A Symbolic-Numerical Algorithm for Solving the Eigenvalue Problem for a Hydrogen Atom in the Magnetic Field: Cylindrical Coordinates

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Abstract. The boundary problem in cylindrical coordinates for the Schrödinger equation describing a hydrogen-like atom in a strong homogeneous magnetic field is reduced to the problem for a set of the longitudinal equations in the framework of the Kantorovich method. The effective potentials of these equations are given by integrals over transversal variable of a product of transverse basis functions depending on the longitudinal variable as a parameter and their first derivatives with respect to the parameter. A symbolic-numerical algorithm for evaluating the transverse basis functions and corresponding eigenvalues which depend on the parameter, their derivatives with respect to the parameter and corresponded effective potentials is presented. The efficiency and accuracy of the algorithm and of the numerical scheme derived are confirmed by computations of eigenenergies and eigenfunctions for the low-excited states of a hydrogen atom in the strong homogeneous magnetic field.

1 Introduction

To solve the problem of photoionization of low-lying excited states of a hydrogen atom in a strong magnetic field [1,2] symbolic-numerical algorithms (SNA) and the Finite Element Method (FEM) code have been elaborated [3,4,5,6]. Next investigations are shown that to impose on boundary conditions for the scattering problem in spherical coordinates (r, θ, φ), one needs to consider solution of this problem in cylindrical coordinates (z, ρ, φ) and to construct an asymptotics of solutions for both small and large values of the longitudinal variable [2,7].

With this end in view we consider a SNA for evaluating the transverse basis functions and eigenvalues depending on a longitudinal parameter, $|z|$, for their derivatives with respect to the $|z|$ and for the effective potentials depended on $|z|$ of the 1-D problem for a set of second order differential equations in the frame of the Kantorovich method (KM) [8]. For solving the above problems on a grid of the longitudinal parameter, $|z|$, from a finite interval, we elaborate the SNA to reduce a transverse eigenvalue problem for a second order ordinary

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differential equation to algebraic one applied the FEM [9,10] or some expansions of the solution over an appropriate basis such that corresponded integrals over transversal variable will be calculated analytically [11,12]. A symbolic algorithm for evaluating the asymptotic effective potentials with respect to the $|z|$, using a series expansion in the Laguerre polynomials, is implemented in MAPLE and is used to continue the calculated numerical values of effective potentials to large values of $|z|$.

The main goal of this paper is to develop a symbolic algorithm for generation of algebraic eigenvalue problem to calculate economically the transverse basis on a grid points of finite interval of the longitudinal parameter, $|z|$, and its continuation from matching point to large $|z|$. The obtained asymptotic of effective potentials at large values of the longitudinal variable are used as input file for an auxiliary symbolic algorithm of evaluation in analytical form the asymptotics of solutions of a set of the second order differential equations with respect to the longitudinal variable, $|z|$, in the KM. The algorithms are explicitly presented and implemented in MAPLE. The developed approach is applied to numerical calculation of effective potentials for the Schrödinger equation describing a hydrogen-like atom in a strong magnetic field. A region of applicability versus a strength of the magnetic field, efficiency and accuracy of the developed algorithms and accompanying numerical schemes is confirmed by computation of eigenenergies and eigenfunctions of a hydrogen atom in the strong homogeneous magnetic field.

The paper is organized as follows. In section 2 we briefly describe a reduction of the 2D-eigenvalue problem to the 1D-eigenvalue problem for a set of the closed longitudinal equations by means of the KM. In section 3 algorithm of generation of an algebraic problem by means of the FEM. We examine the algorithm for evaluating the transverse basis functions on a grid of the longitudinal parameter from a finite interval. In section 4 the algorithm for asymptotic calculation of matrix elements at large values of the longitudinal variable is presented. In section 5 the auxiliary algorithm of evaluation the asymptotics of the longitude solutions at large $|z|$ in the KM. In section 6 the method is applied to calculating the low-lying states of a hydrogen atom in a strong magnetic field. The convergence rate is explicitly demonstrated for typical examples. The obtained results are compared with the known ones obtained in the spherical coordinates to establish of an applicability range of the method. In section 7 the conclusions are made, and the possible future applications of the method are discussed.

2 Statement of the Problem in Cylindrical Coordinates

The wave function $\hat{\Psi}(\rho, z, \varphi) = \Psi(\rho, z)\exp(\imath m\varphi)/\sqrt{2\pi}$ of a hydrogen atom in an axially symmetric magnetic field $\boldsymbol{B} = (0, 0, B)$ in cylindrical coordinates (ρ, z, φ) satisfies the 2D Schrödinger equation

$$-\frac{\partial^2}{\partial z^2}\Psi(\rho, z) + \hat{A}_c\Psi(\rho, z) = \epsilon\Psi(\rho, z), \tag{1}$$

$$\hat{A}_c = \hat{A}_c^{(0)} - \frac{2Z}{\sqrt{\rho^2 + z^2}}, \quad \hat{A}_c^{(0)} = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{m^2}{\rho^2} + m\gamma + \frac{\gamma^2\rho^2}{4},$$

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. Boundary conditions in each $m\sigma$ subspace of the full Hilbert space have the form

$$\lim_{\rho \to 0} \rho \frac{\partial \Psi(\rho, z)}{\partial \rho} = 0, \quad \text{for} \quad m = 0, \quad \text{and} \quad \Psi(0, z) = 0, \quad \text{for} \quad m \neq 0, \tag{2}$$

$$\lim_{\rho \to \infty} \Psi(\rho, z) = 0. \tag{3}$$

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

$$\lim_{z \to 0} \frac{\partial \Psi(\rho, z)}{\partial z} = 0, \quad \sigma = +1, \quad \Psi(\rho, 0) = 0, \quad \sigma = -1, \tag{4}$$

$$\lim_{z \to \pm\infty} \Psi(\rho, z) = 0 \quad \rightarrow \quad \Psi(\rho, \pm |z_{\max}|) = 0. \tag{5}$$

These functions satisfy the additional normalization condition

$$\int_{-z_{\max}}^{z_{\max}} \int_0^{\infty} |\Psi(\rho, z)|^2 \rho d\rho dz = 2 \int_0^{z_{\max}} \int_0^{\infty} |\Psi(\rho, z)|^2 \rho d\rho dz = 1. \tag{6}$$

2.1 Kantorovich Expansion

Consider a formal expansion of the partial solution $\Psi_i^{Em\sigma}(\rho, z)$ of Eqs. (1)–(3), corresponding to the eigenstate $|m\sigma i\rangle$, expanded in the finite set of one-dimensional basis functions $\{\hat{\Phi}_j^m(\rho; z)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(\rho, z) = \sum_{j=1}^{j_{\max}} \hat{\Phi}_j^m(\rho; z) \hat{\chi}_j^{(m\sigma i)}(E, z). \tag{7}$$

In Eq. (7) 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 KM 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 eigenvalue problem

$$\hat{A}_c \hat{\Phi}_j(\rho; z) = \hat{E}_j(z) \hat{\Phi}_j(\rho; z), \tag{8}$$

with the boundary conditions

$$\lim_{\rho \to 0} \rho \frac{\partial \hat{\Phi}_j(\rho; z)}{\partial \rho} = 0, \quad \text{for} \quad m = 0, \quad \text{and} \quad \hat{\Phi}_j(0; z) = 0, \quad \text{for} \quad m \neq 0, \tag{9}$$

$$\lim_{\rho \to \infty} \hat{\Phi}_j(\rho; z) = 0. \tag{10}$$

Since the operator in the left-hand side of Eq. (8) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle \hat{\Phi}_i(\rho;z) \middle| \hat{\Phi}_j(\rho;z) \right\rangle_\rho = \int_0^\infty \hat{\Phi}_i(\rho;z)\hat{\Phi}_j(\rho;z)\rho d\rho = \delta_{ij}, \tag{11}$$

where δ_{ij} is the Kronecker 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 (7)

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \hat{\mathbf{U}}(z) + \hat{\mathbf{Q}}(z)\frac{d}{dz} + \frac{d\hat{\mathbf{Q}}(z)}{dz}\right)\hat{\boldsymbol{\chi}}^{(i)}(z) = \epsilon_i \mathbf{I}\hat{\boldsymbol{\chi}}^{(i)}(z). \tag{12}$$

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

$$\begin{aligned}
\hat{U}_{ij}(z) &= \left(\frac{\hat{E}_i(z) + \hat{E}_j(z)}{2}\right)\delta_{ij} + \hat{H}_{ij}(z), \quad I_{ij} = \delta_{ij}, \\
\hat{H}_{ij}(z) &= \hat{H}_{ji}(z) = \int_0^\infty \frac{\partial\hat{\Phi}_i(\rho;z)}{\partial z}\frac{\partial\hat{\Phi}_j(\rho;z)}{\partial z}\rho d\rho, \\
\hat{Q}_{ij}(z) &= -\hat{Q}_{ji}(z) = -\int_0^\infty \hat{\Phi}_i(\rho;z)\frac{\partial\hat{\Phi}_j(\rho;z)}{\partial z}\rho d\rho.
\end{aligned} \tag{13}$$

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

$$\lim_{z\to 0}\left(\frac{d}{dz} - \hat{\mathbf{Q}}(z)\right)\hat{\boldsymbol{\chi}}^{(i)}(z) = 0, \quad \sigma = +1, \quad \hat{\boldsymbol{\chi}}^{(i)}(0) = 0, \quad \sigma = -1, \tag{14}$$

$$\lim_{z\to\pm\infty}\hat{\boldsymbol{\chi}}^{(i)}(z) = 0 \quad \to \quad \hat{\boldsymbol{\chi}}^{(i)}(\pm z_{\max}) = 0, \tag{15}$$

$$\int_{-z_{\max}}^{z_{\max}}\left(\hat{\boldsymbol{\chi}}^{(i)}(z)\right)^T\hat{\boldsymbol{\chi}}^{(j)}(z)dz = 2\int_0^{z_{\max}}\left(\hat{\boldsymbol{\chi}}^{(i)}(z)\right)^T\hat{\boldsymbol{\chi}}^{(j)}(z)dz = \delta_{ij}. \tag{16}$$

3 Algorithm 1 of Generation of Parametric Algebraic Problems by the Finite Element Method

To solve eigenvalue problem for equation (8) the boundary conditions (9), (10) and the normalization condition (11) with respect to the space variable ρ on an infinite interval are replaced with appropriate conditions (9), (11) and $\hat{\Phi}(\rho_{\max};z) = 0$ on a finite interval $\rho \in [\rho_{\min} \equiv 0, \rho_{\max}]$.

We consider a discrete representation of solutions $\hat{\Phi}(\rho;z)$ of the problem (8) by means of the FEM on the grid, $\Omega^p_{h(\rho)} = (\rho_0 = \rho_{\min}, \rho_j = \rho_{j-1} + h_j, \rho_{\bar{n}} = \rho_{\max})$, in a finite sum in each $z = z_k$ of the grid $\Omega^p_{h(z)}[z_{\min}, z_{\max}]$:

$$\hat{\Phi}(\rho;z)=\sum_{\mu=0}^{\bar{n}p}\Phi_{\mu}^{h}(z)N_{\mu}^{p}(\rho)=\sum_{r=0}^{\bar{n}}\sum_{j=1}^{p}\Phi_{r+p(j-1)}^{h}(z)N_{r+p(j-1)}^{p}(\rho), \tag{17}$$

where $N_{\mu}^{p}(\rho)$ are local functions and $\Phi_{\mu}^{h}(z)$ are node values of $\hat{\Phi}(\rho_{\mu};z)$. The local functions $N_{\mu}^{p}(\rho)$ are piece-wise polynomial of the given order p equals one only in the node ρ_{μ} and equals zero in all other nodes $\rho_{\nu}\neq\rho_{\mu}$ of the grid $\Omega_{h(\rho)}^{p}$, i.e., $N_{\nu}^{p}(\rho_{\mu})=\delta_{\nu\mu}$, $\mu,\nu=0,1,\ldots,\bar{n}p$. The coefficients $\Phi_{\nu}(z)$ are formally connected with solution $\hat{\Phi}(\rho_{j,r}^{p};z)$ in a node $\rho_{\nu}=\rho_{j,r}^{p}$, $r=1,\ldots,p$, $j=0,\ldots,\bar{n}$:

$$\Phi_{\nu}^{h}(z)=\Phi_{r+p(j-1)}^{h}(z)\approx\hat{\Phi}(\rho_{j,r}^{p};z),\quad \rho_{j,r}^{p}=\rho_{j-1}+\frac{h_j}{p}r.$$

The theoretical estimate for the $\mathbf{H^0}$ norm between the exact and numerical solution has the order of

$$|\hat{E}_{m}^{h}(z)-\hat{E}_{m}(z)|\leq c_1|\hat{E}_{m}(z)|\,h^{2p},\quad \left\|\Phi_{m}^{h}(z)-\Phi_{m}(z)\right\|_{0}\leq c_2|\hat{E}_{m}(z)|h^{p+1},$$

where $h=\max_{1<j<\bar{n}}h_j$ is maximum step of grid [9]. It has been shown that we have a possibility to construct schemes with high order of accuracy comparable with the computer one [14]. Let us consider the reduction of differential equations (8) on the interval $\Delta:\ \rho_{\min}<\rho<\rho_{\max}$ with boundary conditions in points $\rho_{\min}$ and $\rho_{\max}$ rewriting in the form

$$\mathbf{A}(z)\hat{\Phi}(\rho;z)=\hat{E}(z)\mathbf{B}(z)\hat{\Phi}(\rho;z), \tag{18}$$

where $\mathbf{A}$ and $\mathbf{B}$ are differential operators. Substituting expansion (17) to (18) and integration with respect to ρ by parts in the interval $\Delta=\cup_{j=1}^{\bar{n}}\Delta_j$, we arrive to a system of the linear algebraic equations

$$\mathbf{a}_{\mu\nu}^{p}\Phi_{\mu}^{h}(z)=\hat{E}(z)\mathbf{b}_{\mu\nu}^{p}\Phi_{\mu}^{h}(z), \tag{19}$$

in framework of the briefly described FEM. Using p-order Lagrange elements [9], we present below an algorithm 1 for construction of algebraic problem (19) by the FEM in the form of conventional pseudocode. It MAPLE realization allow us show explicitly recalculation of indices μ, ν and test of correspondent modules in FORTRAN code.

In order to solve the generalized eigenvalue problem (19), the subspace iteration method [9,10] elaborated by Bathe [10] for the solution of large symmetric banded matrix eigenvalue problems has been chosen. This method uses a skyline storage mode, which stores components of the matrix column vectors within the banded region of the matrix, and is ideally suited for banded finite element matrices. The procedure chooses a vector subspace of the full solution space and iterates upon the successive solutions in the subspace (for details, see [10]). The iterations continue until the desired set of solutions in the iteration subspace converges to within the specified tolerance on the Rayleigh quotients for the

eigenpairs. Generally, 10-16 iterations are required for the subspace iterations to converge the subspace to within the prescribe tolerance. If matrix $\mathbf{a}^p$ in Eq. (19) is not positively defined, problem (19) is replaced by the following problem:

$$\tilde{\mathbf{a}}^p \, \boldsymbol{\Phi}^h = \check{E}^h \, \mathbf{b}^p \, \boldsymbol{\Phi}^h, \quad \tilde{\mathbf{a}}^p = \mathbf{a}^p - \alpha \mathbf{b}^p. \tag{20}$$

The number α (the shift of the energy spectrum) is chosen in such a way that matrix $\tilde{\mathbf{a}}^p$ is positive. The eigenvector of problem (20) is the same, and $\hat{E}^h = \check{E}^h + \alpha$.

Algorithm 1

Input:
$\Delta = \cup_{j=1}^{\bar{n}} \Delta_j = [\rho_{\min}, \rho_{\max}]$, is interval of changing of space variable ρ;
$h_j = \rho_j - \rho_{j-1}$ is a grid step;
$\bar{n}$ is a number of subintervals $\Delta_j = [\rho_{j-1}, \rho_j]$;
p is a order of finite elements;
$\mathbf{A}(z), \mathbf{B}(z)$ are differential operators in Eq. (18);
Output:
N_μ^p is a basis functions in (17);
$\mathbf{a}_{\mu\nu}^p$, $\mathbf{b}_{\mu\nu}^p$ are matrix elements in system of algebraic equations (19);
Local:
$\rho_{j,r}^p$ are nodes;
$\phi_{j,r}^p(\rho)$ are Lagrange elements;
$\mu, \nu = 0, 1, \ldots, \bar{n}p$;

1: for j:=1 to $\bar{n}$ do
  for r:=0 to p do
    $\rho_{j,r}^p = \rho_{j-1} + \frac{h_j}{p} r$
  end for;
end for;
2: $\phi_{j,r}^p(\rho) = \prod_{k \neq r} [(\rho - \rho_{j,k}^p)(\rho_{j,r}^p - \rho_{j,k}^p)^{-1}]$
3: $N_0^p(\rho) := \{\phi_{1,0}^p(\rho), \rho \in \Delta_1; 0, \rho \notin \Delta_1\}$;
  for j:=1 to $\bar{n}$ do
    for r:=1 to $p-1$ do
      $N_{r+p(j-1)}^p(\rho) := \{\phi_{j,r}^p(\rho), \rho \in \Delta_j; 0, \rho \notin \Delta_j, \}$
    end for;
    $N_{jp}^p(\rho) := \{\phi_{j,p}^p(\rho), \rho \in \Delta_j; \phi_{j+1,0}^p(\rho), \rho \in \Delta_{j+1}; 0, \rho \notin \Delta_j \bigcup \Delta_{j+1}\}$;
  end for;
  $N_{\bar{n}p}^p(\rho) := \{\phi_{\bar{n},p}^p(\rho), \rho \in \Delta_{\bar{n}}; 0, \rho \notin \Delta_{\bar{n}}\}$;
4: for μ, ν:=0 to $\bar{n}p$ do
    $\mathbf{a}_{\mu\nu}^p := \int\limits_{\Delta} N_\mu^p(\rho) \mathbf{A}(z) N_\nu^p(\rho) \rho d\rho$; $\quad \mathbf{b}_{\mu\nu}^p := \int\limits_{\Delta} N_\mu^p(\rho) \mathbf{B}(z) N_\nu^p(\rho) \rho d\rho$;
  end for;

Remarks

1. For equation (8) matrix elements of the operator,

$$\hat{A}_c = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + V(\rho;z), \quad V(\rho;z) = -\frac{2Z}{\sqrt{\rho^2+z^2}} + \frac{m^2}{\rho^2} + m\gamma + \frac{\gamma^2\rho^2}{4},$$

between local functions N_μ and N_ν defined in same interval Δ_j calculated by formula

$$\begin{aligned}
(\mathbf{a}(z_k))_{q+p(j-1),r+p(j-1)} &= \int_{-1}^{+1} \left\{ \tfrac{4}{h_j^2}(\phi^p_{j,q})'(\phi^p_{j,r})' + V(\rho;z_k)\phi^p_{j,q}\phi^p_{j,r} \right\} \tfrac{h_j}{2}\rho d\eta, \\
(\mathbf{b}(z_k))_{q+p(j-1),r+p(j-1)} &= \int_{-1}^{+1} \phi^p_{j,q}\phi^p_{j,r}\tfrac{h_j}{2}\rho d\eta.
\end{aligned}$$

2. If integrals do not calculated analytically, for example, like in [11,12], then they have been calculated by numerical methods [9], by means of the Gauss quadrature formulae of the order $p+1$.

3. For calculations matrix elements (19) and the corresponded derivatives of eigenfunctions by z we used algorithm described in [3]. Starting from matching point $z_m < z_{\max}$ of the grid $\Omega^p_{h(z)}[z_{\min}, z_{\max}]$ the calculation has been performed using an asymptotic expansion from next section ($z_m \sim 20$, $z_{\max} \sim 100$).

4. The problem (8)–(10) has been solved using a grid $\Omega^p_{h(\rho)}[\rho_{\min}, \rho_{\max}] = 0(500)4(500)30$ (the number in parentheses denotes the number of finite elements of order $p = 4$ in each interval). As an example, at $m = -1$ and $\gamma = 10$ the calculated the potential curves $\hat{E}_j(z)$, effective potentials $\hat{Q}_{ij}(z)$, $\hat{H}_{ij}(z)$ are shown in Fig. 1.

4 Algorithm 2 of Evaluation the Asymptotics of Effective Potentials at Large $|z|$ in Kantorovich Method

Step 1. In (8) apply the transformation to a scaled variable x

$$x = \frac{\gamma\rho^2}{2}, \;\; \rho = \frac{\sqrt{x}}{\sqrt{\gamma/2}}, \tag{21}$$

and put $\lambda = \hat{E}_j(z)/(2\gamma) = \lambda^{(0)} + m/2 - Z/(\gamma|z|) + \delta\lambda$. Eigenvalue problem reads

$$\left(-\frac{\partial}{\partial x}x\frac{\partial}{\partial x} + \frac{m^2}{4x} + \frac{x}{4} + \frac{m}{2} - \frac{Z}{\gamma\sqrt{\frac{2x}{\gamma}+z^2}} - \lambda \right) \hat{\Phi}_j(x;z) = 0, \tag{22}$$

with a normalization condition

$$\frac{1}{\gamma}\int_0^\infty \hat{\Phi}_j(x;z)^2 dx = 1. \tag{23}$$

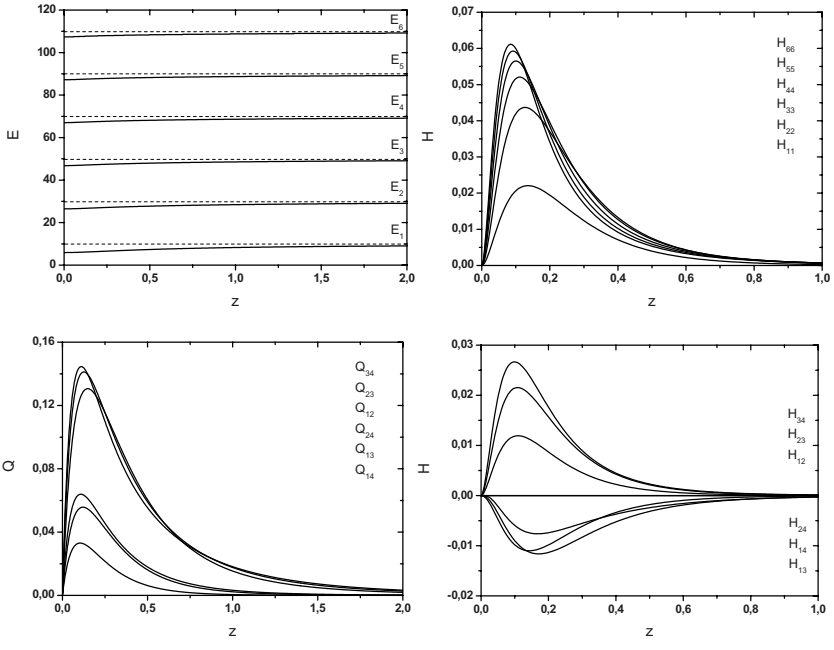

Fig. 1. The behaviour of potential curves $\hat{E}_j(z)$, effective potentials $\hat{Q}_{ij}(z)$ and $\hat{H}_{ij}(z)$ for $\gamma = 10$, $m = -1$

At $Z = 0$ Eq. (22) takes the form

$$L(n)\Phi_{nm}^{(0)}(x) = 0, \qquad L(n) = -\frac{\partial}{\partial x}x\frac{\partial}{\partial x} + \frac{m^2}{4x} + \frac{x}{4} - \lambda^{(0)}, \tag{24}$$

and has the regular and bounded solutions at

$$\lambda^{(0)} = n + (|m| + 1)/2, \tag{25}$$

where transverse quantum number $n \equiv N_\rho = j - 1 = 0, 1, \ldots$ determines the number of nodes of the solution $\Phi_{nm}^{(0)}(x)$ with respect to the variable x. Normalized solutions of Eq. (24), take the form

$$\Phi_{nm}^{(0)}(x) = C_{n|m|}e^{-\frac{x}{2}}x^{\frac{|m|}{2}}L_n^{|m|}(x), \qquad C_{n|m|} = \left[\gamma\frac{n!}{(n+|m|)!}\right]^{\frac{1}{2}}, \tag{26}$$

$$\frac{1}{\gamma}\int_0^\infty \Phi_{nm}^{(0)}(x)\Phi_{n'm}^{(0)}(x)dx = \delta_{nn'}, \tag{27}$$

where $L_n^{|m|}(x)$ are Laguerre polynomials [13].

Step 2. Substituting notation $\delta\lambda = \lambda - \lambda^{(0)} - m/2 + Z/(\gamma|z|) \equiv \hat{E}_j(z)/(2\gamma) - (n + (m + |m| + 1)/2) + Z/(\gamma|z|)$, and decomposition

$$\frac{Z}{\gamma|z|} - \frac{Z}{\gamma\sqrt{\frac{2x}{\gamma}+z^2}} = \sum_{k=1}^{j_{\max}} \frac{V^{(k)}}{|z|^k},$$

$$V^{(k)} = \begin{cases} -(-1)^{k'} \frac{(2k'-1)!!}{k'!} \frac{Z x^{k'}}{\gamma^{k'+1}}, & k = 2k'+1, \quad k' = 1, 2, \ldots, \\ 0, & \text{otherwise}, \end{cases}$$

to Eq. (22) at $Z \neq 0$, transform it in the following form

$$L(n)\hat{\Phi}_j(x;z) + \left(\sum_{k=1}^{j_{\max}} \frac{V^{(k)}}{|z|^k} - \delta\lambda \right) \hat{\Phi}_j(x;z) = 0. \tag{28}$$

Step 3. Solution of equation (28) is found in the form of the perturbation series by inverse powers of $|z|$

$$\delta\lambda = \sum_{k=0}^{k_{\max}} |z|^{-k} \lambda^{(k)}, \quad \Phi_j(x;z) = \sum_{k=0}^{k_{\max}} |z|^{-k} \Phi_n^{(k)}(x). \tag{29}$$

Equating coefficients at the same powers of $|z|$, we arrive to the system of inhomogeneous differential equations with respect to corrections $\lambda^{(k)}$ and $\Phi^{(k)}$

$$\begin{aligned} &L(n)\Phi^{(0)}(x) = 0 \equiv f^{(0)}, \\ &L(n)\Phi^{(k)}(x) = \sum_{p=0}^{k-1} (\lambda^{(k-p)} - V^{(k-p)}) \Phi^{(p)}(x) \equiv f^{(k)}, \quad k \geq 1. \end{aligned} \tag{30}$$

For solving the Eqs. (28) the unnormalized orthogonal basis

$$\Phi_{n+s}(x) = C_{n|m|} e^{-\frac{x}{2}} x^{\frac{|m|}{2}} L_{n+s}^{|m|}(x) = C_{n|m|} C^{-1}_{n+s|m|} \Phi^{(0)}_{n+s,m}(x), \tag{31}$$

$$\langle s|s'\rangle = \int_0^\infty \Phi_{n+s}(x)\Phi_{n+s'}(x)dx = \delta_{ss'}\gamma \frac{n!}{(n+|m|)!} \frac{(n+s+|m|)!}{(n+s)!},$$

has been applied. The operators $L(n)$ and x on the functions $\Phi_{n+s}(x)$ are defined by the relations without fractional powers of quantum numbers n and m

$$\begin{aligned} &L(n)\Phi_{n+s}(x) = s\Phi_{n+s}(x), \\ &x\Phi_{n+s}(x) = -(n+s+|m|)\Phi_{n+s-1}(x) + (2(n+s)+|m|+1)\Phi_{n+s}(x) \\ &\qquad\qquad -(n+s+1)\Phi_{n+s+1}(x). \end{aligned} \tag{32}$$

Step 4. Applying relations (32), the right-hand side $f^{(k)}$ and solutions $\Phi^{(k)}(x)$ of the system (30) are expanded over basis states $\Phi_{n+s}(x)$

$$\Phi_n^{(k)}(x) = \sum_{s=-k}^{k} b_s^{(k)} \Phi_{n+s}(x), \quad f^{(k)} = \sum_{s=-k}^{k} f_s^{(k)} \Phi_{n+s}(x). \tag{33}$$

Then a recurrent set of linear algebraic equations for unknown coefficients $b_s^{(k)}$ and corrections $\lambda^{(k)}$ is obtained

$$sb_s^{(k)} - f_s^{(k)} = 0, \quad s = -k, \ldots, k.$$

that is solved sequentially for $k = 1, 2, \ldots, k_{\max}$:

$$f_0^{(k)} = 0 \quad \to \lambda^{(k)}; \quad b_s^{(k)} = f_s^{(k)}/s, \quad s = -k, \ldots, k, \quad s \neq 0.$$

The initial conditions (25) and $b_s^{(0)} = \delta_{s0}$ are followed from (24) and (27).

Step 5. To obtain the normalized wave function $\hat{\Phi}_j(x; z)$ up to the k-th order, the coefficient $b_0^{(k)}$ are defined by the following relation:

$$b_0^{(k)} = -\frac{1}{2\gamma} \sum_{p=1}^{k-1} \sum_{s'=p-k}^{k-p} \sum_{s=-p}^{p} b_s^{(k-p)} \langle s|s' \rangle b_{s'}^{(p)}, \quad b_0^{(k=1,\ldots,5)} = 0.$$

As an example of output file at steps 1–5, we display nonzero coefficients $\lambda^{(k)}$, $b_s^{(k)}$ of the inverse power series (29), (33) up to $O(|z|^{-5})$:

$$\begin{aligned} &\lambda^{(0)} = n + (|m| + 1)/2, \quad \lambda^{(3)} = Z(2n + |m| + 1)/\gamma^2, \\ &b_0^{(0)} = 1, \quad b_{-1}^{(3)} = -Z(n + |m|)/\gamma^2, \quad b_1^{(3)} = Z(n + 1)/\gamma^2. \end{aligned} \tag{34}$$

Step 6. In scaled variable x the relations of effective potentials $\hat{H}_{ij}(z) = \hat{H}_{ji}(z)$ and $\hat{Q}_{ij}(z) = -\hat{Q}_{ji}(z)$ takes form

$$\hat{H}_{ij}(z) = \frac{1}{\gamma} \int_0^\infty dx \frac{\partial \hat{\Phi}_i(x; z)}{\partial z} \frac{\hat{\partial} \Phi_j(x; z)}{\partial z}, \quad \hat{Q}_{ij}(z) = -\frac{1}{\gamma} \int_0^\infty dx \hat{\Phi}_i(x; z) \frac{\partial \hat{\Phi}_j(x; z)}{\partial z}. \tag{35}$$

For their evaluation the decomposition of solution Eqs. (24) over the normalized orthogonal basis $\Phi_{n+s}^{(0)}$ with the normalized coefficients $b_{n;n+s}^{(k)}$,

$$\Phi_n^{(k)}(x) = \sum_{s=-k}^{k} b_{n;n+s}^{(k)} \Phi_{n+s}^{(0)}, \tag{36}$$

has been applied. The normalized coefficients $b_{n;n+s}^{(k)}$ are calculated via $b_s^{(k)}$,

$$b_{n;n+s}^{(k)} = b_s^{(k)} \sqrt{\frac{n!}{(n + |m|)!} \frac{(n + s + |m|)!}{(n + s)!}} \tag{37}$$

as follows from (33), (36) and (31).

Step 7. In a result of substitution (29), (36) in (35), matrix elements takes form

$$\begin{aligned} \hat{Q}_{jj+t}(z) &= -\sum_{k=0}^{k_{\max}-1} |z|^{-k-1} \sum_{k'=0}^{k} \sum_{s=\max(-k,k'-k-t)}^{\min(k,k-k'-t)} (k - k') b_{n;n+s}^{(k')} b_{n+t;n+s}^{(k-k')}, \\ \hat{H}_{jj+t}(z) &= \sum_{k=0}^{k_{\max}-2} |z|^{-k-2} \sum_{k'=0}^{k} \sum_{s=\max(-k,k'-k-t)}^{\min(k,k-k'-t)} k'(k - k') b_{n;n+s}^{(k')} b_{n+t;n+s}^{(k-k')}. \end{aligned} \tag{38}$$

Collecting of coefficients of (38) at equal powers of $|z|$, algorithm leads to final expansions of eigenvalues and effective potentials of output file

$$\hat{E}_j(z) = \sum_{k=0}^{k_{\max}} |z|^{-k} E_j^{(k)},\ \hat{H}_{ij}(z) = \sum_{k=8}^{k_{\max}} |z|^{-k} H_{ij}^{(k)},\ \hat{Q}_{ij}(z) = \sum_{k=4}^{k_{\max}} |z|^{-k} Q_{ij}^{(k)}. \quad (39)$$

The successful run of the above algorithm was occurs up to $k_{\max} = 16$ (Run time is 95s on Intel Pentuim IV, 2.40 GHz, 512 MB). The some first nonzero coefficients takes form ($j = n + 1$)

$$\begin{aligned}
E_j^{(0)} &= 2\gamma(n + (m + |m| + 1)/2),\\
E_j^{(1)} &= -2Z,\\
E_j^{(3)} &= 2Z(2n + |m| + 1)/\gamma,\\
E_j^{(5)} &= -3Z(2 + 3|m| + 6n^2 + |m|^2 + 6n|m| + 6n)/\gamma^2,\\
E_j^{(6)} &= -2Z^2(2n + |m| + 1)/\gamma^3,\\
Q_{jj+1}^{(4)} &= 3Z\sqrt{n+1}\sqrt{n+|m|+1}/\gamma^2,\\
Q_{jj+1}^{(6)} &= -15Z\sqrt{n+1}\sqrt{n+|m|+1}(2n + |m| + 2)/\gamma^3,\\
Q_{jj+2}^{(6)} &= 15Z\sqrt{n+1}\sqrt{n+2}\sqrt{n+|m|+1}\sqrt{n+|m|+2}/(4\gamma^3),\\
H_{jj}^{(8)} &= 9Z^2(2n^2 + 2n|m| + 2n + |m| + 1)/\gamma^4,\\
H_{jj}^{(10)} &= -90Z^2(2n + |m| + 1)(2n^2 + 2n|m| + 2n + |m| + 2)/\gamma^5,\\
H_{jj+1}^{(10)} &= 45Z^2\sqrt{n+1}\sqrt{n+|m|+1}(n^2 + n|m| + 2n + |m| + 2)/(2\gamma^5),\\
H_{jj+2}^{(8)} &= -9Z^2\sqrt{n+1}\sqrt{n+2}\sqrt{n+|m|+1}\sqrt{n+|m|+2}/\gamma^4,\\
H_{jj+2}^{(10)} &= 90Z^2\sqrt{n+1}\sqrt{n+2}\sqrt{n+|m|+1}\sqrt{n+|m|+2}(2n + |m| + 3)/\gamma^5,\\
H_{jj+3}^{(10)} &= -45Z^2\sqrt{n+1}\sqrt{n+2}\sqrt{n+3}\sqrt{n+|m|+1}\sqrt{n+|m|+2}\sqrt{n+|m|+3}/(2\gamma^5).
\end{aligned}$$

As an example, in Table 1 we show true convergence of partial sums of asymptotic expansions (39) of effective potentials $\hat{Q}_{ij}(z)$ to the corresponding numerical values calculated by algorithm 1, described in section 3.

5 Algorithm 3 of Evaluation the Asymptotics of Solutions at Large $|z|$ in Kantorovich Method

Step 1. We write the set of differential equations (12) at fixed values m, and ϵ in the explicit form for $\chi_{ji_o}(z) \equiv \hat{\chi}_j^{(i_o)}(z)$ and $j = 1, 2, \ldots, j_{\max}$, $i_o = 1, 2, \ldots, N_o$

$$\begin{aligned}
&-\frac{d^2\chi_{ji_o}(z)}{dz^2} - \frac{2Z}{|z|}\chi_{ji_o}(z) - \left(\epsilon - \hat{E}_j(z) - \frac{2Z}{|z|}\right)\chi_{ji_o}(z) + \hat{H}_{jj}(z)\chi_{ji_o}(z)\\
&= \sum_{j'=1, j'\neq j}^{j_{\max}} \left(-\hat{Q}_{jj'}(z)\frac{d}{dz} - \hat{H}_{jj'}(z) - \frac{d\hat{Q}_{jj'}(z)}{dz}\right)\chi_{j'i_o}(z), \qquad (40)
\end{aligned}$$

Table 1. Values of the partial sums (39) depending on $k_{\max}$ for $m=-1$, $Z=1$, $z=10$, $\gamma=10$. The last row contains the corresponding numerical values (n.v.).

i,j	$\hat{Q}_{12},10^{-6}$	$\hat{Q}_{23},10^{-6}$	$\hat{Q}_{34},10^{-5}$	$\hat{Q}_{13},10^{-8}$	$\hat{Q}_{24},10^{-8}$	$\hat{Q}_{14},10^{-11}$
$z^{-4}Q_{ij}^{(4)}$	4.24264069	7.34846923	1.03923048	0	0	0
$+z^{-6}Q_{ij}^{(6)}$	4.17900108	7.16475750	1.00285742	1.29903811	3.18198052	0
$+z^{-7}Q_{ij}^{(7)}$	4.17883137	7.16446356	1.00281585	1.29903811	3.18198052	0
$+z^{-8}Q_{ij}^{(8)}$	4.17972233	7.16857870	1.00394341	1.26266504	3.04833733	7.0000
$+z^{-9}Q_{ij}^{(9)}$	4.17972824	7.16859579	1.00394680	1.26260268	3.04818460	7.0000
$+z^{-10}Q_{ij}^{(10)}$	4.17971489	7.16850321	1.00391243	1.26342108	3.05252800	6.6850
$+z^{-11}Q_{ij}^{(11)}$	4.17971474	7.16850253	1.00391224	1.26342451	3.05254060	6.6846
$+z^{-12}Q_{ij}^{(12)}$	4.17971496	7.16850469	1.00391330	1.26340651	3.05240830	6.6950
$+z^{-13}Q_{ij}^{(13)}$	4.17971496	7.16850471	1.00391331	1.26340638	3.05240762	6.6950
$+z^{-14}Q_{ij}^{(14)}$	4.17971496	7.16850466	1.00391328	1.26340679	3.05241163	6.6947
$+z^{-15}Q_{ij}^{(15)}$	4.17971496	7.16850466	1.00391327	1.26340679	3.05241166	6.6947
$+z^{-16}Q_{ij}^{(16)}$	4.17971496	7.16850466	1.00391328	1.26340678	3.05241154	6.6947
(n.v.)	4.17971496	7.16850466	1.00391328	1.26340678	3.05241154	6.6947

where matrix elements $\hat{Q}_{jj'}(z)$ and $\hat{H}_{jj'}(z)$ have of the form (39).

Note, that at large z, $E_i^{(2)}=H_{ii}^{(2)}=0$, i.e., the centrifugal terms are eliminated and the longitudinal solution has the asymptotic form corresponding to zero angular momentum solutions, or to the one-dimensional problem on a semi-axis:

$$\chi_{ji_o}(z)=\frac{\exp(w(z))}{\sqrt{p_{i_o}}}\phi_{ji_o}(z),\quad \phi_{ji_o}(z)=\sum_{k=0}^{k_{\max}}\phi_{ji_o}^{(k)}|z|^{-k}, \tag{41}$$

where $w(z)=\imath p_{i_o}|z|+\imath\zeta\ln(2p_{i_o}|z|)+\imath\delta_{i_o}$, p_{i_o} is the momentum in the channel, ζ is the characteristic parameter, and δ_{i_o} is the phase shift. The components $\phi_{ji_o}^{(k)}$ satisfy the system of ordinary differential equations

$$\begin{aligned}
&(p_{i_o}^2-2E+E_j^{(0)})\phi_{ji_o}^{(k)}=f_{ji_o}^{(k)}(\phi_{j'i_o}^{(k'=0,\ldots,k-1)},p_{i_o})\\
&\equiv -2(\zeta p_{i_o}+\imath(k-1)p_{i_o}-Z)\phi_{ji_o}^{(k-1)}-(\zeta+\imath(k-2))(\zeta+\imath(k-1))\phi_{ji_o}^{(k-2)}\\
&-\sum_{k'=3}^{k}(E_j^{(k')}+H_{jj}^{(k')})\phi_{ji_o}^{(k-k')}+\sum_{j'=1}^{j_{\max}}\sum_{k'=4}^{k}(-2\imath Q_{jj'}^{(k')}p_{i_o}-H_{jj'}^{(k')})\phi_{j'i_o}^{(k-k')}\\
&+\sum_{j'=1}^{j_{\max}}\sum_{k'=5}^{k}(2k-1-k'-2\imath\zeta)Q_{jj'}^{(k'-1)}\phi_{j'i_o}^{(k-k')},\\
&k=0,1,\ldots,k_{\max},\quad \phi_{ji_o}^{(-1)}\equiv 0,\quad \phi_{ji_o}^{(-2)}\equiv 0,\quad k_{\max}\le j_{\max}-i_o.
\end{aligned} \tag{42}$$

Here index of summation, j', takes integer values, except i_o and j, ($j'=1,\ldots,j_{\max}$, $j'\neq i_o$, $j'\neq j$).

Step 2. From first two equations ($k = 0, 1$) of set (42) we have the leading terms of eigenfunction $\phi^{(0)}_{ji_o}$, eigenvalue $p^2_{i_o}$ and characteristic parameter ζ, i.e initial data for solving recurrence sequence,

$$\phi^{(0)}_{ji_o} = \delta_{ji_o}, \quad p^2_{i_o} = 2E - E^{(0)}_{i_o} \to p_{i_o} = \sqrt{2E - E^{(0)}_{i_o}}, \quad \zeta = Z/p_{i_o}. \tag{43}$$

Open channels have $p^2_{i_o} \geq 0$, and close channels have $p^2_{i_o} < 0$. Lets there are $N_o \leq j_{\max}$ open channels, i.e., $p^2_{i_o} \geq 0$ for $i_o = 1, \ldots N_o$ and $p^2_{i_o} < 0$ for $i_o = N_o + 1, \ldots j_{\max}$.

Step 3. Substituting (43) in (42), we obtain the following recurrent set of algebraic equations for the unknown coefficients $\phi_{ji_o}(z)$ for $k = 1, 2, \ldots, k_{\max}$:

$$(E^{(0)}_{i_o} - E^{(0)}_j)\phi^{(k)}_{ji_o} = f^{(k)}_{ji_o}(\phi^{(k'=0,\ldots,k-1)}_{j'i_o}, p_{i_o}) \tag{44}$$

that is solved sequentially for $k = 1, 2, \ldots, k_{\max}$:

$$\begin{aligned} &\phi^{(k)}_{ji_o} = f^{(k)}_{ji_o}(\phi^{(k'=0,\ldots,k-1)}_{j'i_o}, p_{i_o})/(E^{(0)}_{i_o} - E^{(0)}_j),\ j \neq i_o, \\ &f^{(k+1)}_{i_o i_o}(\phi^{(k'=0,\ldots,k)}_{j'i_o}, p_{i_o}) = 0 \to \phi^{(k)}_{i_o i_o}. \end{aligned} \tag{45}$$

The successful run of the above algorithm was occurs up to $k_{\max} = 16$ (Run time is 167s on Intel Pentuim IV, 2.40 GHz, 512 MB). The some first nonzero coefficients takes form ($j = n + 1$)

$$\begin{aligned}
\phi^{(0)}_{ji_o} &= \delta_{ji_o}, \\
\phi^{(1)}_{ji_o} &= \delta_{ji_o} \imath Z(Z + \imath p_{i_o})/(2p^3_{i_o}), \\
\phi^{(2)}_{ji_o} &= \delta_{ji_o}[\imath E^{(3)}_j/(4p_{i_o}) - Z(Z + \imath p_{i_o})^2(Z + 2\imath p_{i_o})/(8p^6_{i_o})], \\
\phi^{(3)}_{ji_o} &= \delta_{ji_o}[-E^{(3)}_j(3Z^2 + 7\imath p_{i_o} Z - 6p^2_{i_o})/(24p^4_{i_o}) \\
&\qquad - \imath Z(Z + \imath p_{i_o})^2(Z + 2\imath p_{i_o})^2(Z + 3\imath p_{i_o})/(48p^9_{i_o})], \\
\phi^{(4)}_{ji_o} &= \delta_{ji_o}[\imath E^{(5)}_j/(8p_{i_o}) - (E^{(3)}_j)^2/(32p^2_{i_o}) \\
&\qquad - \imath E^{(3)}_j(3Z^4 + 20\imath p_{i_o} Z^3 - 53p^2_{i_o} Z^2 - 66\imath p^3_{i_o} Z + 36p^4_{i_o}))/(96p^7_{i_o}) \\
&\qquad + Z(Z + \imath p_{i_o})^2(Z + 2\imath p_{i_o})^2(Z + 3\imath p_{i_o})^2(Z + 4\imath p_{i_o})/(384p^{12}_{i_o})] \\
&\quad + 2\imath p_{i_o} Q^{(4)}_{ji_o}/(E^{(0)}_{i_o} - E^{(0)}_j).
\end{aligned}$$

Remarks

1. Expansion (41) holds true for $|z_m| \gg \max(Z^2/(2p^3_{i_o}), 2Z(2i_o + |m| - 1)/(8\gamma p^2_{i_o}))$. The choice of a new value of $z_{\max}$ for the constructed expansions of the linearly independent solutions for $p_{i_o} > 0$ is controlled by the fulfillment of the Wronskian condition with a long derivative $D_z \equiv \mathbf{I}d/dz - \mathbf{Q}(z)$

$$Wr(\mathbf{Q}(z); \boldsymbol{\chi}^*(z), \boldsymbol{\chi}(z)) = (\boldsymbol{\chi}^*(z))^T D_z \boldsymbol{\chi}(z) - (D_z \boldsymbol{\chi}^*(z))^T \boldsymbol{\chi}(z) = 2\imath \mathbf{I}_{oo}$$

up to the prescribed accuracy. Here $\mathbf{I}_{oo}$ is the N_o-by-N_o identity matrix.

2. This algorithm can be applied also for evaluation asymptotics of solutions in closed channels $p_{i_o} = \imath\kappa_{i_o}$, $\kappa_{i_o} > 0$.

Table 2. Convergence of the method for the binding energy $\mathcal{E} = \gamma/2 - E$ (in a.u.) of even wave functions $m = -1$, $\gamma = 10$ and $\gamma = 5$ versus the number $j_{\max}$ of coupled equations (40)

$j_{\max}$	$2p_{-1}$ $(\gamma = 10)$	$3p_{-1}$ $(\gamma = 10)$	$2p_{-1}$ $(\gamma = 5)$	$3p_{-1}$ $(\gamma = 5)$
1	1.123 532 554 (3)	0.182 190 992 (2)	0.857 495 336 (9)	0.165 082 403 (4)
2	1.125 069 513 (1)	0.182 282 868 (7)	0.859 374 058 (2)	0.165 234 428 (1)
3	1.125 280 781 (8)	0.182 294 472 (5)	0.859 641 357 (6)	0.165 253 152 (9)
4	1.125 343 075 (2)	0.182 297 825 (6)	0.859 721 942 (4)	0.165 258 606 (4)
6	1.125 381 347 (9)	0.182 299 867 (7)	0.859 772 441 (3)	0.165 261 973 (6)
8	1.125 392 776 (1)	0.182 300 474 (6)	0.859 787 833 (7)	0.165 262 991 (9)
10	1.125 397 502 (9)	0.182 300 725 (2)	0.859 794 289 (0)	0.165 263 418 (0)
12	1.125 399 854 (7)	0.182 300 849 (8)	0.859 797 533 (8)	0.165 263 631 (9)
[6]	1.125 422 341 (8)	0.182 301 494 (7)	0.859 832 622 (6)	0.165 264 273 (1)

6 Applications Algorithms for Solving the Eigenvalue Problem

The efficiency and accuracy of the elaborated SNA and of the corresponded numerical scheme derived are confirmed by computations of eigenenergies and eigenfunctions for the low-excited states of a hydrogen atom in the strong homogeneous magnetic field. These algorithms are used to generate an input file of effective potentials in the Gaussian points $z = z_k$ of the FEM grid $\Omega^p_{h(z)}[z_{\min} = 0, z_{\max}]$ and asymptotic of solutions of a set of longitudinal equations (12)–(16) for the KANTBP code [5]. In Table 2 we show convergence of the method for the binding energy $\mathcal{E} = \gamma/2 - E$ (in a.u.) of the even wave functions at $m = -1$, $\gamma = 10$ and $\gamma = 5$ versus the number $j_{\max}$ of coupled equations (40). The calculations was performed on a grid $\Omega^p_{h(z)} = \{0(200)2(600)150\}$ (the number in parentheses denotes the number of finite elements of order $p = 4$ in each interval). Comparison with corresponding calculations given in spherical coordinates from [1,6] is shown that elaborated method in cylindrical coordinates is applicable for strength magnetic field $\gamma > 5$ and magnetic number m of order of ~ 10. The main goal of the method consists in the fact that for states having preferably a cylindrical symmetry a convergence rate is increased at fixed m with growing values of $\gamma \gg 1$ or the high-$|m|$ Rydberg states at $|m| > 150$ in laboratory magnetic fields $B = 6.10$T ($\gamma = 2.595 \cdot 10^{-5}$ a.u.), such that several equations are provide a given accuracy [7].

7 Conclusion

A new effective method of calculating wave functions of a hydrogen atom in a strong magnetic field is developed. The method is based on the Kantorovich approach to parametric eigenvalue problems in cylindrical coordinates. The rate

of convergence is examined numerically and illustrated by a set of typical examples. The results are in a good agreement with calculations executed in spherical coordinates at fixed m for $\gamma > 5$. The elaborated SNA for calculating effective potentials and asymptotic solutions allows us to generate effective approximations for a finite set of longitudinal equations describing an open channel. The developed approach yields a useful tool for calculation of threshold phenomena in formation and ionization of (anti)hydrogen like atoms and ions in magnetic traps [2,7] and channeling of ions in thin films [15].

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