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POTHMF, a Program to Compute Matrix Elements of the Coupled Radial Equations for a Hydrogen-like Atom in a Homogeneous Magnetic Field

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Abstract. We describe POTHMF, a program to compute matrix elements of the coupled radial equations for a hydrogen-like atom in a homogeneous magnetic field. POTHMF computes with a prescribed accuracy the oblate angular spheroidal functions, which depend on a parameter and corresponding eigenvalues, and the matrix elements, which are integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter. The program, implemented in Maple-Fortran, consists of a package of symbolic-numerical algorithms that reduce a singular two-dimensional boundary value problem for an elliptic second-order partial differential equation to a regular boundary value problem for a system of second-order ordinary differential equations using the Kantorovich method.

1 Introduction

The calculation of the dynamics of electron states of hydrogen-like atoms in a magnetic field in atomic physics is reduced to a boundary value problem for an elliptic second-order partial differential equation in a two-dimensional region for fixed values of the magnetic number and parity [1]. Efficient algorithms for the numerical solution of this problem are based on its reduction to a system of ordinary differential equations by the Kantorovich method, using the oblate angular spheroidal functions [2] as the basis for the expansion of the unknown solution. For an efficient application of the Kantorovich method we elaborate the POTHMF program as a set of symbolic-numerical algorithms for computing the following quantities to a prescribed accuracy [3]:

• oblate angular spheroidal functions on a bounded interval of the parameter values,

• derivatives with respect to the parameter of the angular functions and of the matrix elements (integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter),

• asymptotics of the radial parameter of the eigenfunctions and of the matrix elements that appear as variable coefficients in the system of ordinary differential equations,

• asymptotics of the solutions to the system of ordinary differential equations for small and large values of the radial variable,

• solutions of the boundary value problem for the system of second-order ordinary differential equations.

The program also calculates asymptotic regular and irregular matrix solutions of the system of second-order ordinary differential equations at the end of interval in the radial variable needed for solving the corresponded boundary problem with third-type boundary conditions.

2 The problem statement

The Schrödinger equation for the hydrogen atom in an axially symmetric magnetic field $\mathbf{B} = (0, 0, B)$ in spherical coordinates $(r, \eta = \cos\theta, \varphi)$ can be written as the 2D-equation in the region $\Omega = \{0 < r < \infty, -1 < \eta < 1\}$ [1]

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\hat{A}^{(0)}(r,\eta)}{r^2} - \frac{2Z}{r} - \epsilon \right) \Psi(r,\eta) = 0. \qquad (1)$$

The operator $\hat{A}^{(0)}(r,\eta) = A^{(0)}(r,\eta) + \gamma m r^2$, where $A^{(0)}(r,\eta)$ is given by

$$A^{(0)}(r,\eta) = -\frac{\partial}{\partial \eta}(1-\eta^2)\frac{\partial}{\partial \eta} + \frac{m^2}{1-\eta^2} + \left(\frac{\gamma r^2}{2}\right)^2 (1-\eta^2). \qquad (2)$$

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, and the atomic units $(a.u.)$ $\hbar = m_e = e = 1$ are used under the assumption of infinite mass of the nucleus having charge Z. In these expressions, $\epsilon = 2E$ is the doubled energy (in Rydbergs, 1Ry=(1/2) $a.u.$) of the state $|m\sigma\rangle$ at fixed values of m and z-parity; $\sigma = \pm 1$; $\Psi \equiv \Psi_{m\sigma}(r,\theta) = (\Psi_m(r,\theta) + \sigma\Psi_m(r,\pi-\theta))/\sqrt{2}$ is the corresponding wave function. The wave functions $\Psi_i^{Em\sigma}(r,\eta)\exp(\imath m\varphi)/\sqrt{2\pi}$ with fixed parity σ and azimuthal quantum number m is expanded over the one-dimensional basis, $\Phi_j^{m\sigma}(\eta; r)$,

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

with unknown radial vector-solutions $\chi_j^{(m\sigma i)}(E, r)$. The basis functions are solutions of the eigenvalue problem for the angular oblate spheroidal functions[2]

$$\hat{A}^{(0)}(r,\eta)\Phi_j(\eta; r) = E_j(r)\Phi_j(\eta; r), \quad I_{ij}(r) = \int_{-1}^{1} \Phi_i(\eta; r)\Phi_j(\eta; r)d\eta = \delta_{ij}. \qquad (3)$$

Thus, the Schrödinger equation in the 2D-region, $\Omega = \{R^1_+ \times [-1,1]\}$, is reduced to a set of coupled differential equations

$$\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\mathbf{U}(r)}{r^2} + \mathbf{Q}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{d\,r^2\mathbf{Q}(r)}{dr}\right)\boldsymbol{\chi}^{(i)}(r) = \epsilon_i\,\mathbf{I}\boldsymbol{\chi}^{(i)}(r). \quad (4)$$

The matrix of effective potentials $\mathbf{U}(r)$ and $\mathbf{Q}(r)$ of $j_{\max} \times j_{\max}$ are given by

$$U_{ij}(r) = \frac{E_i(r) + E_j(r)}{2}\delta_{ij} - 2Zr\delta_{ij} + r^2 H_{ij}(r), \quad I_{ij} = \delta_{ij}, \quad (5)$$

$$H_{ij}(r) = \int_{-1}^{1}\frac{\partial\Phi_i(\eta;r)}{\partial r}\frac{\partial\Phi_j(\eta;r)}{\partial r}d\eta, \quad Q_{ij}(r) = -\int_{-1}^{1}\Phi_i(\eta;r)\frac{\partial\Phi_j(\eta;r)}{\partial r}d\eta.$$

The wave function $\boldsymbol{\chi}(r) = \{\chi_j^{(m\sigma i)}(E,r)\}_{j=1}$ satisfies the following boundary conditions at $r \to 0$

$$\lim_{r\to 0} r^2\left(\mathbf{I}\frac{d}{dr} - \mathbf{Q}(r)\right)\boldsymbol{\chi}(r) = 0, \quad (6)$$

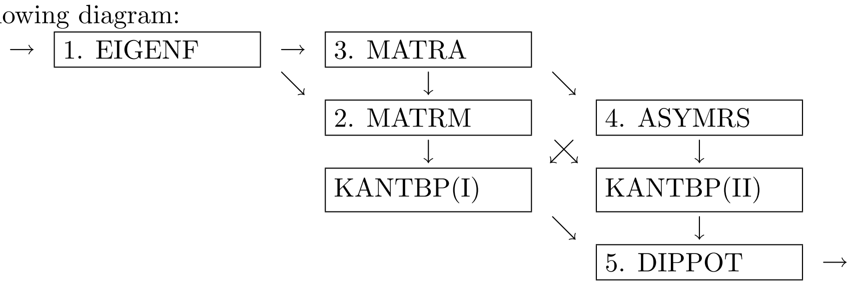
and at large $r = r_{\max} \gg 1$

$$\boldsymbol{\chi}(r) = 0, \quad \text{for the discrete spectrum,} \quad (7)$$

$$\left(\mathbf{I}\frac{d}{dr} - \mathbf{Q}(r)\right)\boldsymbol{\chi}(r) = \mu(r)\boldsymbol{\chi}(r), \quad \text{for the continuous spectrum.} \quad (8)$$

Note, the energy $\epsilon \equiv \epsilon(r_{\max})$ plays the role of eigenvalues of the boundary problem (4)–(7) on a finite interval $0 \le r \le r_{\max}$, while the unknown parameters $\mu \equiv \mu(r_{\max}, \epsilon)$ at fixed value of ϵ play the role of eigenvalues of the logarithmic normal derivative matrix of the solution of the boundary problem (4)–(6), (8).

To reduce the system of radial equations to the finite interval $r \in (0, r_{\max})$ with homogeneous boundary conditions of the third type, symbolic algorithms for evaluating asymptotics of the effective potentials and the solutions of radial equations at small and large values of r are elaborated. The resulting system of radial equations, which contains the first-derivative coupling terms, is solved using the finite element method by means of the KANTBP program, implemented in FORTRAN. POTHMF calculates energy values, the reaction matrix and unknown radial vector-solutions, and the photoionization cross-sections. POTHMF prepares input files for KANTBP and has the structure given by the following diagram:



In procedure EIGENF, the eigenvalue problem for one-dimension differential equation is reduced to the algebraic eigenvalue problem, which is solved for a finite set of values of parameter r.
In procedure MATRM, using solutions of the algebraic eigenvalue problem above, the parametric derivatives of the basis functions, $\partial\Phi_j(\eta;r)/\partial r$ and matrix elements $Q_{ij}(r)$, $H_{ij}(r)$, $\partial Q_{ij}(r)/\partial r$, etc, are calculated.
In procedure MATRA, the asymptotic solutions of the algebraic eigenvalue problem generated in EIGENF as well as its matrix elements are calculated as a power series in the parameter r^2 and its inverse.
In procedure ASYMRS, using asymptotics of matrix elements, the asymptotics of the fundamental radial solutions at small and large values r are calculated and the needed boundary conditions for a reduced interval $[0, r_{max}]$ are generated.
In procedure DIPPOT, the transition matrix elements are evaluated using the results of program KANTBP.

3 The procedure EIGENF

In procedure EIGENF, the eigenvalue problem for a one-dimensional differential equation is reduced to the algebraic eigenvalue problem, which is solved for a finite set of values of parameter r.

We obtain eigenfunctions $\Phi_j(\eta;\hat{r})$ in the form of a series expansion at fixed values $\sigma = \pm 1$ and m,

$$\Phi_j(\eta;\hat{r}) = \sum_{s=(1-\sigma)/2}^{s_{\max}} c_{sj}^{m\sigma}(\hat{r}) P_{|m|+s}^{|m|}(\eta). \tag{9}$$

Here, s is an even (odd) integer at $\sigma = (-1)^s = \pm 1$ until $s_{\max} = 2(N_{\max} - 1) + (1-\sigma)/2$, where $N_{\max}$ is the number of even or odd terms of expansion, and $P_{|m|+s}^{|m|}(\eta)$ are the normalized associated Legendre polynomials defined by the relation [2]:

$$-\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}P_{|m|+s}^{|m|}(\eta) + \frac{m^2}{1-\eta^2}P_{|m|+s}^{|m|}(\eta) = \lambda_s^{m\sigma}(0)P_{|m|+s}^{|m|}(\eta), \tag{10}$$

$$\lambda_s^{m\sigma}(0) = (|m|+s)(|m|+s+1), \quad s = 2(j-1) + (1-\sigma)/2,$$

$$\int_{-1}^{1} P_{|m|+s}^{|m|}(\eta) P_{|m|+s'}^{|m|}(\eta) d\eta = \delta_{ss'}. \tag{11}$$

The coefficients $c_{sj}^{m\sigma}(\hat{r})$ satisfy the relation

$$\sum_{s=(1-\sigma)/2}^{s_{\max}} c_{sj}^{m\sigma}(\hat{r}) c_{sj'}^{m\sigma}(\hat{r}) = \delta_{jj'}. \tag{12}$$

The eigenvalue problem for eigenvectors $\mathbf{c}_j = \{c_{sj}^{m\sigma}(\hat{r})\}_{(1-\sigma)/2}^{s_{\max}}$, and eigenvalues $\lambda_j(\hat{r})$ take the form

$$\mathbf{A}^{(0)}\mathbf{c}_j = \lambda_j(\hat{r})\mathbf{c}_j, \tag{13}$$

where matrix $\mathbf{A}^{(0)}$ is the symmetric tridiagonal $N_{\max} \times N_{\max}$ matrix:

$$A^{(0)}_{ss-2} = A^{(0)}_{s-2s} = \frac{-p^2}{(2s+2|m|-1)}\sqrt{\frac{(s-1)s(s+2|m|-1)(s+2|m|)}{(2s+2|m|-3)(2s+2|m|+1)}},$$
$$A^{(0)}_{ss} = (s+|m|)(s+|m|+1) + 2p^2\frac{(s^2+s+2s|m|+2m^2+|m|-1)}{(2s+2|m|-1)(2s+2|m|+3)}. \quad (14)$$

The expansion (9), which provides stability of the numerical calculation with double precision arithmetic (the relative machine precision is $eps \approx 2 \cdot 10^{-16}$), was implemented using the subroutine DSTEVR from the LAPACK Fortran Library [4]. The orthogonality relations (12) were computed with an accuracy of the order of *eps*.

3.1 Finding the optimal value of $s_{\max}$ and the matching point $R_{\rm match}$ of numerical and asymptotic solutions

At large s elements of matrix $\mathbf{A}^{(0)}$ (14) take the form

$$A^{(0)}_{ss} = \frac{(2s+2|m|+1)^2-1}{4} + \frac{p^2}{2} + O(s^{-2}), \quad A^{(0)}_{ss\pm2} = -\frac{p^2}{4} + O(s^{-2}). \quad (15)$$

On intervals $s \in (s_b, s_e)$ at $s_b, s_e \gg 1$, we suppose that the elements of matrix $\mathbf{A}^{(0)}$ have slow dependence on s. Therefore, for a given value of λ, the solution of the algebraic problem (13), (15) will be represented in the form

$$c_s = xc_{s+2}, \quad c_{s-2} = xc_s. \quad (16)$$

From (16), (13), and (15) we have the following algebraic equation with respect to factor x

$$x + x^{-1} = d \equiv p^{-2}\left((2s+2|m|+1)^2 - 1 - 4\lambda + 2p^2\right). \quad (17)$$

For $s > s_2$, where $s_2 = (\sqrt{4\lambda+1} - 2|m| - 1)/2$ is determined from equation (17) at $d = 2$, equation (17) has two real solutions. One of them,

$$x_s = p^{-2}\left(\sqrt{(s-s_2)(s+s_2+2|m|+1)} + \sqrt{p^2+(s-s_2)(s+s_2+2|m|+1)}\right)^2, \quad (18)$$

exceeds unity by its absolute value and the other, x^{-1}, is smaller than one. Thus, the solution of (16) with decreased coefficients c_s at increased s exists. For $s < s_2$ we have two solutions with oscillating coefficients c_s. Then, the solution of Eq. (17) allows us to determine an algorithm for evaluating $s_{\max}$:

$$\prod_{s=s_2}^{s_{\max}-1} x_s < 1/eps, \qquad \prod_{s=s_2}^{s_{\max}} x_s > 1/eps. \quad (19)$$

We need an approximate value of the eigenvalue λ for the above calculation. If we use the fact all diagonal elements $A^{(0)}_{ss}$ of the tridiagonal matrix $\mathbf{A}^{(0)}$ and eigenvalues $\varepsilon_j(p)$ or $\lambda_j(p)$ increased by the number j, then we can obtain the upper bound of the eigenvalue λ_N with the help of Wilkinson's shift [5]:

$$shift = G + A^{(0)}_{s_N s_N} + \sqrt{G^2 + (A^{(0)}_{s_N s_N - 2})^2}, \quad G = \frac{A^{(0)}_{s_N-2 s_N-2} - A^{(0)}_{s_N s_N}}{2}, \quad (20)$$

where $s_N = 2(N-1) + (1-\sigma)/2$. But $shift \gg \lambda_N$ at $p \gg 1$. In this case we use an asymptotic expression of the eigenvalue (29) at $p \geq 2s_N$, since the asymptotic expression gives an upper bound of the eigenvalue.

The matching point R_{match} of the numerical and asymptotic solution is calculated by the MATRA algorithm as follows:

$$r_{\text{match}} = \max(r_\varepsilon, r_h, r_q),\ r_\varepsilon = \sqrt[18]{\frac{|\varepsilon^{(18)}_N|}{eps}},\ r_h = \sqrt[18]{\frac{|H^{(18)}_{NN}|}{eps}},\ r_q = \sqrt[17]{\frac{|Q^{(17)}_{NN-1}|}{eps}}, \quad (21)$$

since $|\varepsilon^{(2k)}_j| < \gamma|\varepsilon^{(2k+2)}_j|$, $|Q^{(2k-1)}_{jj'}| < \gamma|Q^{(2k+1)}_{jj'}|$, $|H^{(2k)}_{jj'}| < \gamma|H^{(2k+2)}_{jj'}|$ and $|Q^{(17)}_{jj'}| \leq |Q^{(17)}_{NN-1}|$, $|H^{(18)}_{jj'}| \leq |H^{(18)}_{NN}|$.

4 The procedure MATRM

In the procedure MATRM, based on solutions of the above algebraic eigenvalue problem, the parametric derivatives of the basis functions $\partial\Phi_j(\eta; r)/\partial r$ and matrix elements $Q_{ij}(r)$, $H_{ij}(r)$, $\partial Q_{ij}(r)/\partial r$, etc., are calculated.

The derivatives of functions $\Phi_j(\theta; r)$ at fixed values of $\sigma = \pm 1$ and m can be represented as the following expansion in terms of the normalized Legendre polynomials (9):

$$\Phi^{(n)}_j(\theta; r) = \sum_{s=(1-\sigma)/2}^{s_{\max}} c^{(n)}_{sj} P^{|m|}_{|m|+s}(\eta), \quad c^{(n)}_{sj} \equiv \frac{\partial^n c_{sj}(r)}{\partial r^n}, \quad (22)$$

where $\mathbf{c}^{(0)} \equiv \mathbf{c}_j$ and $\lambda^{(0)} \equiv \lambda_j(r)$.

Following (12)–(13), we solve the following linear recurrence system of algebraic equations:

$$(\mathbf{A}^{(0)}\mathbf{c}^{(k)} - \mathbf{c}^{(k)}\lambda^{(0)}) + (\mathbf{A}^{(k)}\mathbf{c}^{(0)} - \mathbf{c}^{(0)}\lambda^{(k)}) = \mathbf{b}_{(k)}, \quad \mathbf{A}^{(k)} \equiv \frac{\partial^k \mathbf{A}^{(0)}}{\partial r^k},$$
$$\mathbf{b}_{(k)} \equiv \sum_{n=1}^{k-1} \frac{k!}{n!(k-n)!}(\mathbf{c}^{(k-n)}\lambda^{(n)} - \mathbf{A}^{(n)}\mathbf{c}^{(k-n)}), \qquad \mathbf{b}_{(1)} \equiv 0. \quad (23)$$

From the normalization condition (12) we obtain the required additional equality

$$\sum_{n=0}^{k} \frac{k!}{n!(k-n)!} \mathbf{c}^{(k-n)T} \mathbf{c}^{(n)} = 0, \quad (24)$$

providing the uniqueness of the solution (23). The details of the algebraic realization of the algorithm are given in [3].

5 The procedure MATRA

In procedure MATRA, the asymptotic solutions of the algebraic eigenvalue problem generated in EIGENF and the matrix elements are calculated as a power series of the parameter r^2 and its inverse at small and large values r.

At step 1 we go from coordinate $\eta \in [0,1]$ (or $\eta \in [-1,0]$) to the new coordinate y using the formula $y = 2p(1-\eta)$ (or $y = 2p(1+\eta)$).
At steps 2 and 3 we go from the set of functions $\Phi_j(y)$ to the set of functions $F_n(y)$

$$\Phi_j(y) = \exp\left(-\frac{y}{2}\right)\left(\frac{y}{4p}\right)^{|m|/2}\left(1-\frac{y}{4p}\right)^{|m|/2} F_n(y), \tag{25}$$

that are found as a sum of Laguerre polynomials $L^{|m|}_{n+s}(y)$ [2] with unknowns $C_n(s,r)$

$$F_n(y) = 2^{|m|+1/2} p^{(|m|+1)/2} \sum\nolimits_s C_n(s,r) L^{|m|}_{n+s}(y). \tag{26}$$

In step 4, where we evaluate integrals, we change the domain from $[0,2p]$ to $[0,\infty)$, and then drop exponentially small terms. Step 5 finds $C_n(s,r)$ and λ_n as a series expansion

$$C_n(s,r) = c^{(0)}_{s,n} + \sum_{k=1}^{k_{\max}} \frac{c^{(k)}_{s,n}}{(4p)^k}, \quad \lambda_n = 4p\left[\frac{|m|+1}{2} + \beta^{(0)}_n + \sum_{k=1}^{k_{\max}} \frac{\beta^{(k)}_n}{(4p)^k}\right]. \tag{27}$$

Substituting (27) in the result of step 3 and equating coefficients at the same powers of p, we arrive at a system of recurrence relations for evaluating coefficients $\beta^{(k)}_n$ and $c^{(k)}_{s,n}$ (except $c^{(k)}_{0,n}$):

$$s c^{(k)}_{s,n} = ((n_s+|m|+1)(2n_s+|m|+1) - (n_s+|m|)(|m|+1)) c^{(k-1)}_{s,n} \tag{28}$$
$$-n_s(n_s+|m|) c^{(k-1)}_{s-1,n} - (n_s+|m|+1)(n_s+1) c^{(k-1)}_{s+1,n} + \sum_{k'=1}^{k-|s|} \beta^{(k')}_n c^{(k-k')}_{s,n},$$

with initial conditions $\beta^{(0)}_n = n$, $c^{(0)}_{s,n} = \delta_{s0}\sqrt{n!/(n+|m|)!}$.
In step 6, substituting (27) the coefficients $c^{(k)}_{s,j}$ evaluated in step 5 for expressions of the matrix elements evaluated in step 4, we easily find the matrix elements as a series expansion of inverse powers of r

$$r^{-2}\varepsilon_j(r) = \sum_{k=0}^{k_{\max}} \frac{\varepsilon^{(2k)}_j}{r^{2k}}, \quad H_{jj'}(r) = \sum_{k=1}^{k_{\max}} \frac{H^{(2k)}_{jj'}}{r^{2k}}, \quad Q_{jj'}(r) = \sum_{k=1}^{k_{\max}} \frac{Q^{(2k-1)}_{jj'}}{r^{2k-1}}. \tag{29}$$

6 Procedure ASYMRS

In procedure ASYMRS, using asymptotics of matrix elements, the asymptotics of the fundamental radial solutions at small and large values r are calculated and the needed boundary conditions for a reduced interval $[0, r_{max}]$ are generated. Now let us consider the asymptotic solution

$$\chi_{ji_o}(r) = R(p_{i_o}, r)\phi_{ji_o}(r) + \frac{dR(p_{i_o}, r)}{dr}\psi_{ji_o}(r), \tag{30}$$

where $R(p_{i_o}, r) = p_{i_o}^{-1/2} r^{-1}(\imath F_0(p_{i_o}, r) + G_0(p_{i_o}, r))/2$, $F_0(p_{i_o}, r)$ and $G_0(p_{i_o}, r)$ are the Coulomb regular and irregular functions, respectively [2]. The function $R(p_{i_o}, r)$ satisfies the differential equation

$$\frac{d^2R(p_{i_o}, r)}{dr^2} + \frac{2}{r}\frac{dR(p_{i_o}, r)}{dr} + \left(p_{i_o}^2 + \frac{2Z}{r}\right)R(p_{i_o}, r) = 0. \tag{31}$$

Substituting the function (30) into Eq. (4) using (31) and extracting the coefficients for the Coulomb function and its derivative, we arrive at two coupled differential equations with respect to the unknown functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$. Then we expand the functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$ in the inverse power series of r:

$$\phi_{ji_o}(r) = \sum\nolimits_{k=0}^{k_{\max}} \phi_{ji_o}^{(k)} r^{-k}, \quad \psi_{ji_o}(r) = \sum\nolimits_{k=0}^{k_{\max}} \psi_{ji_o}^{(k)} r^{-k}. \tag{32}$$

After substituting the expansions (29), (32) to the given coupled differential equations and equating the coefficients of the same powers of r, we compute a set of recurrence relations with respect to the unknown coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$

$$\begin{aligned}
&\left(p_{i_o}^2 - 2E + \varepsilon_j^{(0)}\right)\phi_{ji_o}^{(k)} - 2p_{i_o}^2(k-1)\psi_{ji_o}^{(k-1)} - (k-2)(k-3)\phi_{ji_o}^{(k-2)} \\
&\qquad -2Z(2k-3)\psi_{ji_o}^{(k-2)} + \sum_{k'=1}^{k}\left(\varepsilon_j^{(k')} + H_{jj}^{(k')}\right)\phi_{ji_o}^{(k-k')} \\
&= \sum_{j'=1, j'\neq j}^{N}\sum_{k'=1}^{k}\Bigg[\left((2k-k'-3)Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')}\right)\phi_{j'i_o}^{(k-k')} \\
&\qquad + \left(2p_{i_o}^2 Q_{jj'}^{(k')} + 4ZQ_{jj'}^{(k'-1)}\right)\psi_{j'i_o}^{(k-k')}\Bigg],
\end{aligned} \tag{33}$$

$$\begin{aligned}
&\left(p_{i_o}^2 - 2E + \varepsilon_j^{(0)}\right)\psi_{ji_o}^{(k)} + 2(k-1)\phi_{ji_o}^{(k-1)} - k(k-1)\psi_{ji_o}^{(k-2)} \\
&+ \sum_{k'=1}^{k}\left(\varepsilon_j^{(k')} + H_{jj}^{(k')}\right)\psi_{ji_o}^{(k-k')} \\
&= \sum_{j'=1, j'\neq j}^{N}\sum_{k'=1}^{k}\left[\left((2k-k'+1)Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')}\right)\psi_{j'i_o}^{(k-k')} - 2Q_{jj'}^{(k')}\phi_{j'i_o}^{(k-k')}\right].
\end{aligned} \tag{34}$$

From the first four equations of the set (33), (34) for $\phi_{i_oi_o}^{(0)}$, $\phi_{j_0i_o}^{(0)}$, $\psi_{i_oi_o}^{(0)}$, $\psi_{j_0i_o}^{(0)}$, we obtain the leading terms of the eigenfunction, the eigenvalue $p_{i_o}^2$, i.e., the initial data for solving the recurrence equations (33), (34),

$$\phi^{(0)}_{j_0 i_o} = \delta_{j_0 i_o}, \quad \psi^{(0)}_{j_0 i_o} = 0, \quad p^2_{i_o} = 2E - \varepsilon^{(0)}_{i_o}. \tag{35}$$

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

In addition, it should be noted that at large r the linearly independent functions (30) satisfy the Wronskian-type relation

$$\mathbf{W}(\mathbf{Q}(r); \boldsymbol{\chi}^*(r), \boldsymbol{\chi}(r)) = \frac{\imath}{2}\mathbf{I}_{oo}, \tag{36}$$

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

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

These relations will be used to examine the accuracy of the above expansion. The calculations of the above asymptotics were performed using MATRA and ASYMRS implemented in MAPLE 8.

7 Procedure DIPPOT

In procedure DIPPOT, the transition matrix elements are evaluated using the results of program KANTBP.

Let us construct the longitudinal and transversal dipole matrix elements $D^{(m\sigma\sigma')}_{jj'}(r)$ and $P^{(mm'\sigma)}_{jj'}(r)$ with the photon polarized along the z axis and along the XOY plane, respectively. Using the expression (9), the above matrix elements can be written in the form

$$D^{(m\sigma\sigma')}_{jj'}(r) = \delta_{|\sigma+\sigma'|0}\, r \sum_{s=s(\sigma)}^{s_{\max}} \sum_{s'=s(\sigma')}^{s_{\max}} c^{m\sigma}_{sj}(r) c^{m\sigma'}_{s'j'}(r) \delta_{|s-s'|1} \frac{\sqrt{s_>}\sqrt{s_> + 2|m|}}{\sqrt{4(s_> + |m|)^2 - 1}},$$

$$P^{(mm'\sigma)}_{jj'}(r) = \delta_{|m-m'|1} \frac{r}{\sqrt{2}} \sum_{s=s(\sigma)}^{s_{\max}} \sum_{s'=s(\sigma')}^{s_{\max}} c^{m\sigma}_{sj}(r) c^{m'\sigma}_{s'j'}(r) \tag{37}$$

$$\times \left\{ \delta_{ss'+2} \sqrt{\frac{s(s-1)}{4(s+m_<)^2 - 1}} - \delta_{ss'} \sqrt{\frac{(s+2m_<+1)(s+2m_<+2)}{(2s+2m_<+1)(2s+2m_<+3)}} \right\},$$

where $s(\sigma) = (1-\sigma)/2$, $s_> = \max(s, s')$ and $m_< = \min(|m|, |m'|)$.

Using the coefficients $c^{(k)}_{s,j}$ obtained in sections 3 and 4, one can easily find longitudinal and transversal dipole matrix elements as the series expansion by the inverse power of r without the exponential terms

$$D^{(m\sigma\sigma')}_{jj'}(r) = r \sum_{k=0}^{k_{\max}} r^{-2k} D^{(2k)}_{jj'}, \quad P^{(mm'\sigma)}_{jj'}(r) = -\sum_{k=0}^{k_{\max}} r^{-2k} P^{(2k)}_{jj'}. \tag{38}$$

8 Conclusion

Using elaborated algorithms, for large r one could build asymptotic expansions in the inverse powers of r needed for calculation with a given accuracy of the required set of basis functions for all values of parameter r [3]. As a consequence, at large values of the radial variable r, the potential curves, radial matrix elements, and dipole transition matrix elements are calculated using asymptotic formulae and matching points $r_{\mathrm{match}} < r_{\mathrm{max}}$ that are found automatically from the interval of integration $0 \le r \le r_{\mathrm{max}}$. Thus, we can build a more efficient algorithm for solving the partial algebraic eigenvalue problem depending on parameter r with an automatic choice of Wilkinson's shift [5]. Thus, we give a constructive *solution of the key problem* to build up a nonsymmetric matrix logarithmic derivative, i.e., **R**-matrix in an adiabatic (parametrically dependent) basis in terms of the recalculation matrix for solution of a boundary problem with the boundary conditions of the third type from the inner region to the outer region.
The LONG WRITE UP of POTHMF and KANTBP will be published in Computer Physics Communications.

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