

A SYMBOLIC-NUMERICAL ALGORITHM FOR SOLVING THE EIGENVALUE PROBLEM FOR A HYDROGEN ATOM IN THE MAGNETIC FIELD: CYLINDRICAL COORDINATES

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Contents of the talk

- 1 The Kantorovich reduction of the 2D-eigenvalue problem to the 1D-eigenvalue problem for a set of the closed longitudinal equations.
- 2 The FEM algorithm for evaluating the transverse basis functions on a grid of the longitudinal parameter from a finite interval and calculation of matrix elements.
- 3 The symbolic algorithm for asymptotic calculation of matrix elements at large values of the longitudinal variable $|z|$.
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- 5 The calculation of the low-lying states of a hydrogen atom in a strong magnetic field with help of the FEM using the KANTBP program.
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Statement of the problem in cylindrical coordinates

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

$$\hat{\Psi}(\rho, z, \varphi) = \Psi(\rho, z) \frac{\exp(im\varphi)}{\sqrt{2\pi}} \quad (1)$$

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

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

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

in the region Ω_c : $0 < \rho < \infty$ and $-\infty < z < \infty$.

Here $m = 0, \pm 1, \dots$ 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

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

$$\Psi(0, z) = 0, \quad \text{for } m \neq 0, \quad (5)$$

$$\lim_{\rho \rightarrow \infty} \Psi(\rho, z) = 0. \quad (6)$$

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,

$$\lim_{z \rightarrow \pm \infty} \Psi(\rho, z) = 0 \quad \rightarrow \quad \Psi(\rho, \pm z_{\max}) = 0. \quad (7)$$

These functions satisfy the additional normalization condition

$$\int_{-z_{\max}}^{z_{\max}} \int_0^{\infty} |\Psi(\rho, z)|^2 \rho d\rho dz = 1. \quad (8)$$

The asymptotic boundary condition for the continuum wave function will be considered below.

Kantorovich expansion

Consider a formal expansion of the partial solution $\Psi_i^{Em\sigma}(\rho, z)$ of Eqs. (2)–(6), corresponding to the eigenstate $|m\sigma i\rangle$, expanded in the finite set of one-dimensional basis functions $\{\hat{\Phi}_j^m(\rho; z)\}_{j=1}^{j_{\max}}$

$$\Psi_i^{Em\sigma}(\rho, z) = \sum_{j=1}^{j_{\max}} \hat{\Phi}_j^m(\rho; z) \hat{\chi}_j^{(m\sigma i)}(E, z). \quad (9)$$

In Eq. (9) the functions $\hat{\chi}^{(i)}(z) \equiv \hat{\chi}^{(m\sigma i)}(E, z)$, $(\hat{\chi}^{(i)}(z))^T = (\hat{\chi}_1^{(i)}(z), \dots, \hat{\chi}_{j_{\max}}^{(i)}(z))$ are unknown, and the surface functions $\hat{\Phi}(\rho; z) \equiv \hat{\Phi}^m(\rho; z) = \hat{\Phi}^m(\rho; -z)$, $(\hat{\Phi}(\rho; z))^T = (\hat{\Phi}_1(\rho; z), \dots, \hat{\Phi}_{j_{\max}}(\rho; z))$ 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

$$\hat{A}_c \hat{\Phi}_j(\rho; z) = \hat{E}_j(z) \hat{\Phi}_j(\rho; z), \quad (10)$$

with the boundary conditions

$$\lim_{\rho \rightarrow 0} \rho \frac{\partial \hat{\Phi}_j(\rho; z)}{\partial \rho} = 0, \quad \text{for } m = 0, \quad \text{and} \quad \hat{\Phi}_j(0; z) = 0, \quad \text{for } m \neq 0, \quad (11)$$

$$\lim_{\rho \rightarrow \infty} \hat{\Phi}_j(\rho; z) = 0. \quad (12)$$

Since the operator in the left-hand side of Eq. (10) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle \hat{\Phi}_i(\rho; z) \left| \hat{\Phi}_j(\rho; z) \right. \right\rangle_{\rho} = \int_0^{\infty} \hat{\Phi}_i(\rho; z) \hat{\Phi}_j(\rho; z) \rho d\rho = \delta_{ij}, \quad (13)$$

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 $\hat{\chi}^{(i)}(z)$ of the expansion (9)

$$\left(-\mathbf{I} \frac{d^2}{dz^2} + \hat{\mathbf{U}}(z) + \hat{\mathbf{Q}}(z) \frac{d}{dz} + \frac{d\hat{\mathbf{Q}}(z)}{dz} \right) \hat{\chi}^{(i)}(z) = \epsilon_i \mathbf{I} \hat{\chi}^{(i)}(z). \quad (14)$$

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

$$\begin{aligned} \hat{U}_{ij}(z) &= \left(\frac{\hat{E}_i(z) + \hat{E}_j(z)}{2} \right) \delta_{ij} + \hat{H}_{ij}(z), \quad I_{ij} = \delta_{ij}, \\ \hat{H}_{ij}(z) &= \hat{H}_{ji}(z) = \int_0^\infty \frac{\partial \hat{\Phi}_i(\rho; z)}{\partial z} \frac{\partial \hat{\Phi}_j(\rho; z)}{\partial z} \rho d\rho, \\ \hat{Q}_{ij}(z) &= -\hat{Q}_{ji}(z) = - \int_0^\infty \hat{\Phi}_i(\rho; z) \frac{\partial \hat{\Phi}_j(\rho; z)}{\partial z} \rho d\rho. \end{aligned} \quad (15)$$

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

$$\lim_{z \rightarrow 0} \left(\frac{d}{dz} - \hat{\mathbf{Q}}(z) \right) \hat{\chi}^{(i)}(z) = 0, \quad \sigma = +1, \quad \hat{\chi}^{(i)}(0) = 0, \quad \sigma = -1, \quad (16)$$

$$\lim_{z \rightarrow \pm\infty} \hat{\chi}^{(i)}(z) = 0 \quad \rightarrow \quad \hat{\chi}^{(i)}(\pm z_{\max}) = 0, \quad (17)$$

$$\int_{-z_{\max}}^{z_{\max}} \left(\hat{\chi}^{(i)}(z) \right)^T \hat{\chi}^{(j)}(z) dz = 2 \int_0^{z_{\max}} \left(\hat{\chi}^{(i)}(z) \right)^T \hat{\chi}^{(j)}(z) dz = \delta_{ij}. \quad (18)$$

The asymptotic boundary condition for the continuum wave function will be considered below.

Algorithm 1 of generation of parametric algebraic problems by the Finite Element Method

To solve eigenvalue problem for equation (10) the boundary conditions (11), (12) and the normalization condition (13) with respect to the space variable ρ on an infinite interval are replaced with appropriate conditions (11), (13) 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 (10) by means of the FEM on the grid, $\Omega_{h(\rho)}^p = (\rho_0 = \rho_{\min}, \rho_j = \rho_{j-1} + h_j, \rho_{\bar{n}} = \rho_{\max})$, in a finite sum in each $z = z_k$ of the grid $\Omega_{h(z)}^p [z_{\min}, z_{\max}]$:

$$\hat{\Phi}(\rho; z) = \sum_{\mu=0}^{\bar{n}p} \Phi_{\mu}^h(z) N_{\mu}^p(\rho) = \sum_{r=0}^{\bar{n}} \sum_{j=1}^p \Phi_{r+p(j-1)}^h(z) N_{r+p(j-1)}^p(\rho), \quad (19)$$

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.,

$N_{\nu}^p(\rho_{\mu}) = \delta_{\nu\mu}$, $\mu, \nu = 0, 1, \dots, \bar{n}p$. The coefficients $\Phi_{\nu}(z)$ are formally connected with solution $\hat{\Phi}(\rho_{j,r}^p; z)$ in a node $\rho_{\nu} = \rho_{j,r}^p$, $r = 1, \dots, p$, $j = 0, \dots, \bar{n}$:

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

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. It has been shown that we have a possibility to construct schemes with high order of accuracy comparable with the computer one. Let us consider the reduction of differential equations (10) on the interval $\Delta : \rho_{\min} < \rho < \rho_{\max}$ with boundary conditions in points ρ_{\min} and ρ_{\max} rewriting in the form

$$\mathbf{A}(z)\hat{\Phi}(\rho; z) = \hat{E}(z)\mathbf{B}(z)\hat{\Phi}(\rho; z), \quad (20)$$

where \mathbf{A} and \mathbf{B} are differential operators. Substituting expansion (19) to (20) 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

$$\mathbf{a}_{\mu\nu}^p \Phi_{\mu}^h(z) = \hat{E}(z) \mathbf{b}_{\mu\nu}^p \Phi_{\mu}^h(z), \quad (21)$$

in framework of the briefly described FEM. Using p -order Lagrange elements, we present below an algorithm 1 for construction of algebraic problem (21) 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.

Algorithm 2 of evaluation the asymptotics of effective potentials at large $|z|$ in Kantorovich method

Step 1. In (10) apply the transformation to a scaled variable x

$$x = \frac{\gamma\rho^2}{2}, \quad \rho = \frac{\sqrt{x}}{\sqrt{\gamma/2}}, \quad (22)$$

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

$$\left(-\frac{\partial}{\partial x} x \frac{\partial}{\partial x} + \frac{m^2}{4x} + \frac{x}{4} + \frac{m}{2} - \frac{Z}{\gamma\sqrt{\frac{2x}{\gamma} + z^2}} - \lambda \right) \hat{\Phi}_j(x; z) = 0, \quad (23)$$

with a normalization condition

$$\frac{1}{\gamma} \int_0^\infty \hat{\Phi}_j(x; z)^2 dx = 1. \quad (24)$$

At $Z = 0$ Eq. (23) takes the form

$$L(n)\Phi_{nm}^{(0)}(x) = 0, \quad L(n) = -\frac{\partial}{\partial x}x\frac{\partial}{\partial x} + \frac{m^2}{4x} + \frac{x}{4} - \lambda^{(0)}, \quad (25)$$

and has the regular and bounded solutions at

$$\lambda^{(0)} = n + (|m| + 1)/2, \quad (26)$$

where transverse quantum number $n \equiv N_\rho = j - 1 = 0, 1, \dots$ determines the number of nodes of the solution $\Phi_{nm}^{(0)}(x)$ with respect to the variable x . Normalized solutions of Eq. (25), take the form

$$\Phi_{nm}^{(0)}(x) = C_{n|m|} e^{-\frac{x}{2}} x^{\frac{|m|}{2}} L_n^{|m|}(x), \quad C_{n|m|} = \left[\gamma \frac{n!}{(n + |m|)!} \right]^{\frac{1}{2}}, \quad (27)$$

$$\frac{1}{\gamma} \int_0^\infty \Phi_{nm}^{(0)}(x) \Phi_{n'm}^{(0)}(x) dx = \delta_{nn'}, \quad (28)$$

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

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

$$\frac{Z}{\gamma|z|} - \frac{Z}{\gamma\sqrt{\frac{2x}{\gamma} + z^2}} = \sum_{k=1}^{j_{\max}} \frac{V(k)}{|z|^k},$$
$$V(k) = \begin{cases} -(-1)^{k'} \frac{(2k'-1)!!}{k'!} \frac{Zx^{k'}}{\gamma^{k'+1}}, & k = 2k' + 1, \quad k' = 1, 2, \dots, \\ 0, & \text{otherwise,} \end{cases}$$

to Eq. (23) at $Z \neq 0$, transform it in the following form

$$L(n)\hat{\Phi}_j(x; z) + \left(\sum_{k=1}^{j_{\max}} \frac{V(k)}{|z|^k} - \delta\lambda \right) \hat{\Phi}_j(x; z) = 0. \quad (29)$$

Step 3.

Solution of equation (29) is found in the form of the perturbation series by inverse powers of $|z|$

$$\delta\lambda = \sum_{k=0}^{k_{\max}} |z|^{-k} \lambda^{(k)}, \quad \Phi_j(x; z) = \sum_{k=0}^{k_{\max}} |z|^{-k} \Phi_n^{(k)}(x). \quad (30)$$

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

$$\begin{aligned} L(n)\Phi^{(0)}(x) &= 0 \equiv f^{(0)}, \\ L(n)\Phi^{(k)}(x) &= \sum_{p=0}^{k-1} (\lambda^{(k-p)} - V^{(k-p)})\Phi^{(p)}(x) \equiv f^{(k)}, \quad k \geq 1. \end{aligned} \quad (31)$$

For solving the Eqs. (29) the unnormalized orthogonal basis

$$\begin{aligned}\Phi_{n+s}(x) &= C_{n|m|} e^{-\frac{x}{2}} x^{\frac{|m|}{2}} L_{n+s}^{|m|}(x) = C_{n|m|} C_{n+s|m|}^{-1} \Phi_{n+s,m}^{(0)}(x), \quad (32) \\ \langle s|s' \rangle &= \int_0^\infty \Phi_{n+s}(x) \Phi_{n+s'}(x) dx = \delta_{ss'} \gamma \frac{n!}{(n+|m|)!} \frac{(n+s+|m|)!}{(n+s)!},\end{aligned}$$

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

$$\begin{aligned}L(n)\Phi_{n+s}(x) &= s\Phi_{n+s}(x), \quad (33) \\ x\Phi_{n+s}(x) &= -(n+s+|m|)\Phi_{n+s-1}(x) + (2(n+s)+|m|+1)\Phi_{n+s}(x) \\ &\quad - (n+s+1)\Phi_{n+s+1}(x).\end{aligned}$$

Step 4.

Applying relations (33), the right-hand side $f^{(k)}$ and solutions $\Phi^{(k)}(x)$ of the system (31) are expanded over basis states $\Phi_{n+s}(x)$

$$\Phi_n^{(k)}(x) = \sum_{s=-k}^k b_s^{(k)} \Phi_{n+s}(x), \quad f^{(k)} = \sum_{s=-k}^k f_s^{(k)} \Phi_{n+s}(x). \quad (34)$$

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

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

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

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

The initial conditions (26) and $b_s^{(0)} = \delta_{s0}$ are followed from (25) and (28).

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:

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

As an example of output file at steps 1–5, we display nonzero coefficients $\lambda^{(k)}$, $b_s^{(k)}$ of the inverse power series (30), (34) up to $O(|z|^{-5})$:

$$\begin{aligned} \lambda^{(0)} &= n + (|m| + 1)/2, & \lambda^{(3)} &= Z(2n + |m| + 1)/\gamma^2, \\ b_0^{(0)} &= 1, & b_{-1}^{(3)} &= -Z(n + |m|)/\gamma^2, & b_1^{(3)} &= Z(n + 1)/\gamma^2. \end{aligned} \quad (35)$$

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

$$\hat{H}_{ij}(z) = \frac{1}{\gamma} \int_0^{\infty} dx \frac{\partial \hat{\Phi}_i(x; z)}{\partial z} \frac{\partial \hat{\Phi}_j(x; z)}{\partial z}, \quad \hat{Q}_{ij}(z) = -\frac{1}{\gamma} \int_0^{\infty} dx \hat{\Phi}_i(x; z) \frac{\partial \hat{\Phi}_j(x; z)}{\partial z}. \quad (36)$$

For their evaluation the decomposition of solution Eqs. (25) over the normalized orthogonal basis $\Phi_{n+s}^{(0)}$ with the normalized coefficients $b_{n;n+s}^{(k)}$,

$$\Phi_n^{(k)}(x) = \sum_{s=-k}^k b_{n;n+s}^{(k)} \Phi_{n+s}^{(0)}, \quad (37)$$

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

$$b_{n;n+s}^{(k)} = b_s^{(k)} \sqrt{\frac{n!}{(n+|m|)!} \frac{(n+s+|m|)!}{(n+s)!}} \quad (38)$$

as follows from (34), (37) and (32).

Step 7.

In a result of substitution (30), (37) in (36), matrix elements takes form

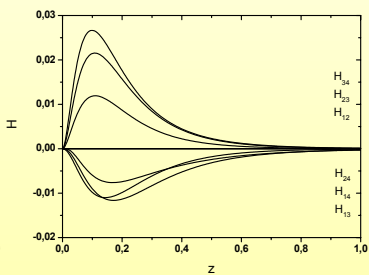
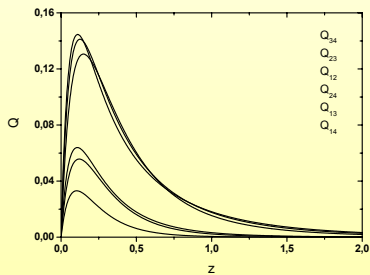
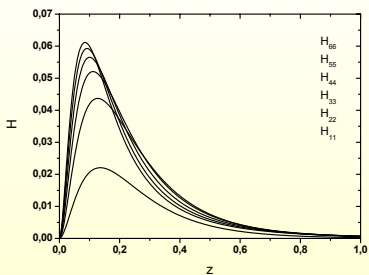
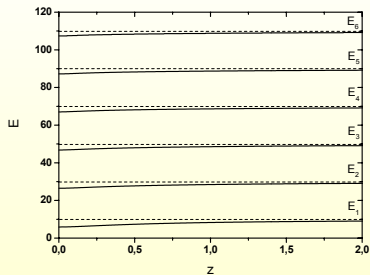
$$\begin{aligned}\hat{Q}_{jj+t}(z) &= - \sum_{k=0}^{k_{\max}-1} |z|^{-k-1} \sum_{k'=0}^k \sum_{s=\max(-k, k'-k-t)}^{\min(k, k-k'-t)} (k-k') b_{n;n+s}^{(k')} b_{n+t;n+s}^{(k-k')}, \\ \hat{H}_{jj+t}(z) &= \sum_{k=0}^{k_{\max}-2} |z|^{-k-2} \sum_{k'=0}^k \sum_{s=\max(-k, k'-k-t)}^{\min(k, k-k'-t)} k'(k-k') b_{n;n+s}^{(k')} b_{n+t;n+s}^{(k-k')}. \quad (39)\end{aligned}$$

Collecting of coefficients of (39) at equal powers of $|z|$, algorithm leads to final expansions of eigenvalues and effective potentials of output file

$$\hat{E}_j(z) = \sum_{k=0}^{k_{\max}} |z|^{-k} E_j^{(k)}, \quad \hat{H}_{ij}(z) = \sum_{k=8}^{k_{\max}} |z|^{-k} H_{ij}^{(k)}, \quad \hat{Q}_{ij}(z) = \sum_{k=4}^{k_{\max}} |z|^{-k} Q_{ij}^{(k)}. \quad (40)$$

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

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



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

Values of the partial sums (40) 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	$\hat{Q}_{12}, 10^{-6}$	$\hat{Q}_{23}, 10^{-6}$	$\hat{Q}_{34}, 10^{-5}$	$\hat{Q}_{13}, 10^{-8}$	$\hat{Q}_{24}, 10^{-8}$
$z^{-4} Q_{ij}^{(4)}$	4.24264069	7.34846923	1.03923048	0	0
$+z^{-6} Q_{ij}^{(6)}$	4.17900108	7.16475750	1.00285742	1.29903811	3.18198052
$+z^{-7} Q_{ij}^{(7)}$	4.17883137	7.16446356	1.00281585	1.29903811	3.18198052
$+z^{-8} Q_{ij}^{(8)}$	4.17972233	7.16857870	1.00394341	1.26266504	3.04833733
$+z^{-9} Q_{ij}^{(9)}$	4.17972824	7.16859579	1.00394680	1.26260268	3.04818460
$+z^{-10} Q_{ij}^{(10)}$	4.17971489	7.16850321	1.00391243	1.26342108	3.05252800
$+z^{-11} Q_{ij}^{(11)}$	4.17971474	7.16850253	1.00391224	1.26342451	3.05254060
$+z^{-12} Q_{ij}^{(12)}$	4.17971496	7.16850469	1.00391330	1.26340651	3.05240830
$+z^{-13} Q_{ij}^{(13)}$	4.17971496	7.16850471	1.00391331	1.26340638	3.05240762
$+z^{-14} Q_{ij}^{(14)}$	4.17971496	7.16850466	1.00391328	1.26340679	3.05241163
$+z^{-15} Q_{ij}^{(15)}$	4.17971496	7.16850466	1.00391327	1.26340679	3.05241166
$+z^{-16} Q_{ij}^{(16)}$	4.17971496	7.16850466	1.00391328	1.26340678	3.05241154
(n.v.)	4.17971496	7.16850466	1.00391328	1.26340678	3.05241154

Algorithm 3 of evaluation the asymptotics of solutions at large $|z|$ in Kantorovich method

Step 1. We write the set of differential equations (14) at fixed values m , and ϵ in the explicit form for $\chi_{j i_o}(z) \equiv \hat{\chi}_j^{(i_o)}(z)$ and $j = 1, 2, \dots, j_{\max}$, $i_o = 1, 2, \dots, N_o$

$$\begin{aligned} & -\frac{d^2 \chi_{j i_o}(z)}{dz^2} - \frac{2Z}{|z|} \chi_{j i_o}(z) - \left(\epsilon - \hat{E}_j(z) - \frac{2Z}{|z|} \right) \chi_{j i_o}(z) + \hat{H}_{jj}(z) \chi_{j i_o}(z) \\ & = \sum_{j'=1, j' \neq j}^{j_{\max}} \left(-\hat{Q}_{jj'}(z) \frac{d}{dz} - \hat{H}_{jj'}(z) - \frac{d\hat{Q}_{jj'}(z)}{dz} \right) \chi_{j' i_o}(z), \end{aligned} \quad (41)$$

where matrix elements $\hat{Q}_{jj'}(z)$ and $\hat{H}_{jj'}(z)$ have of the form (40).

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:

$$\chi_{ji_o}(z) = \frac{\exp(w(z))}{\sqrt{p_{i_o}}} \phi_{ji_o}(z), \quad \phi_{ji_o}(z) = \sum_{k=0}^{k_{\max}} \phi_{ji_o}^{(k)} |z|^{-k}, \quad (42)$$

where $w(z) = \nu p_{i_o} |z| + \nu \zeta \ln(2p_{i_o} |z|) + \nu \delta_{i_o}$, 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

$$\begin{aligned}
 (p_{i_o}^2 - 2E + E_j^{(0)})\phi_{ji_o}^{(k)} &= f_{ji_o}^{(k)}(\phi_{j'i_o}^{(k'=0, \dots, k-1)}, p_{i_o}) \\
 &\equiv -2(\zeta p_{i_o} + \iota(k-1)p_{i_o} - Z)\phi_{ji_o}^{(k-1)} - (\zeta + \iota(k-2))(\zeta + \iota(k-1))\phi_{ji_o}^{(k-2)} \\
 &\quad - \sum_{k'=3}^k (E_j^{(k')} + H_{jj}^{(k')})\phi_{ji_o}^{(k-k')} + \sum_{j'=1}^{j_{\max}} \sum_{k'=4}^k (-2\iota Q_{jj'}^{(k')} p_{i_o} - H_{jj'}^{(k')})\phi_{j'i_o}^{(k-k')} \\
 &\quad + \sum_{j'=1}^{j_{\max}} \sum_{k'=5}^k (2k-1-k'-2\iota\zeta)Q_{jj'}^{(k'-1)}\phi_{j'i_o}^{(k-k')}, \\
 k = 0, 1, \dots, k_{\max}, \quad \phi_{ji_o}^{(-1)} &\equiv 0, \quad \phi_{ji_o}^{(-2)} \equiv 0, \quad k_{\max} \leq j_{\max} - i_o. \quad (43)
 \end{aligned}$$

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

Step 2.

From first two equations ($k = 0, 1$) of set (43) we have the leading terms of eigenfunction $\phi_{ji_o}^{(0)}$, eigenvalue $p_{i_o}^2$ and characteristic parameter ζ , i.e initial data for solving recurrence sequence,

$$\phi_{ji_o}^{(0)} = \delta_{ji_o}, \quad p_{i_o}^2 = 2E - E_{i_o}^{(0)} \rightarrow p_{i_o} = \sqrt{2E - E_{i_o}^{(0)}}, \quad \zeta = Z/p_{i_o}. \quad (44)$$

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 $i_o = 1, \dots, N_o$ and $p_{i_o}^2 < 0$ for $i_o = N_o + 1, \dots, j_{\max}$.

Step 3.

Substituting (44) in (43), we obtain the following recurrent set of algebraic equations for the unknown coefficients $\phi_{j i_o}(z)$ for $k = 1, 2, \dots, k_{\max}$:

$$(E_{i_o}^{(0)} - E_j^{(0)})\phi_{j i_o}^{(k)} = f_{j i_o}^{(k)}(\phi_{j' i_o}^{(k'=0, \dots, k-1)}, p_{i_o}) \quad (45)$$

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

$$\begin{aligned} \phi_{j i_o}^{(k)} &= f_{j i_o}^{(k)}(\phi_{j' i_o}^{(k'=0, \dots, k-1)}, p_{i_o}) / (E_{i_o}^{(0)} - E_j^{(0)}), \quad j \neq i_o, \\ f_{i_o i_o}^{(k+1)}(\phi_{j' i_o}^{(k'=0, \dots, k)}, p_{i_o}) &= 0 \rightarrow \phi_{i_o i_o}^{(k)}. \end{aligned} \quad (46)$$

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

$$\phi_{ji_o}^{(0)} = \delta_{ji_o},$$

$$\phi_{ji_o}^{(1)} = \delta_{ji_o} i Z(Z + \nu p_{i_o}) / (2p_{i_o}^3),$$

$$\phi_{ji_o}^{(2)} = \delta_{ji_o} [i E_j^{(3)} / (4p_{i_o}) - Z(Z + \nu p_{i_o})^2 (Z + 2\nu p_{i_o}) / (8p_{i_o}^6)],$$

$$\phi_{ji_o}^{(3)} = \delta_{ji_o} [-E_j^{(3)} (3Z^2 + 7\nu p_{i_o} Z - 6p_{i_o}^2) / (24p_{i_o}^4) \\ - i Z(Z + \nu p_{i_o})^2 (Z + 2\nu p_{i_o})^2 (Z + 3\nu p_{i_o}) / (48p_{i_o}^9)],$$

$$\phi_{ji_o}^{(4)} = \delta_{ji_o} [i E_j^{(5)} / (8p_{i_o}) - (E_j^{(3)})^2 / (32p_{i_o}^2) \\ - i E_j^{(3)} (3Z^4 + 20\nu p_{i_o} Z^3 - 53p_{i_o}^2 Z^2 - 66\nu p_{i_o}^3 Z + 36p_{i_o}^4) / (96p_{i_o}^7) \\ + Z(Z + \nu p_{i_o})^2 (Z + 2\nu p_{i_o})^2 (Z + 3\nu p_{i_o})^2 (Z + 4\nu p_{i_o}) / (384p_{i_o}^{12})] \\ + 2\nu p_{i_o} Q_{ji_o}^{(4)} / (E_{i_o}^{(0)} - E_j^{(0)}).$$

Remarks:

1. Expansion (42) holds true for $|z_m| \gg \max(Z^2/(2p_{i_o}^3), 2Z(2i_o + |m| - 1)/(8\gamma p_{i_o}^2))$. 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 $D_z \equiv \text{Id}/dz - \mathbf{Q}(z)$

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

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

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

Applications algorithms for solving the eigenvalue problem

The symbolic-numerical algorithms are used to generate an input file of effective potentials in the Gaussian points $z = z_k$ of the FEM grid $\Omega_{h(z)}^p [z_{\min} = 0, z_{\max}]$ and asymptotic of solutions of a set of longitudinal equations (14)–(18) for the KANTBP code (Chuluunbaatar, O., et al: KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach. accepted in Comput. Phys. Commun. (2007)). The calculations was performed on a grid $\Omega_{h(z)}^p = \{0(200)2(600)150\}$ (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 (Dimova, M.G., Kaschiev, M.S., Vinitisky, S.I.: The Kantorovich method for high-accuracy calculations of a hydrogen atom in a strong magnetic field: low-lying excited states. Journal of Physics B: At. Mol. Phys. **38** (2005) 2337–2352) given in the last line of the Table is shown that elaborated method in cylindrical coordinates is applicable for strength magnetic field $\gamma > 5$ and magnetic number m of order of ~ 10 .

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.

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)
	1.125 422 341 (8)	0.182 301 494 (7)	0.859 832 622 (6)	0.165 264 273 (1)

Conclusion

- A set of symbolic-numerical algorithms for 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 of the Kantorovich expansion 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 symbolic-numerical algorithms for calculating effective potentials and asymptotic solutions allows us to generate effective approximations for a finite set of longitudinal equations describing an open channel to have the low upper estimations.
- 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 $B = 6.10\text{T}$ ($\gamma = 2.595 \cdot 10^{-5}$ a.u.), such that several equations are provide a given accuracy.
- 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 and channeling of ions in thin films .

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