\theta |\Psi(r_{\max},\theta)|^2 d\theta. \tag{10}$$

Standard theorems[15] ensure the existence of a function $\lambda(r_{\max})$ such that Eq. (9) is satisfied at any finite $r = r_{\max} < \infty$.[16]

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

Consider a formal expansion of the total wave function Ψ and the partial solution $\Psi_i^{m\sigma}(r,\theta,\sqrt{\epsilon})$ that corresponds to the state $|m\sigma i>$ using the finite set of one-dimensional basis functions $\{\Phi_j^{m\sigma}(\theta;r)\}_{j=1}^{j_{max}}$

$$\Psi(r,\theta,\varphi,\sqrt{\epsilon},\theta',\varphi') = \sum_{m'=-|m_{max}|}^{|m_{max}|} \sum_{\sigma=o,e} \frac{\exp(-\imath m'\varphi')}{\sqrt{2\pi}} \sum_{i=1}^{j_{max}} \Psi_i^{m'\sigma}(r,\theta,\varphi,\sqrt{\epsilon})\Phi_i^{m'\sigma}(\theta';r\to\infty), \tag{11}$$

$$\Psi_i^{m\sigma}(r,\theta,\varphi,\sqrt{\epsilon}) = \sum_{m=-|m_{max}|}^{|m_{max}|} \frac{\exp(\imath m\varphi)}{\sqrt{2\pi}} \Psi_i^{m\sigma}(r,\theta,\sqrt{\epsilon}), \quad \Psi_i^{m\sigma}(r,\theta,\sqrt{\epsilon}) = \sum_{j=1}^{j_{max}} \Phi_j^{m\sigma}(\theta;r)\chi_j^{(m\sigma i)}(r\sqrt{\epsilon}).$$

The matrix functions $\boldsymbol{\chi}(r) \equiv \{\boldsymbol{\chi}^{(i)}(r)\}_{i=1}^{j_{max}}$ composed of the vector functions, $(\boldsymbol{\chi}^{(i)})^T = (\chi_1^{(i)}(r),\ldots,\chi_{j_{max}}^{(i)}(r))$ are unknown, and the surface functions $(\Phi(\theta;r))^T = (\Phi_1(\theta;r),\ldots,\Phi_{j_{max}}(\theta;r))$ form an orthonormal basis for each value of the radius r which is treated here as a parameter.

In the Kantorovich approach the functions $\Phi_i(\theta;r)$ and the potential curves $E(r)$ (in Ry) are determined as the solutions of the following one-dimensional parametric eigenvalue problem:

$$-\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\Phi(\theta;r)}{\partial\theta} + r^2\sin\theta V(r,\theta)\Phi(\theta;r) = E(r)\sin\theta\Phi(\theta;r), \tag{12}$$

with the boundary conditions

$$\lim_{\theta\to 0}\sin\theta\frac{\partial\Phi}{\partial\theta} = 0, \quad \text{if} \quad m=0, \quad \text{and} \quad \Phi(0;r)=0, \quad \text{if} \quad m\neq 0, \tag{13}$$

$$\frac{\partial\Phi}{\partial\theta}(\frac{\pi}{2};r) = 0, \quad 0\le r<\infty, \quad \text{for the even parity state } (\sigma=+1), \tag{14}$$

$$\Phi(\frac{\pi}{2};r) = 0, \quad 0\le r<\infty, \quad \text{for the odd parity state } (\sigma=-1). \tag{15}$$

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 Φ with respect to the angular variable θ in the interval $0<\theta<\pi$. Since the operator in the left-hand side of (12) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle \Phi_i((\rho;\Omega) \middle| \Phi_j(\rho;\Omega)\right\rangle_\Omega = 4\pi\int_0^{\pi/2}\sin\theta\Phi_i(\theta;r)\Phi_j(\theta;r)d\theta = \delta_{ij}, \tag{16}$$

where δ_{ij} is the Kronecker δ–symbol. The problem (12)–(15) is solved for each value of the field parameter,γ, i.e. $\Phi(\theta;r) \equiv \Phi(\theta;r,\gamma)$ and $E(r) \equiv E(r,\gamma)$, and for each value of the radial variable $r \in \omega_r$, where $\omega_r = (r_1,r_2,\ldots,r_k,\ldots)$ is a given set of values of r.

Table 1. Comparison of the classification of a free hydrogen atom in the spherical coordinates with the adiabatic classification of a hydrogen atom in a magnetic field with strength γ in the spherical and cylindrical coordinate systems, respectively.

λ	N	l	m	σ	N_θ	N_r	N_ρ	$N_{\lvert z\rvert}$	$\epsilon^{th}_{m\sigma j}$	j
1	1	s	0	1	0	0	0	0	γ	1
1	2	s	0	1	0	1	0	1	γ	1
-1	2	p	0	-1	1	0	0	0	γ	1
-1	2	p	-1	1	0	0	0	0	γ	1
-1	2	p	1	1	0	0	0	0	3γ	1

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[11] with respect to the variable $\eta = \cos\theta$:

$$-\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial\Phi(\eta;\hat{r})}{\partial\eta} + \left(\frac{m^2}{1-\eta^2} + \left(\frac{\hat{r}^2}{2}\right)^2 (1-\eta^2)\right)\Phi(\eta;\hat{r}) = \hat{\tilde{E}}(\hat{r})\Phi(\eta;\hat{r}). \tag{17}$$

This means that for small r the asymptotic form of the eigenvalues $E_j(r)$, $j = 1,2,3,\ldots$ at fixed values m and σ is defined by the values of the orbital quantum number, $l = s,p,d,f,\ldots$: $E_j(0) = l(l+1)$, $l = 0,1,2,3,\ldots$, where $j = (l-|m|)/2+1$ 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 Φ 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 asymptotic form of eigenvalues $E_j(r)$, $j = 1,2,3,\ldots$ at fixed values of m and σ is defined by the values of the transversal quantum number, N_ρ: $\lim_{r\to\infty} E_j(r,\gamma)r^{-2} = \epsilon_j^{th}(\gamma) = \gamma(2N_\rho + |m| + m + 1)$, $N_\rho = 0,1,2,3,\ldots$, where $j = N_\rho + 1$ (see Fig. 1). The values of the transversal quantum number N_ρ, i.e., the number of nodes of the eigenfunction Φ with respect to the transversal variable $\rho = r\sin\theta$ on semi-axis, are expressed via the number of nodes N_θ of the solution Φ: $N_\rho = 1/2 \cdot N_\theta$ 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.,

$$\lim_{r\to\infty} \tilde{E}_j(r,\gamma)r^{-2} = \gamma(2N_\rho + |m| + 1). \tag{18}$$

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 (11) into the variational problem (7), and using Eqs. (12), (15), (16) and the identity

$$4\pi\int_0^{\pi/2}\left(\sin\theta\frac{\partial\Phi_i(\theta;r)}{\partial\theta}\frac{\partial\Phi_j(\theta;r)}{\partial\theta} + r^2\sin\theta V(r,\theta)\Phi_i(r,\theta)\Phi_j(\theta;r)\right)d\theta = \frac{E_i(r)+E_j(r)}{2}\delta_{ij}, \tag{19}$$

which follows from these equations, 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) $(\boldsymbol{\chi}^{(i)}(r))^T = (\chi_1^{(i)}(r), \chi_2^{(i)}(r), \ldots, \chi_{j_{max}}^{(i)}(r))$ of the expansion (11)

$$-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\boldsymbol{\chi}^{(i)}}{dr} + \frac{\mathbf{U}(\mathbf{r})}{r^2}\boldsymbol{\chi}^{(i)} + \mathbf{Q}(r)\frac{d\boldsymbol{\chi}^{(i)}}{dr} + \frac{1}{r^2}\frac{d[r^2\mathbf{Q}(r)\boldsymbol{\chi}^{(i)}]}{dr} = \epsilon_i\,\mathbf{I}\boldsymbol{\chi}^{(i)}, \qquad \lim_{r\to 0} r^2\frac{\partial\boldsymbol{\chi}^{(i)}}{\partial r} = 0, \tag{20}$$

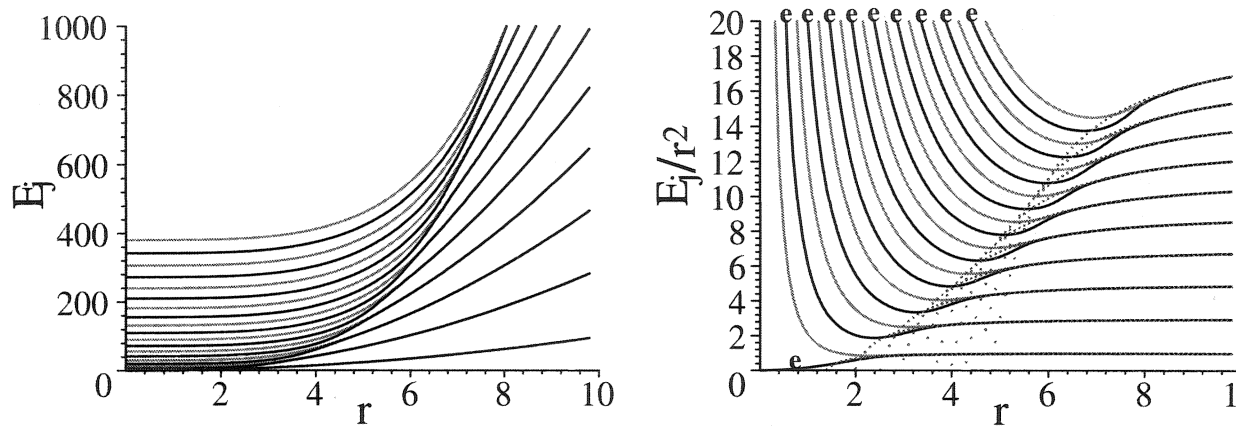

Figure 1. The behavior of the potential curves $E_j(r)$, $j=1,2,\ldots$ at $m=0$ and $\gamma=1$ for some first even $j=(l-|m|)/2+1$ (marked by the symbol "e") and for odd $j=(l-|m|+1)/2$ states. The dotted lines show the asymptotic behavior of the potential curves at large r.

Here $\mathbf{I}$, $\mathbf{U}(r)$, and $\mathbf{Q}(r)$ are finite $j_{max}\times j_{max}$ matrices, whose elements are given by the relations (see Figs. 2-3)

$$U_{ij}(r)=\frac{E_i(r)+E_j(r)}{2}\delta_{ij}+2Zr+r^2H_{ij}(r),\qquad H_{ij}(r)=H_{ji}(r)=4\pi\int_0^{\pi/2}\sin\theta\frac{\partial\Phi_i}{\partial r}\frac{\partial\Phi_j}{\partial r}d\theta,$$
$$Q_{ij}(r)=-Q_{ji}(r)=-4\pi\int_0^{\pi/2}\sin\theta\Phi_i\frac{\partial\Phi_j}{\partial r}d\theta,\quad I_{ij}=\delta_{ij},\quad i,j=1,2,\ldots,j_{max}. \tag{21}$$

The discrete spectrum solutions are governed by the asymptotic boundary condition and orthonormality conditions

$$\lim_{r\to\infty}r^2\boldsymbol{\chi}^{(i)}=0\qquad\to\qquad\boldsymbol{\chi}^{(i)}(r_{\max})=0,\qquad\int_0^{r_{\max}}r^2(\boldsymbol{\chi}^{(i)}(r))^T\boldsymbol{\chi}^{(j)}(r)dr=\delta_{ij}. \tag{22}$$

For the continuum solution $\boldsymbol{\chi}^{(i)}(r))$ we can alternatively require that the projections of (9) onto all adiabatic functions hold

$$\left\langle\Phi_i(r;\theta)\left|\frac{\partial\boldsymbol{\Psi}(r,\theta)}{\partial r}-\lambda\,\boldsymbol{\Psi}(r,\theta)\right.\right\rangle_\Omega=0,\quad r=r_{\max}, \tag{23}$$

that leads to the third-type boundary conditions at fixed values of energy ϵ and radial variable $r=r_{\max}$

$$\left(\frac{\partial\boldsymbol{\chi}^{(i)}(r)}{\partial r}(\boldsymbol{\chi}^{(i)})^{-1}(r)-\mathbf{Q}(r)-\lambda_i\right)\boldsymbol{\chi}^{(i)}(r)=0,\quad r=r_{\max}. \tag{24}$$

From here on λ_i and $\boldsymbol{\chi}^{(i)}(r_{\max})$ will be the set of eigenvalues $\boldsymbol{\Lambda}=\{\delta_{ij}\lambda_i\}_{ij=1}^{N_\rho+1}$ corresponding to the set of eigenvectors $\boldsymbol{\chi}(r_{\max})\equiv\{\boldsymbol{\chi}^{(i)}(r_{\max})\}_{i=1}^{N_\rho+1}$ of the eigenvalue problem

$$\frac{d\boldsymbol{\chi}(r_{\max})}{dr}-\mathbf{Q}(r_{\max})\boldsymbol{\chi}(r_{\max})=\boldsymbol{\chi}(r_{\max})\boldsymbol{\Lambda}, \tag{25}$$

that can be reduced to the following one by averaging the variational problem (10):

$$\langle\boldsymbol{\Pi}\rangle_\Omega-r_{\max}^2\boldsymbol{\chi}^T(r_{\max})\boldsymbol{\chi}(r_{\max})\boldsymbol{\Lambda}=0.$$

Here $\boldsymbol{\chi}(r_{\max})$ is normalized as follows

$$r_{\max}^2 \boldsymbol{\chi}^T(r_{\max})\boldsymbol{\chi}(r_{\max}) = \mathbf{I}. \tag{26}$$

Multiplying (25) from the right by $r_{\max}^2 \boldsymbol{\chi}^T(r_{\max})$ and using the relation between the transposed and left pseudo-inverse of $\boldsymbol{\chi}(r_{\max})$,

$$\boldsymbol{\chi}^{-1}(r_{\max}) \equiv r_{\max}^2 \boldsymbol{\chi}^T(r_{\max}), \tag{27}$$

yields the relation between $\boldsymbol{\chi}(r_{\max})$ and its derivative

$$\frac{d\boldsymbol{\chi}(r_{\max})}{dr} = \mathbf{P}\boldsymbol{\chi}(r_{\max}), \qquad \mathbf{P} \equiv r_{\max}^2 \Big(\boldsymbol{\chi}(r_{\max})\, \boldsymbol{\Lambda} \boldsymbol{\chi}^T(r_{\max}) + \mathbf{Q}(r_{\max})\boldsymbol{\chi}(r_{\max})\, \boldsymbol{\chi}^T(r_{\max}) \Big). \tag{28}$$

Below we will consider the $\mathbf{P}$ matrix of dimension $j_{max} \times j_{max}$, which is a constant matrix for any normalization of $\boldsymbol{\chi}(r_{\max})$.

The application of the Kantorovich approach makes the above problems equivalent to the following ones:

- Calculation of the potential curves $E_i(r)$ and the eigenfunctions $\Phi_i(\theta; r)$ of the spectral problem (12)–(15) for a given set of $r \in \omega_r$ at fixed values $|m|$ and $\gamma = 1$.
- Calculation of the derivatives $\dfrac{\partial \Phi}{\partial r}$ and computation of the corresponding integrals (see (21)), necessary for obtaining the matrix elements of radial coupling $U_{ij}(r)$ and $Q_{ij}(r)$.
- Calculation of the scaled energies $\hat{\epsilon}$ and radial wave functions $\chi(r)$ as solutions of one-dimensional eigenvalue problem (20)–(25) at fixed values m, $\gamma = 1$ and effective charge $\hat{Z} = Z/\sqrt{\gamma}$, analysis of the convergence of these solutions depending on the number of channels j_{max} and recalculation of the scaled energies to the initial ones $\epsilon = \hat{\epsilon}\gamma$.
- Calculation of matrices Λ, P and the reaction matrix R (using Eqs. (28), (36)) corresponding to the radial wave functions $\chi(r)$ as the solutions of one-dimensional eigenvalue problem (20)–(25) at the fixed values of m, $\gamma = 1$ and $\hat{Z} = Z/\sqrt{\gamma}$, and the scaled energies $\hat{\epsilon}$. Examination of the convergence of these solutions depending on the number of channels j_{max}.

Note, that in the diagonal approximation $i = j$ of the problem (20)–(21), the so-called adiabatic approximation, the number of nodes N_r of the solution $\chi(r)$ 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 Φ 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 $\chi(|z|)$ with respect to the longitudinal variable $z = r\cos\theta$ on semi-axis. This means that the solution $\chi(z)$ on an axis is defined as follows: $\chi_{m\sigma}(z) = (\chi_m(\rho, z) + \sigma\chi_m(\rho, -z))/2$, or reduced to the solution $\chi(|z|)$ of the 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 asymptotic behavior of eigenvalues $E_j(r)$ at large r, we can express the binding energy $\mathcal{E}$ via the eigenvalues ϵ of the problem (20)–(21) as follows: $\mathcal{E} = (\epsilon_{m\sigma j}^{th}(\gamma) - \epsilon)/2$ (in a.u.), where $\epsilon_{m\sigma j}^{th}(\gamma)$ is the full threshold shift $\epsilon_{m\sigma j}^{th}(\gamma) = \gamma(2N_\rho + |m| + m + 1)$ or the reduced one $\epsilon_{m\sigma}^{th}(\gamma) = \gamma(|m| + m + 1)$, respectively (see, for example, Table 1).

4. ASYMPTOTIC BEHAVIOR OF SOLUTION

We write the set of differential equations (21) at fixed values m, σ and $\epsilon = 2E$ in the explicit form

$$
\begin{aligned}
&-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\chi_{ji}(r)}{dr} - \frac{2Z}{r}\chi_{ji}(r) - \left(\epsilon - \frac{E_j(r)}{r^2}\right)\chi_{ji}(r) + H_{jj}(r)\chi_{ji}(r) \\
&= \sum_{j'=1, j'\neq j}^{j_{max}} \left(-Q_{jj'}(r)\frac{d\chi_{j'i}(r)}{dr} - H_{jj'}(r)\chi_{j'i}(r) - \frac{1}{r^2}\frac{d\left(r^2 Q_{jj'}(r)\chi_{j'i}(r)\right)}{dr}\right), \quad i,j = 1,\dots,j_{max}. \qquad (29)
\end{aligned}
$$

At small r the asymptotic values of the matrix elements E_j, $H_{jj'}$ and $Q_{jj'}$, characterized by $l = 2j - 2 + |m|$ for even states and by $l = 2j - 1 + |m|$ for odd states, have the form

$$
\begin{aligned}
E_l &= l(l+1) + \gamma m r^2 + \frac{\gamma^2 r^4}{2}\frac{l^2 + l - 1 + |m|^2}{(2l-1)(2l+3)} + \frac{\gamma^4 r^8}{8}\frac{(20l + 20l^2 + 33)|m|^4}{(2l-3)(2l-1)^3(2l+3)^3(2l+5)} \\
&\quad + \frac{\gamma^4 r^8}{8}\frac{(-24l^4 - 48l^3 + 2l^2 + 26l - 30)|m|^2 + 4l^6 + 12l^5 - 3l^4 - 26l^3 + 2l^2 + 17l - 3}{(2l-3)(2l-1)^3(2l+3)^3(2l+5)} + O(r^{12}), \\
Q_{ll+2} &= \frac{\gamma^2 r^3}{2}\frac{\sqrt{(l+1)^2 - |m|^2}\sqrt{(l+2)^2 - |m|^2}}{\sqrt{2l+1}(2l+3)^2\sqrt{2l+5}} + \frac{\gamma^4 r^7}{2}\frac{\sqrt{(l+1)^2 - |m|^2}\sqrt{(l+2)^2 - |m|^2}(4|m|^2 - 1)}{(2l-1)\sqrt{2l+1}(2l+3)^4\sqrt{2l+5}(2l+7)} + O(r^{11}), \\
Q_{ll+4} &= \frac{\gamma^4 r^7}{8}\frac{\sqrt{(l+1)^2 - |m|^2}\sqrt{(l+2)^2 - |m|^2}\sqrt{(l+3)^2 - |m|^2}\sqrt{(l+4)^2 - |m|^2}}{\sqrt{2l+1}(2l+3)^2(2l+5)^2(2l+7)^2\sqrt{2l+9}} + O(r^{11}), \\
H_{ll} &= \frac{\gamma^4 r^6}{2}\Big((16l^4 + 32l^3 + 248l^2 + 232l + 201)|m|^4 + (-10l^2 - 224l^4 - 96l^5 + 118l - 288l^3 - 32l^6 - 195)|m|^2 \\
&\quad + 16l^8 + 64l^7 + 46l + 40l^6 - 127l^4 - 104l^5 + 71l^2 - 6l^3 - 6\Big)\Big/\Big((2l-3)(2l-1)^4(2l+3)^4(2l+5)\Big) + O(r^{10}), \\
H_{ll+4} &= -\frac{\gamma^4 r^6}{4}\frac{\sqrt{(l+1)^2 - |m|^2}\sqrt{(l+2)^2 - |m|^2}\sqrt{(l+3)^2 - |m|^2}\sqrt{(l+4)^2 - |m|^2}}{\sqrt{2l+1}(2l+3)^2(2l+5)(2l+7)^2\sqrt{2l+9}} + O(r^{10}).
\end{aligned}
$$

This asymptotic behavior of the effective potentials allows us to use the above boundary conditions at $r \to 0$ to find regular and bound solutions.

At large r the asymptotic form of the matrix elements by inverse power of r (i.e., without exponential terms) is of the form

$$
\begin{aligned}
&r^{-2}E_n(r) = E_n^{(0)} + r^{-2}E_n^{(2)} + r^{-4}E_n^{(4)} + r^{-6}E_n^{(6)} + r^{-8}E_n^{(8)} + \dots, \qquad (30) \\
&Q_{n_l,n_r}(r) = r^{-1}Q^{(1)}_{n_l,n_r} + r^{-3}Q^{(3)}_{n_l,n_r} + r^{-5}Q^{(5)}_{n_l,n_r} + \dots, \quad H_{n_l,n_r}(r) = r^{-2}H^{(2)}_{n_l,n_r} + r^{-4}H^{(4)}_{n_l,n_r} + r^{-6}H^{(6)}_{n_l,n_r} + \dots.
\end{aligned}
$$

In these formulas the asymptotic quantum numbers n_l, n_r denote the transversal quantum numbers N_ρ, N'_ρ that are connected with the unified numbers j, j' by the above mentioned formulas $n_l = j - 1$, $n_r = j' - 1$. Below we display the matrix elements with $m = 0$; Q is an antisymmetric matrix with the elements

$$
\begin{aligned}
Q^{(1)}_{n_l,n_r} &= (n_l+1)\delta_{n_l+1,n_r} - (n_r+1)\delta_{n_l,n_r+1}, \\
Q^{(3)}_{n_l,n_r} &= (n_l+1)(n_l+2)\delta_{n_l+2,n_r}/(2\gamma) - (n_r+1)(n_r+2)\delta_{n_l,n_r+2}/(2\gamma) \\
&\quad + (n_l+1)^2\delta_{n_l+1,n_r}/\gamma - (n_r+1)^2\delta_{n_l,n_r+1}/\gamma, \\
Q^{(5)}_{n_l,n_r} &= (n_l+1)(n_l+2)(n_l+3)\delta_{n_l+3,n_r}/(4\gamma^2) - (n_r+1)(n_r+2)(n_r+3)\delta_{n_l,n_r+3}/(4\gamma^2) \\
&\quad + (n_l+1)(n_l+2)(2n_l+3)\delta_{n_l+2,n_r}/(\gamma^2) - (n_r+1)(n_r+2)(2n_r+3)\delta_{n_l,n_r+2}/(\gamma^2) \\
&\quad + (n_l+1)(13n_l^2 + 26n_l + 12)\delta_{n_l+1,n_r}/(4\gamma^2) - (n_r+1)(13n_r^2 + 26n_r + 12)\delta_{n_l,n_r+1}/(4\gamma^2),
\end{aligned}
$$

H is a symmetric matrix with the elements

$$
H^{(2)}_{n_l,n_r} = -(n_l+1)(n_l+2)\delta_{n_l+2,n_r} - (n_r+1)(n_r+2)\delta_{n_l,n_r+2} + (2n_r^2 + 2n_r + 1)\delta_{n_l,n_r},
$$

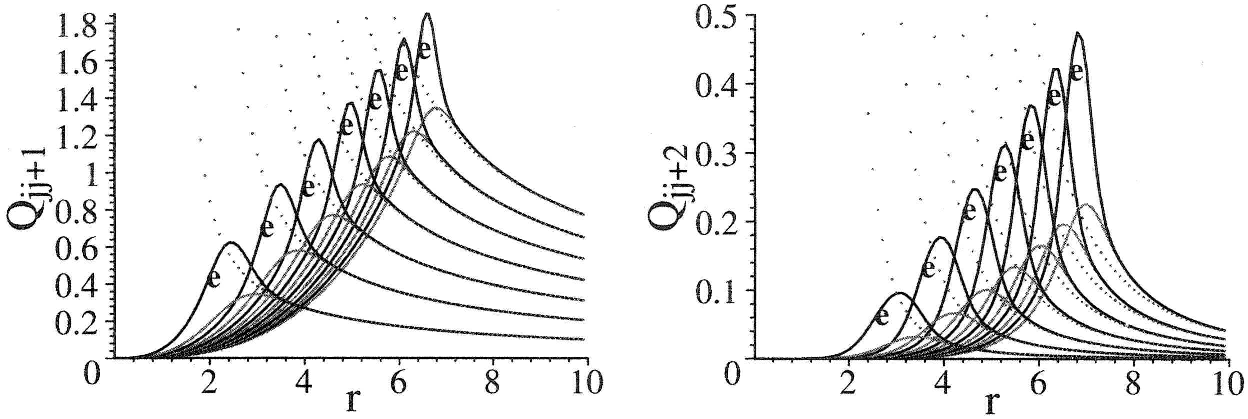

Figure 2. Some radial potentials Q_{ij} for even (marked by symbol "e") and odd parity at $m = 0$ and $\gamma = 1$. The dotted lines are asymptotic potentials at large r.

$$
\begin{aligned}
H^{(4)}_{n_l,n_r} &= -(n_l+1)(n_l+2)(n_l+3)\delta_{n_l+3,n_r}/\gamma - (n_r+1)(n_r+2)(n_r+3)\delta_{n_l,n_r+3}/\gamma \\
&\quad -(n_l+1)(n_l+2)(2n_l+3)\delta_{n_l+2,n_r}/\gamma - (n_r+1)(n_r+2)(2n_r+3)\delta_{n_l,n_r+2}/\gamma \\
&\quad +(n_l+1)(n_l^2+2n_l+2)\delta_{n_l+1,n_r}/\gamma + (n_r+1)(n_r^2+2n_r+2)\delta_{n_l,n_r+1}/\gamma \\
&\quad +2(2n_r+1)(n_r^2+n_r+1)\delta_{n_l,n_r}/\gamma, \\
H^{(6)}_{n_l,n_r} &= -3(n_l+1)(n_l+2)(n_l+3)(n_l+4)\delta_{n_l+4,n_r}/(4\gamma^2) - 3(n_r+1)(n_r+2)(n_r+3)(n_r+4)\delta_{n_l,n_r+4}/(4\gamma^2) \\
&\quad -(n_l+1)(n_l+2)^2(n_l+3)\delta_{n_l+3,n_r}/(\gamma^2) - (n_r+1)(n_r+2)^2(n_r+3)\delta_{n_l,n_r+3}/(\gamma^2) \\
&\quad -(n_l+1)(n_l+2)(14n_l^2+42n_l+31)\delta_{n_l+2,n_r}/(2\gamma^2) - (n_r+1)(n_r+2)(14n_r^2+42n_r+31)\delta_{n_l,n_r+2}/(2\gamma^2) \\
&\quad +(n_l+1)^2(5n_l^2+10n_l+16)\delta_{n_l+1,n_r}/(\gamma^2) + (n_r+1)^2(5n_r^2+10n_r+16)\delta_{n_l,n_r+1}/(\gamma^2) \\
&\quad +(31n_r^4+62n_r^3+95n_r^2+64n_r+16)\delta_{n_l,n_r}/(2\gamma^2),
\end{aligned}
$$

E corresponds to the diagonal matrix of potential curves, i.e., the eigenvalue of the parametric problem

$$
\begin{aligned}
E^{(0)}_n &= \gamma(2n+1), \\
E^{(2)}_n &= -2n^2-2n-1, \\
E^{(4)}_n &= \gamma^{-1}(-2n^3-3n^2-2n-1/2), \\
E^{(6)}_n &= \gamma^{-2}(-5n^4-10n^3-10n^2-5n-1), \\
E^{(8)}_n &= \gamma^{-3}(-42n^2-23/8-17n-165n^4/4-111n^3/2-33n^5/2).
\end{aligned}
$$

Note, that at large r $E^{(2)}_j + H^{(2)}_{jj} = 0$, i.e., the centrifugal terms are eliminated and the radial solution has the asymptotic form corresponding to zero angular momentum radial solutions, or to the one-dimensional problem on a semi-axis :

$$\chi_{ji_o}(r) = \frac{1}{r\sqrt{p_{i_o}}}\exp(\imath p_{i_o} r + \imath\,\alpha \ln r)\phi_{ji_o}(r), \quad \phi_{ji_o}(r) = \sum\nolimits_{k=0}^{k_{max}} \phi^{(k)}_{ji_o} r^{-k}. \tag{31}$$

As a result of substituting the expansion (31) into (29) and equating the coefficients of expansion for the same powers of r we arrive at the set of recurrence relations with respect to unknown coefficients $\phi^{(k)}_{ji_o}$, $j, i_o = 1, \ldots, j_{max}$. The first four coefficients have the form

$$
\begin{aligned}
&(p^2_{i_o} - 2E + E^{(0)}_{i_o})\phi^{(0)}_{i_oi_o} = 0, \qquad (p^2_{i_o} - 2E + E^{(0)}_{j_0})\phi^{(0)}_{j_0i_o} = 0, \\
&(p^2_{i_o} - 2E + E^{(0)}_{i_o})\phi^{(1)}_{i_oi_o} + (2p_{i_o}\alpha - 2Z)\phi^{(0)}_{i_oi_o} = -2\imath p_{i_o}\sum\nolimits_{j_0} Q^{(1)}_{i_oj_0}\phi^{(0)}_{j_0i_o},
\end{aligned}
$$

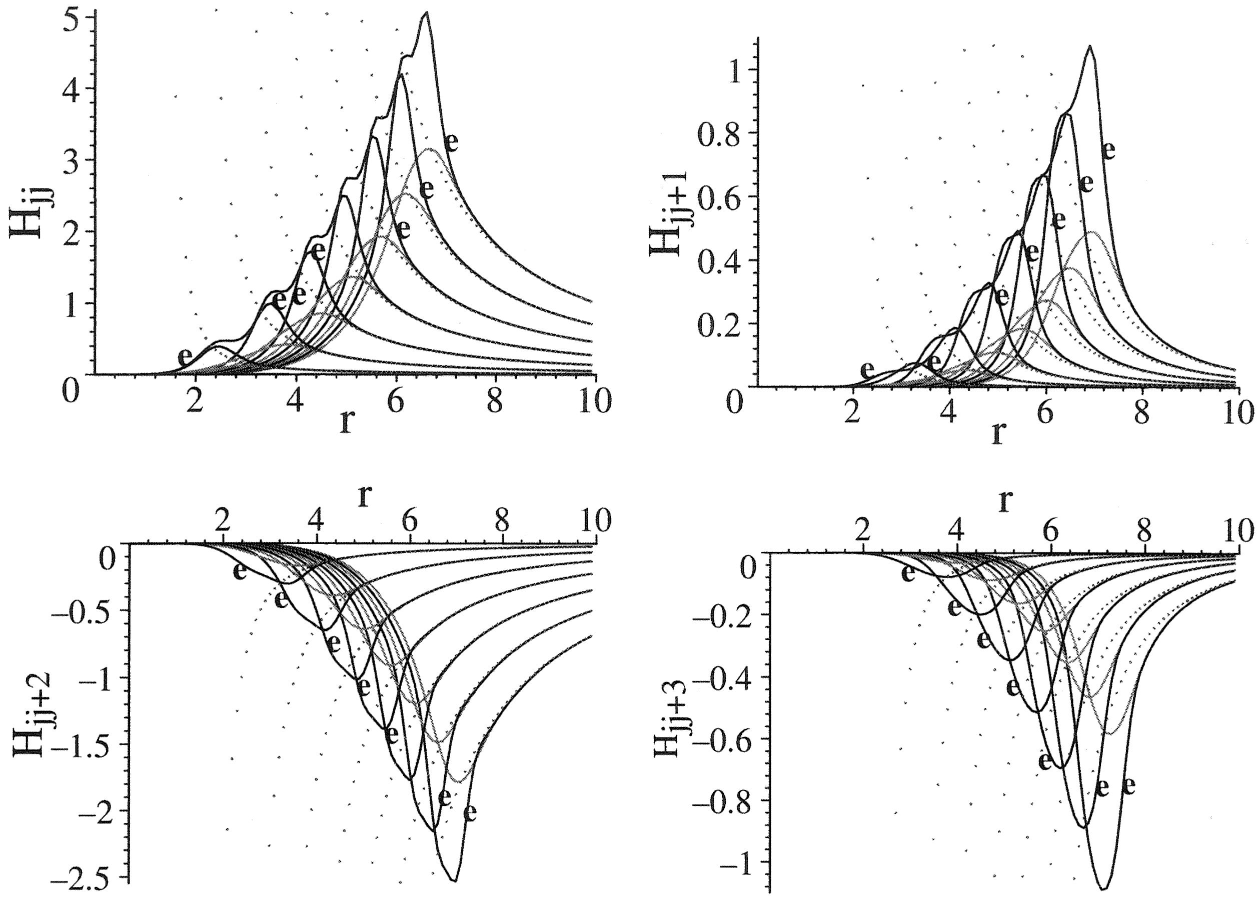

Figure 3. Some potentials H_{ij} for even (marked by the symbol "e") and odd parity at $m = 0$ and $\gamma = 1$. The dotted lines are asymptotic potentials at large r.

$$
\begin{aligned}
&(p_{i_o}^2 - 2E + E_{j_1}^{(0)})\phi^{(1)}_{j_1 i_o} + (2p_{i_o}\alpha - 2Z)\phi^{(0)}_{j_1 i_o} = -2\imath\, p_{i_o} Q^{(1)}_{j_1 i_o}\phi^{(0)}_{i_o i_o} - 2\imath\, p_{i_o}\sum\nolimits_{j_0} Q^{(1)}_{j_1 j_0}\phi^{(0)}_{j_0 i_o}, \\
&(p_{i_o}^2 - 2E + E_{i_o}^{(0)})\phi^{(2)}_{i_o i_o} + (2p_{i_o}\alpha - 2Z + 2\imath\, p_{i_o})\phi^{(1)}_{i_o i_o} + (\imath\,\alpha + \alpha^2)\phi^{(0)}_{i_o i_o} \\
&= -2\imath\, p_{i_o}\sum\nolimits_{j_1} Q^{(1)}_{i_o j_1}\phi^{(1)}_{j_1 i_o} + \sum\nolimits_{j_1}(Q^{(1)}_{i_o j_1}(1 - 2\imath\,\alpha) - H^{(2)}_{i_o j_1})\phi^{(0)}_{j_1 i_o}, \\
&(p_{i_o}^2 - 2E + E_{j_2 j_2}^{(0)})\phi^{(2)}_{j_2 i_o} + (2p_{i_o}\alpha - 2Z + 2\imath\, p_{i_o})\phi^{(1)}_{j_2 i_o} + (\imath\,\alpha + \alpha^2)\phi^{(0)}_{j_2 i_o} = -2\imath\, p_{i_o} Q^{(1)}_{j_2 i_o}\phi^{(1)}_{i_o i_o} \\
&+(Q^{(1)}_{j_2 i_o}(1 - 2\imath\,\alpha) - H^{(2)}_{j_2 i_o})\phi^{(0)}_{i_o i_o} - 2\imath\, p_{i_o}\sum\nolimits_{j_1} Q^{(1)}_{j_2 j_1}\phi^{(1)}_{j_1 i_o} + \sum\nolimits_{j_1}(Q^{(1)}_{j_2 j_1}(1 - 2\imath\,\alpha) - H^{(2)}_{j_2 j_1})\phi^{(0)}_{j_1 i_o}, \ldots.
\end{aligned}
\tag{32}
$$

Here $j_k, k = 0, 1, 2, ..., k_{max}$ take integer values, except i_o, $(j_k = 1, 2, ..., j_{max}, j_k \neq i_o)$. In the summation we put also $j_k \neq j_{k+1}$. From the first three equations of the set (32) we get the leading terms of the eigenfunction, the eigenvalue and the characteristic parameter, i.e., the initial data for solving the recurrence sequence,

$$\phi^{(0)}_{j_0 i_o} = \delta_{j_0 i_o}, \quad p_{i_o}^2 = 2E - E_{i_o}^{(0)} \to p_{i_o} = \pm\sqrt{2E - E_{i_o}^{(0)}}, \quad \alpha = Z/p_{i_o}.$$

Substituting these initial data into the next equations of the set (32), we get a step-by-step procedure for determining the series coefficients $\phi^{(k)}_{j i_o}$

$$\phi^{(1)}_{j_1 i_o} = \frac{2\imath\, p_{i_o} Q^{(1)}_{j_1 i_o}}{E^{(0)}_{i_o} - E^{(0)}_{j_1}}, \qquad \phi^{(1)}_{i_o i_o} = -\sum_{j_1} Q^{(1)}_{i_o j_1}\phi^{(1)}_{j_1 i_o} + \frac{\imath\,(Z^2 + Z p_{i_o}\imath\,)}{2p^3_{i_o}}, \tag{33}$$

$$\phi^{(2)}_{j_2 i_o} = \frac{2\imath\, p_{i_o} Q^{(1)}_{j_2 i_o}\phi^{(1)}_{i_o i_o}}{E^{(0)}_{i_o} - E^{(0)}_{j_2}} + \frac{2\imath\, p_{i_o}\sum_{j_1} Q^{(1)}_{j_2 j_1}\phi^{(1)}_{j_1 i_o}}{E^{(0)}_{i_o} - E^{(0)}_{j_2}} + \frac{2\imath\, p_{i_o}\phi^{(1)}_{j_2 i_o}}{E^{(0)}_{i_o} - E^{(0)}_{j_2}} + \frac{\imath\,(-\imath\, H^{(2)}_{j_2 i_o} p_{i_o} + 2ZQ^{(1)}_{j_2 i_o} + \imath\, Q^{(1)}_{j_2 i_o} p_{i_o})}{2p_{i_o}(E^{(0)}_{i_o} - E^{(0)}_{j_2})},$$

$$\phi^{(2)}_{i_o i_o} = \imath\,(Z^2 + 3\imath\, Z p_{i_o} - 2p^2_{i_o})\frac{\phi^{(1)}_{i_o i_o}}{(4p^3_{i_o})} - \sum_{j_2}(2ZQ^{(1)}_{i_o j_2} + 3\imath\, Q^{(1)}_{i_o j_2} p_{i_o} - \imath H^{(2)}_{i_o j_2} p_{i_o})\frac{\phi^{(1)}_{j_2 i_o}}{(4p^2_{i_o})} - \sum_{j_2} Q^{(1)}_{i_o j_2}\phi^{(2)}_{j_2 i_o}/2, \ldots$$

Substituting the explicit asymptotic form of the matrix elements (30) into (33), we get the explicit expression of these coefficients $\phi^{(k)}_{j i_o}$ via the values of the number of a state (or channel) $i_o = n_o + 1$ and the number of current equation $j = 1, ..., j_{max}$. Note, that if $j_{max} \geq i_o + k$, then all nonzero terms in the above sums of Eqs. (33) should be included into the evaluation of each nonzero element $\phi^{(k)}_{j i_o}$ of the order k. For example, at $j_{max} \geq i_o + k$ and $k = 0, 1, 2$ such elements take the form

$$\begin{aligned}
\phi^{(0)}_{n_o n_o} &= 1,\\
\phi^{(1)}_{n_o-1 n_o} &= \imath\,\frac{p_{n_o} n_o}{\gamma},\\
\phi^{(1)}_{n_o n_o} &= \left[\imath\,\frac{Z^2}{2p^3_{n_o}} - \frac{Z}{2p^2_{n_o}}\right] - \imath\,\frac{p_{n_o}(2n_o+1)}{\gamma},\\
\phi^{(1)}_{n_o+1 n_o} &= \imath\,\frac{p_{n_o}(n_o+1)}{\gamma},\\
\phi^{(2)}_{n_o-2 n_o} &= -\frac{n_o(n_o-1)p^2_{n_o}}{2\gamma^2} - \frac{n_o(n_o-1)}{4\gamma},\\
\phi^{(2)}_{n_o-1 n_o} &= \imath\,\frac{Z n_o}{2p_{n_o}\gamma} + \frac{2p^2_{n_o} {n_o}^2}{\gamma^2} - \frac{n_o}{2\gamma} - \frac{n_o Z^2}{p^2_{n_o}\gamma},\\
\phi^{(2)}_{n_o n_o} &= \left[\imath\,\frac{Z}{4p^3_{n_o}} + \frac{5Z^2}{8p^4_{n_o}} - \imath\,\frac{Z^3}{2p^5_{n_o}} - \frac{Z^4}{8p^6_{n_o}}\right] + \frac{(2n_o+1)Z^2}{2p^2_{n_o}\gamma} - \frac{(3{n_o}^2+3n_o+1)p^2_{n_o}}{\gamma^2} + \frac{2n_o+1}{2\gamma},\\
\phi^{(2)}_{n_o+1 n_o} &= \imath\,\frac{Z(n_o+1)}{2p_{n_o}\gamma} + \frac{2p^2_{n_o}(n_o+1)^2}{\gamma^2} - \frac{n_o+1}{2\gamma} - \frac{(n_o+1)Z^2}{p^2_{n_o}\gamma},\\
\phi^{(2)}_{n_o+2 n_o} &= -\frac{(n_o+1)(n_o+2)p^2_{n_o}}{2\gamma^2} - \frac{(n_o+1)(n_o+2)}{4\gamma}.
\end{aligned} \tag{34}$$

The solution of the scattering problem with $N_\rho + 1$ open channels for $p^2_{i_o} \geq 0$ at $i_o = 1, ..., N_\rho + 1$, and with remaining closed channels for $p^2_{i_c} < 0$ at $i_c = N_\rho + 2, ..., j_{max}$, is defined by two independent fundamental asymptotic solutions $\boldsymbol{\chi}^*$, $\boldsymbol{\chi}$ (corresponding to the signs '−', '+' of $\exp(\mp\imath p_{i_o})$) of Eqs. (29) and the scattering matrix $\mathbf{S}$

$$\chi^{(ph)}_{j i_o} = -(2\imath\,)^{-1}\left(\chi^*_{j i_o} - \sum_{j'=1}^{N_\rho+1}\chi_{j,j'}S_{j' i_o}\right), \quad i_o = 1, ..., N_\rho + 1, \quad j = 1, ..., j_{max},$$

It is defined also by two independent fundamental asymptotic solutions $\boldsymbol{\chi}^s(r) = \Im(\boldsymbol{\chi})$, $\boldsymbol{\chi}^c(r) = \Re(\boldsymbol{\chi})$ (corresponding to 'sine', 'cosine') of Eqs (29) and the reaction matrix $\mathbf{R}$

$$\boldsymbol{\chi}^{(p)} = \boldsymbol{\chi}^{(ph)}(\mathbf{I} - \imath\,\mathbf{R}), \quad \mathbf{S} = (\mathbf{I} + \imath\,\mathbf{R})(\mathbf{I} - \imath\,\mathbf{R})^{-1}, \quad \boldsymbol{\chi} = \boldsymbol{\chi}^s + \boldsymbol{\chi}^c\mathbf{R}.$$

Using the formula (28), we obtain the expression of the reaction matrix $\mathbf{R}$ via the above calculated matrix $\mathbf{P}$:

$$\left(\mathbf{P}\boldsymbol{\chi}^c(r_{\max}) - \frac{d\boldsymbol{\chi}^c(r_{\max})}{dr}\right)\mathbf{R} = \left(\frac{d\boldsymbol{\chi}^s(r_{\max})}{dr} - \mathbf{P}\boldsymbol{\chi}^s(r_{\max})\right). \tag{35}$$

Note, that for the general case the left and right matrices of (35) are rectangular matrices. Therefore, multiplying (35) from the left by the matrix

$$\left(\boldsymbol{\chi}^s(r_{\max}) + \frac{d\boldsymbol{\chi}^s(r_{\max})}{dr}\right)^T \neq 0,$$

we obtain the following formula for the reaction matrix: **R**

$$\mathbf{R} = \mathbf{O}^{-1}\mathbf{Y}, \tag{36}$$

where

$$\mathbf{O} = \left(\boldsymbol{\chi}^s(r_{\max}) + \frac{d\boldsymbol{\chi}^s(r_{\max})}{dr}\right)^T \left(\mathbf{P}\boldsymbol{\chi}^c(r_{\max}) - \frac{d\boldsymbol{\chi}^c(r_{\max})}{dr}\right),$$

$$\mathbf{Y} = \left(\boldsymbol{\chi}^s(r_{\max}) + \frac{d\boldsymbol{\chi}^s(r_{\max})}{dr}\right)^T \left(\frac{d\boldsymbol{\chi}^s(r_{\max})}{dr} - \mathbf{P}\boldsymbol{\chi}^s(r_{\max})\right),$$

are square matrices of the dimension $(N_\rho + 1) \times (N_\rho + 1)$.

In terms of the above definitions the ionization cross-section is given by the formula

$$\sigma_\omega = \frac{4\pi^2}{c}\omega \sum\nolimits_{N_\rho} \left|\left\langle \Psi_{E,N_\rho,\sigma,m} \left| r\cos\theta \right| \Psi_{N_z=0,N_\rho=0,\sigma=1,m=0} \right\rangle\right|^2,$$

$$\left\langle \Psi_{E,N_\rho,\sigma,m} \left| r\cos\theta \right| \Psi_{N_z=0,N_\rho=0,\sigma=1,m=0} \right\rangle$$

$$= \sum_{j,j'=1}^{j_{max}} \int_0^{r_{max}} r^2 dr \chi_{ji}(E, N_\rho, \sigma = -1, m = 0) \langle j \left| r\cos\theta \right| j' \rangle \chi_{j'i}(N_z = 0, N_\rho = 0, \sigma = 1, m = 0)$$

where $\omega = E - E(N_z = 0, N_\rho = 0, \sigma = 1, m = 0)$ is the frequency of radiation, $E(N_z = 0, N_\rho = 0, \sigma = 1, m = 0)$ is the energy of the initial bound state $\Psi_{N_z=0,N_\rho=0,\sigma=1,m=0}$, and $\Psi_{E,N_\rho,\sigma,m}$ is the continuum function with the energy $2E$ (of the ejected electron) above the first threshold ($N_\rho = 0$, $\sigma = -1$), $\epsilon^{th}_{m\sigma j}(\gamma) = \gamma$ or the second threshold ($N_\rho = 1$, $\sigma = -1$), $\epsilon^{th}_{m\sigma j}(\gamma) = 3\gamma$. Note, that the continuum spectrum is beginning with $2E \geq \gamma = 0.1$; till the second threshold, $\gamma \leq 2E < 3\gamma$ we have only one open channel ($N_\rho = 0$), while between the second and the third thresholds, i.e., $3\gamma \leq 2E < 5\gamma$, we have two open channels ($N_\rho = 0$ and $N_\rho = 1$).

5. THE EFFECTIVE APPROXIMATION FOR KANTOROVICH METHOD (KM)

To obtain the effective approximation for the KM, we consider the system of close-coupled radial equations (20) and neglect the coupling of the states $|j>$ and $|j\prime>$ not connected with the open channel $|0>$. This can be useful for sufficiently large effective charge $\hat{Z} = Z/\sqrt{\gamma}$, when the contribution of the adiabatic correction is sufficiently small. It is useful from physical viewpoint to understand the asymptotic boundary conditions in the open channel. We introduce the so-called effective adiabatic approximation (EAA), in which we project these equations onto the open channel $|i>=|0>$ by means of a canonical transformation. The new solution $\chi^{new}_{ii} \equiv \chi^{new}_{ii}(r)$ is connected with the old solutions $\chi_{ji} \equiv \chi_{ji}(r)$ of the system (20) by the relation

$$\chi^{new}_{ii} = \sum\nolimits_j T_{ij}\chi_j \approx \sum\nolimits_{j,j\prime=1}^{j_{max}} < i \mid e^{\imath S^{(2)}} \mid j\prime >< j\prime \mid e^{\imath S^{(1)}} \mid j > \chi_{ji}, \tag{37}$$

Restricting the expansions of the exponents to the second order, i.e., expressing $\exp(iS^{(1)}) \approx 1 + \imath S^{(1)} + (\imath S^{(1)})^2/2$ and $\exp(iS^{(2)}) \approx 1 + \imath S^{(2)}$, we define the non-diagonal matrix elements of the generator $S^{(1)}$ and $S^{(2)}$ in such a way

$$\imath S^{(1)}_{ij} = (1 - \delta_{ij})\Delta^{-1}_{ij}\left(H_{ij} + Q_{ij}\frac{d}{dr} + \frac{1}{r^2}\frac{d}{dr}r^2 Q_{ij}\right), \tag{38}$$

$$\imath S^{(2)}_{ij} = (1 - \delta_{ij})2\Delta^{-2}_{ij}Q_{ij}V_{jj}{}', \quad \Delta_{ij} = \Delta_{ij}(r) = V_{ii} - V_{jj},$$

that the right-hand side of Eq. (20) is eliminated up to the accuracy of the order of $O(\max_{ij}|\Delta^{-3}_{ij})$, and determine the inverse operator for the open channel $|\,0\,\rangle$

$$\chi_j = T^{-1}_{j0}\chi^{new}_0, \quad \chi^{new}_0 = \sum_j T_{0j}\chi_j, \qquad \langle\, 0\,|\,T\,|\,0\,\rangle = \langle\, 0\,|\,T^{-1}\,|\,0\,\rangle = 1 = \langle\, 0\,|\,0\,\rangle. \tag{39}$$

This leads to a projection of the above system of equations onto the channel $|0\rangle$

$$\sum_{ij} T_{0i}(H^{old}-2E)_{ij}T^{-1}_{j0}\chi^{new}_0 = (H^{new}_{00}-2E)\chi^{new}_0 = 0,$$

$$-\frac{1}{r^2}\frac{d}{dr}\frac{r^2}{\mu(r)}\frac{d\chi^{new}_0(r)}{dr} + \frac{\mu'(r)}{\mu^2(r)r}\chi^{new}_0(r) + [\hat{U}_{eff}-2E]\chi^{new}_0(r) = 0. \tag{40}$$

The new solution $\psi \equiv \mu^{-1/2}\chi^{new}_{ii}(r)$ in such a diagonal representation satisfies the following equation

$$-\frac{1}{r^2}(r^2\psi')' + \mu^{1/2}(\mu^{-1/2})''\psi + \mu[\hat{U}_{ad}+\delta U-2E]\psi = 0, \qquad \lim_{r\to 0} r^2\frac{d\psi}{dr} = 0. \tag{41}$$

where the modified scalar product and adiabatic potential are defined by

$$<\psi|\psi> = \int_0^\infty dr r^2\mu\psi\psi, \qquad \hat{U}_{ad} = V_{ii} = \frac{U_{ii}}{r^2}.$$

The effective potential $\hat{U}_{eff}(r)$ is defined as a sum of the adiabatic potential $\hat{U}_{ad}(r)$ and the *effective nonadiabatic correction* $\delta U(r)$, $\mu(r)$ can be regarded as an *effective mass*, defined as the inverse of the sum of unity and the effective mass correction $W_{ii}(r)$:

$$\mu^{-1}(r) = 1 + W_{ii}(r), \quad W_{ii}(r) = -4\sum\nolimits_{j\neq i}^{j_{max}} Q_{ij}(r)Q_{ji}(r)\Delta^{-1}_{ij}(r),$$

$$\delta U(r) = \sum\nolimits_{j\neq i}^{j_{max}} (\Delta^{-1}_{ij}V^{(1)}_{ij} + \Delta^{-2}_{ij}V^{(2)}_{ij} + \Delta^{-3}_{ij}V^{(3)}_{ij}). \tag{42}$$

Here we use the expressions

$$V^{(1)}_{ij} = \sum\nolimits_{s=1}^{4} V^{(1,s)}_{ij} = H^2_{ij} - (Q'_{ij})^2 + 2Q_{ij}H'_{ij} - 2Q_{ij}Q''_{ij},$$

$$V^{(2)}_{ij} = \sum\nolimits_{s=1}^{3} V^{(2,s)}_{ij} = H_{ij}Q_{ij}(\Sigma'_{ij}-\Delta'_{ij}) + Q_{ij}Q'_{ij}(\Sigma'_{ij}+3\Delta'_{ij}) + Q^2_{ij}(\Sigma''_{ij}+\Delta''_{ij}),$$

$$V^{(3)}_{ij} = Q^2_{ij}(\Sigma'_{ij}+\Delta'_{ij})(\Sigma'_{ij}-2\Delta'_{ij}), \qquad \Delta_{ij} = \Delta_{ij}(r) = V_{ii}-V_{jj}, \qquad \Sigma_{ij} = \Sigma_{ij}(r) = V_{ii}+V_{jj}.$$

In the above formulas all the terms are functions of r, and the symbol "$'$" denotes a derivative with respect to r. At large r the leading terms of $W_{ii}(r)$ and $\delta U(r)$ calculated using the asymptotic basis functions read as $W_{ii}(r) = W^{as}_{ii}/r^2 + O(1/r^4)$, $\delta U(r) = \delta U^{as}/r^4 + O(1/r^6)$, where $-W^{as}_{ii} =< i|\rho^2|i >= 4(n+1/2)/\gamma$ is the mean value of the transversal variable, $\rho^2 = (r\sin\theta)^2$, characterizing the electron precession around the z axis in the magnetic field γ, while $\delta U^{as} = -1/2(4n^3+5n^2-4n-3)/\gamma$ is the asymptotic value of the electron polarizability.

6. THE EFFECTIVE APPROXIMATION: ASYMPTOTIC BEHAVIOR OF RADIAL SOLUTIONS

For the elastic scattering states with given value $2E(q) = q^2 + \epsilon^{(0)}_0$ we rewrite the problem in the form

$$(\hat{H}_{eff}-q^2)\psi \equiv -\frac{1}{r^2}(r^2\psi')' + \mu^{1/2}(\mu^{-1/2})''\psi + \mu[\hat{U}_{eff}-2E(q)]\psi = 0. \tag{43}$$

For the function $\chi^{eff} = r(\mu)^{1/2}\psi$ this equation has a conventional form

$$\left(\frac{d}{dr}\mu^{-1}(r)\frac{d}{dr} - U_{eff}(r) + q^2\right)\chi^{eff}_{00}(r) = 0, \tag{44}$$

where the effective potential $U_{eff}(r)$ is defined by

$$U_{eff}(r) = V_{00}(r) + \delta U(r) - \frac{2Z}{r} - \epsilon^{(0)}_0. \tag{45}$$

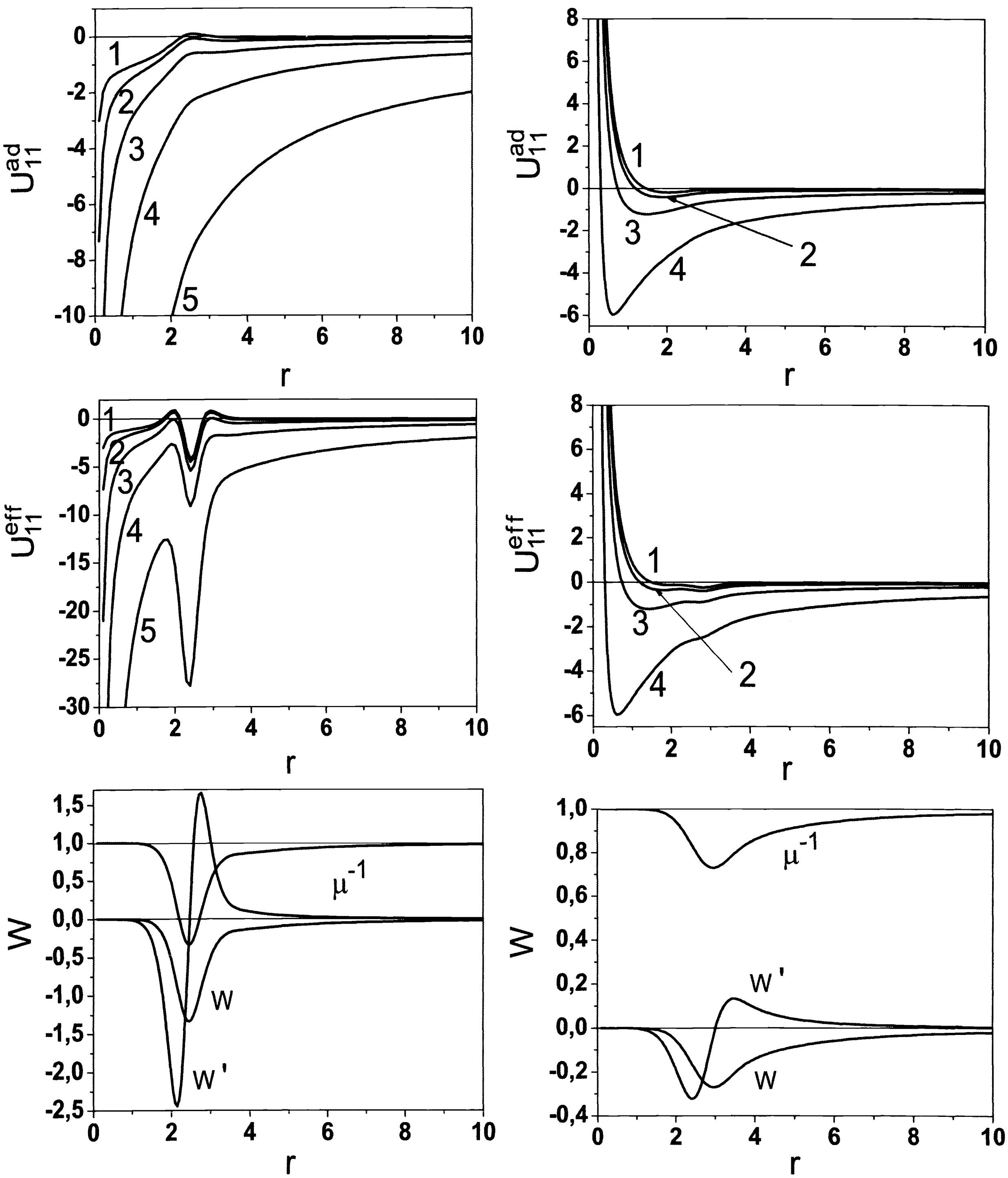

Figure 4. The adiabatic potential $\hat{U}_{ad}(r)$ and the effective adiabatic potential $\hat{U}_{eff}(r)$ for a set of curves 1, 2, 3, 4, 5 for $\gamma = 100,\ 10,\ 1,\ 0.1,\ 0.01$, $m = 0$, in cyclotron frequency units ($\hat{Z} = Z/\sqrt{\gamma}$, $\hat{r} = r/\sqrt{\gamma}$, $\hat{\epsilon} = \epsilon/\gamma$). The effective mass correction W_{11}, its derivative W'_{11} and inverse effective mass μ^{-1} at $\gamma = 1$ for first even (left panel) and odd(right panel) states.

For large values of r, using the asymptotic values $W_{00}^{(j_{max})}$ of $r^2 W(r)$ and $\delta U_{00}^{(j_{max})}$ of $r^4 \delta U(r)$ from (42) it is reduced to the following one:

$$\left(-\frac{d}{dr}\left(1+\frac{W_{00}^{(j_{max})}}{r^2}\right)\frac{d}{dr}-\frac{2Z}{r}+\frac{\delta U_{00}^{(j_{max})}}{r^4}-q^2\right)\bar{\chi}_{00}^{as}(r)=0, \tag{46}$$

and to an accuracy of the order $O(r^{-4})$, Eq. (44) reads

$$\left[\frac{d^2}{dr^2}-\frac{2W_{00}^{(j_{max})}}{r^3}\frac{d}{dr}+\frac{2Z}{r}+q^2\left(1-\frac{W_{00}^{(j_{max})}}{r^2}\right)-\frac{\delta U_{00}^{(j_{max})}}{r^4}\right]\bar{\chi}_{00}^{as}(r)=0. \tag{47}$$

For $qW_{00}^{(N)}/(2r) \ll 1$ the continuous spectrum solutions can be expressed in the form

$$\begin{aligned}\bar{\chi}_{00}^{as}(r) &\sim \sin\left[qr\left(1-\frac{W_{00}^{(j_{max})}}{2r^2}\right)+\frac{Z}{q}\ln(2qr)+\delta^{j_{max})}\right]\\ &\approx \sin(qr+\frac{Z}{q}\ln(2qr)+\delta^c+\delta^{(j_{max})})-q\frac{W_{00}^{(j_{max})}}{2r}\cos(qr+\frac{Z}{q}\ln(2qr)+\delta^c+\delta^{(j_{max})}),\end{aligned} \tag{48}$$

where $\delta^{(j_{max})} \equiv \delta^{(j_{max})}(q)$ is the required phase shift of the elastic scattering in the open channel $|\,0\,\rangle$ derived from the known Coulomb phase shift $\delta^c = arg\Gamma(1-\frac{\imath Z}{q}))$.

Remembering that $r^2 = \rho^2 + z^2$ and $z \sim r(1-\rho^2/(2r^2))$ in the asymptotic region $\rho/r \ll 1$, one should introduce the following definition of the *mean position* operator in the new representation $\chi^{new} = T\chi$

$$r_{mean}^{new} = \langle\chi^{new}|\hat{r}_{mean}^{new}|\chi^{new}\rangle = \langle\chi|T^{-1}\hat{r}_{mean}^{new}T|\chi\rangle = \langle\chi|\hat{r}_{mean}|\chi\rangle = r_{mean}.$$

Here the *mean position* operator $\hat{r}_{mean}^{new} = r$ plays the role of the longitudinal coordinate z in the new representation χ^{new}, i.e., the delocalization of z is contained in the new radial functions $\chi^{new} = T\chi$. In the old representation χ the mean position operator $\hat{r}_{mean}$ is defined as

$$\hat{r}_{mean} = T^{-1}\hat{r}_{mean}^{new}T = T^{-1}rT = r + \delta\hat{r},$$

where $\delta\hat{r}$ is the delocalization of the longitudinal coordinate z, which in the asymptotic region $\rho/r \ll 1$ has the order of $\rho^2/(2r)$, i.e.,

$$\hat{r}_{mean} \to T^{-1}rT \approx \langle z\rangle.$$

Note, that the transformation changes only the form of the radial solutions, and the longitudinal coordinate z is restored only in the total expansion of the wave function. If we omit the non-adiabatic terms, the solution exibits the adiabatic behavior

$$\chi^{ad} \sim \sin(qr+\delta^{ad}),$$

then we can look for the obvious difference between the true phase shift δ, the j_{max}-th approximation $\delta^{(j_{max})}$ and the adiabatic phase shift δ^{ad},

$$\delta^{(j_{max})} = \delta^{ad} - q\frac{W_{00}^{(j_{max})}}{2r}, \quad \delta = \lim_{j_{max}\to\infty}\delta^{(j_{max})} = \delta^{ad} + q\frac{\langle 0|\rho^2|0\rangle}{2r}. \tag{49}$$

7. NUMERICAL RESULTS

In this section we present our numerical results for the energy spectrum of a hydrogen atom in the magnetic field. Ten eigensolutions ($n_{max} = 10$) of the problem (12)–(15) are calculated which amounts to solving ten equations of the system (20). The problem (12)–(15) was solved also using the conventional expansion[11] of regular and

Table 2. Convergence of the method for the energy $E(N=9, N_r=0,2,4,6,8,\ m=0,\ \sigma=+1)$ (in a.u.) of even states with the number of coupled channels $n_{max}=8$, $\gamma=1.472\times10^{-5}$ and the shift=0.0112.

N_r	$n_{max}=2$	$n_{max}=4$	$n_{max}=6$	$n_{max}=8$
0	-0.00781242971347	-0.00617279526323	-0.00617279808777	-0.00617279808777
2	-0.00781225974455	-0.00617270287945	-0.00617274784933	-0.00617274784933
4	-0.00617272642538	-0.00617258450255	-0.00617268955914	-0.00617268955914
6	-0.00617245301145	-0.00617243588598	-0.00617258283911	-0.00617258283911
8	-0.00499982705326	-0.00499993540325	-0.00617243586258	-0.00617243586258

Table 3. Convergence of the method for the energy $E(N=9, N_r=1,3,5,7,\ m=0,\ \sigma=-1)$ (in a.u.) of odd states with the number of coupled channels $n_{max}=8$, $\gamma=1.472\times10^{-5}$ and the shift=0.0112.

N_r	$n_{max}=2$	$n_{max}=4$	$n_{max}=6$	$n_{max}=8$
1	-0.00617276008813	-0.00617279765740	-0.00617279765755	-0.00617279765755
3	-0.00617254499872	-0.00617272898894	-0.00617272898991	-0.00617272898992
5	-0.00499987886194	-0.00617264137929	-0.00617264137970	-0.00617264137970
7	-0.00499954507256	-0.00617251430932	-0.00617251430935	-0.00617251430935

bound solutions of Eq. (17). The results coincide with the calculations by FEM[4] with ten digits. In Figs. 1, 2 and 3 the numerical values of the effective potentials are compared with their asymptotic values.

The finite-element grid of r has been chosen as follows : 0 (100) 3 (70) 20 (80) 100 (the number in parentheses denotes the number of finite elements of the order $k=4$ in each interval). This grid is composed of 999 nodes. The maximum number of unknowns of the system (20) ($n_{max}=10$) is 9990. The calculated energy values and the rate of convergence of the method versus the number of basis functions for $n=9$, $m=0$ and $\gamma=1.472\times10^{-5}$ are shown in Tables 2-3. The probability density isolines of the Zeeman wave states $|N,\nu,m\rangle$ with even parity $\sigma=+1$ in a homogeneous magnetic field are shown in Fig. 5.

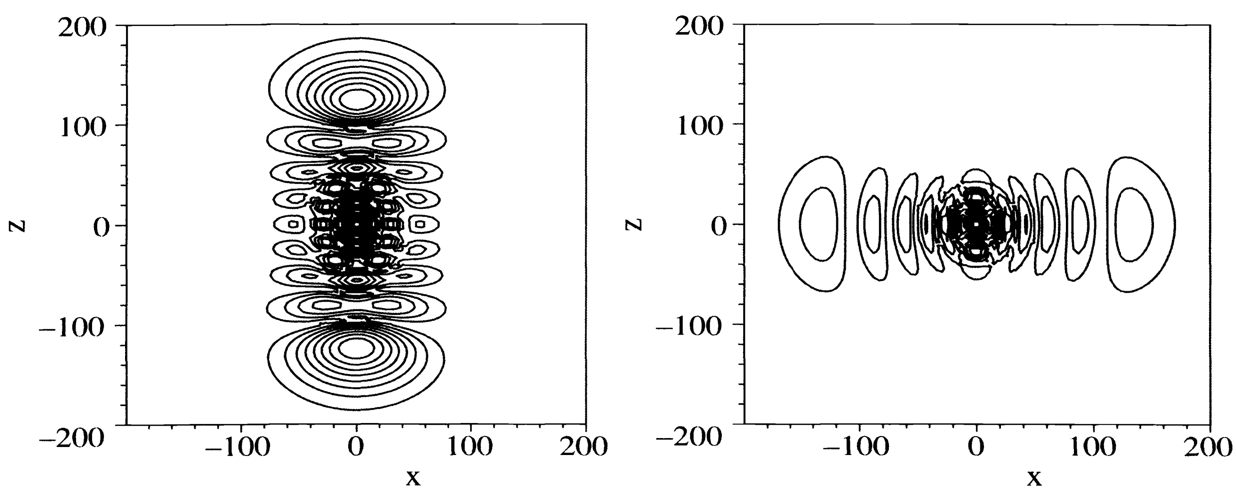

Figure 5. The probability density isolines of the Zeeman wave states $|N,\nu,m\rangle$ with even parity $\sigma=+1$ and $m=0$ in the homogeneous magnetic field for the minimal energy correction $|9,0,0\rangle$ and (rhs) (left panel) and the maximal energy correction $|9,8,0\rangle$ (right panel).

8. CONCLUSIONS

A new effective method of calculating the wave functions of a hydrogen atom in a strong magnetic field is developed basing 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 spectral parametric problem for a one-dimensional equation in the angular variable and a finite set of ordinary second-order differential equations in the radial variable. A canonical transformation is considered to approximate the finite set of radial equations by means of a new radial equation describing the open channel. The rate of convergence is examined numerically and the analysis is illustrated with a set of typical examples. The results are in good agreement with calculations by other authors. The developed approach yields a good tool for the calculations of threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps.

9. ACKNOWLEDGMENTS

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