## ADIABATIC REPRESENTATION

## FOR A HYDROGEN LIKE ATOM PHOTOIONIZATION IN A MAGNETIC FIELD <sup>1</sup>

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In collaboration with:

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<sup>&</sup>lt;sup>1</sup>This talk is presented to International Conference on Muon Catalyzed Fusion and Related Topics (MCF-07), 18–21 June 2007.

#### 1. Contents of review

- 1. A new effective method of calculating wave functions of discrete and continuous spectra of a hydrogen atom in a strong uniform magnetic field is developed based on the adiabatic approach, known in mathematics as the Kantorovich method, to parametric boundary problems in spherical coordinates <sup>2</sup>.
- 2. The two-dimensional boundary problems for the Schrödinger equation at a fixed magnetic quantum number and a spatial parity is reduced to a spectral parametric problem for a one-dimensional equation by the angular variable for the angular oblate spheroidal functions and to boundary problems for a finite set of the ordinary second-order differential equations by the radial variable with effective potentials.
- 3. All needed asymptotics of set of adaptive basis functions, matrix elements of radial coupling and radial solutions are calculated in an analytic form to reduce interval of integration in the corresponded boundary problems and to achieve economy of computer resources.

<sup>&</sup>lt;sup>2</sup>M.S. Kaschiev, S.I. Vinitsky, and F.R. Vukajlović, Hydrogen atom H and  $H_2^+$  in strong magnetic fields. Phys. Rev. A 22 (1980) 557–559.

M.G. Dimova, M.S. Kaschiev, and S.I. Vinitsky, 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.

O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, et al, Application of Kantorovich method for calculations of a hydrogen atom photoionization in a strong magnetic field. Proc. SPIE 6537 (2007).

- The rate of convergence is investigated firstly numerically and is illustrated with a number of typical examples.
- 5. The method is applied to calculations of the photo-ionization cross-sections of a hydrogen atom in the magnetic field that will be provide a true threshold behavior.
- 6. Further applications of the method to the photo-ionization and -recombination of a hydrogen-like atom in the magnetic field <sup>3</sup>, and channeling of atoms or ions in a confinement potential <sup>4</sup> are briefly discussed.

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 $<sup>^{3}</sup>V.V.$  Serov, V.L. Derbov, and S.I. Vinitsky, Laser-stimulated recombination of antihydrogen in magnetic field via quasistationary state. Opt.&Spectr. 102 (2007).

O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, et al, Calculation of a hydrogen atom photoionization in a strong magnetic field by using the angular oblate spheroidal functions, submitted to J. of Physics A.

<sup>&</sup>lt;sup>4</sup>Yu.N. Demkov and J.D. Meyer, A sub-atomic microscope, superfocusing in channeling and close encounter atomic and nuclear reactions. Eur. Phys. J. B 42 (2004) 361–365.

- 1. Contents
- 2. Statement of the problem in cylindrical coordinates  $(1 \le \gamma)$
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- 2.2.2. Asymptotic form "incident wave + waves going out from the center"
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  - 3. Statement of the problem in spherical coordinates ( $0 \le \gamma < 10^4$ )
  - 3.1. Kantorovich expansion of solution over basis of angular spheroidal functions
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  - 4.1. Asymptotics of matrix elements of radial coupling at large r
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  - 4.3. Correspondence of asymptotic solutions in spherical coordinates to cylindrical ones

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- 5. The scattering states and the photoionization cross sections
- 5.1. Eigenchannel function
- 5.2. reaction matrix
- 5.3. "Ingoing" wave function
- 5.4. The photoionization cross section
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FIG. 1. Antiprotons are loaded from below (left), into the trap electrodes below the rotatable electrode. Positrons are simultaneously loaded from above (right) into the electrodes above the rotatable electrode.

ATRAP Apparatus G. Gabrielse et al (ATRAP Collaboration), PRL **93**, 073401 (2004)

Projections of cylindrical and spherical coordinate systems in the zx plane for a hydrogen atom or scattering of an electron with a proton in a homogeneous magnetic field  $\vec{B} = (0, 0, B)$ .

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## 2. Statement of the problem in cylindrical coordinates

In cylindrical coordinates  $(\rho, z, \varphi)$  the wave function

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

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

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

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

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

Here  $m = 0, \pm 1, \ldots$  is the magnetic quantum number,  $\gamma = B/B_0$ ,  $B_0 \cong 2.35 \times 10^5 T$  is a dimensionless parameter which determines the field strength B.

We use the atomic units (a.u.)  $\hbar=m_e=e=1$  and assume the mass of the nucleus to be infinite.

In these expressions  $\epsilon=2E,~E$  is the energy (expressed in Rydbergs, 1~Ry=(1/2)~a.u.) of the bound state  $|m\sigma\rangle$  with fixed values of m and z-parity  $\sigma=\pm 1$ , and  $\Psi(\rho,z)\equiv \Psi^{m\sigma}(\rho,z)=\sigma\Psi^{m\sigma}(\rho,-z)$  is the corresponding wave function.

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

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

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

$$\lim_{\rho \to \infty} \Psi(\rho, z) = 0.$$
(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  $|z| = z_{\text{max}} \gg 1$ , namely,

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

These functions satisfy the additional normalization condition

$$\int_{-z_{\text{max}}}^{z_{\text{max}}} \int_{0}^{\infty} |\Psi(\rho, z)|^2 \rho d\rho dz = 1.$$
(8)

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

#### 2.1. Galerkin expansion

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

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

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

$$\hat{A}_c \tilde{\Phi}_j(\rho) = \tilde{E}_j \tilde{\Phi}_j(\rho), \tag{10}$$

with the boundary conditions

$$\lim_{\rho \to 0} \rho \frac{\partial \tilde{\Phi}_j(\rho)}{\partial \rho} = 0, \quad \text{for} \quad m = 0, \tag{11}$$

$$\tilde{\Phi}_j(0) = 0, \quad \text{for} \quad m \neq 0, \tag{12}$$

$$\lim_{\rho \to \infty} \Phi_j(\rho) = 0.$$
(13)

The above eigenvalue problem has the exact solution  $^{5}$  at fixed m

$$\tilde{\Phi}_{j}(\rho) = \sqrt{\frac{\gamma N_{\rho}!}{(N_{\rho} + |m|)!}} \exp\left(-\frac{\gamma \rho^{2}}{4}\right) \left(\frac{\gamma \rho^{2}}{2}\right)^{\frac{|m|}{2}} L_{N_{\rho}}^{|m|}\left(\frac{\gamma \rho^{2}}{2}\right),$$

$$\tilde{E}_{j} = \gamma(2N_{\rho} + |m| + m + 1),$$
(14)

where  $N_{\rho} = j - 1$  is the transversal quantum number and  $L_{N_{\rho}}^{[m]}(x)$  is the associated Laguerre polynomial. Note, that Galerkin expansion follows from Kantorovich expansion at  $z \to \infty$ , i.e., parametric basis functions  $\hat{\Phi}_j(\rho; z)$  and corresponding potential curves  $\hat{E}_j(z)$  transform into the above basis functions and eigenvalues

$$\tilde{\Phi}_{j}(\rho) = \lim_{z \to \pm \infty} \hat{\Phi}_{j}(\rho; z),$$

$$\lim_{z \to \pm \infty} \hat{E}_{j}(z) = \tilde{E}_{j} = \epsilon^{th}_{m\sigma j}(\gamma) = \gamma(2N_{\rho} + |m| + m + 1).$$
(15)

<sup>&</sup>lt;sup>5</sup>L.G.Mardoyan, G.S.Pogosyan, A.N.Sissakian and V.M.Ter-Antonyan. The quantum systems with hidden symmetry. Interbasis expansions, Dubna, JINR, 2004.

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  $\epsilon$  and the coefficients  $\tilde{\chi}^{(i)}(z)$  of the expansion (9)

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \tilde{\mathbf{U}}(z)\right)\tilde{\boldsymbol{\chi}}^{(i)}(z) = \epsilon_i \,\mathbf{I}\tilde{\boldsymbol{\chi}}^{(i)}(z),\tag{16}$$

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

$$\tilde{U}_{ij}(z) = \frac{\tilde{E}_i + \tilde{E}_j}{2} \delta_{ij} - \int_0^\infty \tilde{\Phi}_i(\rho) \frac{2Z}{\sqrt{\rho^2 + z^2}} \tilde{\Phi}_j(\rho) \rho d\rho.$$
(17)

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

$$\lim_{z \to \pm \infty} \tilde{\boldsymbol{\chi}}^{(i)}(z) = 0 \to \quad \tilde{\boldsymbol{\chi}}^{(i)}(\pm z_{\max}) = 0,$$
(18)

$$\int_{-z_{\max}}^{z_{\max}} \left( \tilde{\boldsymbol{\chi}}^{(i)}(z) \right)^T \tilde{\boldsymbol{\chi}}^{(j)}(z) dz = \delta_{ij}.$$
(19)

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

# 2.2. Relation between the parity functions and the functions having physical scattering asymptotic form in cylindrical coordinates<sup>6</sup>

The asymptotic form of the coefficients  $\hat{\chi}^{(n)}(z)$  of the **Galerkin** expansion (9) with fixed  $m, \sigma$  and  $\epsilon = 2E$  for *n*-th solution in open channels is

$$\chi_{Em\sigma n'n}(z \to \pm \infty) = \begin{cases} \frac{a_{\pm 1n'n}}{\sqrt{p_{n'}}} \cos\left(p_{n'}z + \frac{Z}{p_{n'}}\frac{z}{|z|}\ln(2p_{n'}|z|) + \frac{z}{|z|}\delta_{\pm 1n}\right), & \\ \sigma = \pm 1, & \\ \frac{a_{\pm 1n'n}}{\sqrt{p_{n'}}} \sin\left(p_{n'}z + \frac{Z}{p_{n'}}\frac{z}{|z|}\ln(2p_{n'}|z|) + \frac{z}{|z|}\delta_{\pm 1n}\right), & \\ \sigma = -1, & \\ \sigma = -1, & \end{cases}$$
(20)

where  $p_n = \sqrt{2E - \epsilon_{m\sigma n}^{th}} \ge 0$  and  $n, n' = 1, \ldots, N_o, \ \delta_{\sigma n} = \delta_n^{\sigma} + \delta_n^c - (\sigma + 1)\pi/4$ are the phase shifts,  $\delta_n^{\sigma}$  and  $\delta_n^c$  are the eigenchannel short-range and Coulomb phase shifts,  $a_{\sigma n'n} = C_{n'n}^{\sigma}$  are the amplitudes or mixed parameters and  $N_o = \max(n: 2E \ge \epsilon_{m\sigma n}^{th})$  is the number of open channels, i.e.  $N_o$  is the number of Landau thresholds open at the energy E.

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<sup>&</sup>lt;sup>6</sup>O. Chuluunbaatar et al, Proc. SPIE 6537 (2007)

2.2.1. Eigenchannel solutions Eq. (20) is rewritten in the matrix form so that

$$\boldsymbol{\chi}_{E\sigma}(z \to \pm \infty) = \begin{cases} \begin{cases} \frac{1}{2} \mathbf{X}^{(+)}(z) \mathbf{A}_{+1} + \frac{1}{2} \mathbf{X}^{(-)}(z) \mathbf{A}_{+1}^{*}, & \\ \sigma = +1, & \\ \frac{1}{2\imath} \mathbf{X}^{(+)}(z) \mathbf{A}_{-1} - \frac{1}{2\imath} \mathbf{X}^{(-)}(z) \mathbf{A}_{-1}^{*}, & z > 0, \\ \sigma = -1, & \\ & \sigma = -1, & \\ \\ \begin{cases} \frac{1}{2} \mathbf{X}^{(+)}(z) \mathbf{A}_{+1}^{*} + \frac{1}{2} \mathbf{X}^{(-)}(z) \mathbf{A}_{+1}, & \\ \sigma = +1, & \\ \frac{1}{2\imath} \mathbf{X}^{(+)}(z) \mathbf{A}_{-1}^{*} - \frac{1}{2\imath} \mathbf{X}^{(-)}(z) \mathbf{A}_{-1}, & \\ \sigma = -1, & \\ \end{cases}$$
(21)

where

$$X_{n'n}^{(\pm)}(z) = p_{n'}^{-1/2} \exp\left(\pm i p_{n'} z \pm i \frac{Z}{p_{n'}} \frac{z}{|z|} \ln(2p_{n'}|z|)\right) \delta_{n'n},$$
(22)  
$$A_{\sigma n'n} = a_{\sigma n'n} \exp(i \delta_{\sigma n}).$$

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continue spectrum states haven asymptotic (20–22) for  $\sigma = -1$ , Z = 1,  $\gamma = 1$  and m = 0 with energy E = 1.7 a.u. above second threshold  $1/2\epsilon_{m2}^{th} = 1.5$ .

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

$$\boldsymbol{\chi}_{E\hat{v}}^{(+)}(z \to \pm \infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\hat{\mathbf{T}}, & z > 0, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\hat{\mathbf{R}}, & z < 0, \\ \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\hat{\mathbf{R}}, & z > 0, \\ \mathbf{X}^{(-)}(z)\hat{\mathbf{T}}, & z < 0, \end{cases} & \hat{v} = \leftarrow, \end{cases}$$
(23)

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

$$\begin{array}{c|c} \chi_{E \rightarrow}^{(+)}(z \rightarrow \pm \infty) & \chi_{E \leftarrow}^{(+)}(z \rightarrow \pm \infty) \\ \hline \\ \chi^{(+)(z)} & & \\ \hline \\ \chi^{(-)(z)\hat{\mathbf{R}}} & \mathbf{X}^{(+)(z)\hat{\mathbf{T}}} & \mathbf{X}^{(-)(z)\hat{\mathbf{T}}} & \mathbf{X}^{(+)(z)\hat{\mathbf{R}}} \\ z < 0 & z > 0 & z < 0 & z > 0 \end{array}$$

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

$$\boldsymbol{\chi}_{E \stackrel{\leftarrow}{\leftarrow}}^{(+)}(z) = \boldsymbol{\chi}_{E,+1}(z) \mathbf{B}_{+1} \pm \imath \boldsymbol{\chi}_{E,-1}(z) \mathbf{B}_{-1}.$$
(24)

It is easy to show that  ${\bf B}_\sigma=[{\bf A}_\sigma^*]^{-1},$  and the transmission  $\hat{\bf T}$  and reflection  $\hat{\bf R}$  amplitude matrices take the form

$$\hat{\mathbf{T}} = \frac{1}{2} (\mathbf{A}_{+1} \mathbf{B}_{+1} + \mathbf{A}_{-1} \mathbf{B}_{-1}) = \frac{1}{2} (-\tilde{\mathbf{S}}_{+1} + \tilde{\mathbf{S}}_{-1}),$$
(25)  
$$\hat{\mathbf{R}} = \frac{1}{2} (\mathbf{A}_{+1} \mathbf{B}_{+1} - \mathbf{A}_{-1} \mathbf{B}_{-1}) = \frac{1}{2} (-\tilde{\mathbf{S}}_{+1} - \tilde{\mathbf{S}}_{-1}),$$

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where  $\check{\mathbf{S}}_{\sigma}$  is the scattering matrix at fixed  $\sigma$ .

2.2.3. asymptotic form "waves going into the center + outgoing wave"

However, to calculate the ionization cross section it is necessary to use the function having the asymptotic form "waves going into the center + outgoing wave", that is

$$\boldsymbol{\chi}_{E\hat{v}}^{(-)}(z \to \pm \infty) = \begin{cases} \left\{ \begin{array}{ll} \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\hat{\mathbf{R}}^{\dagger}, & z > 0, \\ \mathbf{X}^{(+)}(z)\hat{\mathbf{T}}^{\dagger}, & z < 0, \\ \left\{ \begin{array}{ll} \mathbf{X}^{(-)}(z)\hat{\mathbf{T}}^{\dagger}, & z > 0, \\ \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\hat{\mathbf{R}}^{\dagger}, & z < 0, \end{array} \right., \quad \hat{v} = \leftarrow, \end{cases}$$
(26)

or  $\boldsymbol{\chi}_{E\overrightarrow{\leftarrow}}^{(-)}(z) = \boldsymbol{\chi}_{E,+1}(z)\mathbf{B}_{+1}^* \pm \imath \boldsymbol{\chi}_{E,-1}(z)\mathbf{B}_{-1}^*$ . Note, that  $\left(\boldsymbol{\chi}_{E\overrightarrow{\leftarrow}}^{(-)}(z)\right)^* = \boldsymbol{\chi}_{E\overleftarrow{\rightarrow}}^{(+)}(z)$ . The functions are normalized so that

$$\sum_{n''=1}^{j_{\max}} \int_{-\infty}^{\infty} \left( \chi_{E'm\hat{v}'n''n'}^{(\pm)}(z) \right)^* \chi_{Em\hat{v}n''n}^{(\pm)}(z) dz = 2\pi \delta(E'-E) \delta_{\hat{v}'\hat{v}} \delta_{n'n}.$$
(27)

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$$\begin{array}{c|c} \boldsymbol{\chi}_{E\rightarrow}^{(-)}(z\rightarrow\pm\infty) & \boldsymbol{\chi}_{E\leftarrow}^{(-)}(z\rightarrow\pm\infty) \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(+)(z)}\hat{\boldsymbol{r}}^{\dagger} & \boldsymbol{X}^{(-)(z)}\hat{\boldsymbol{R}}^{\dagger} & \boldsymbol{X}^{(+)(z)}\hat{\boldsymbol{R}}^{\dagger} & \boldsymbol{X}^{(-)(z)}\hat{\boldsymbol{r}}^{\dagger} \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(+)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(+)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(+)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} \\ \hline \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)} & \boldsymbol{\chi}_{E\rightarrow}^{(-)(z)}$$



Profiles of total wave functions  $|\Psi_{Em}^{(-)}|$  (a,c) and  $|\Psi_{Em}^{(-)}|$  (b,d) in the zx plane of the continuous spectrum with Z = 1, m = 0 and  $\gamma = 1 \times 10^{-1}$ . The states with the energy E = 0.05885 a.u. (a,b) correspond to the resonance transmission ( $|T|^2 = 1$ ,  $|R|^2 = 0$ ), while those with the energy E = 0.11692 a.u. (c,d) correspond to the total reflection ( $|T|^2 = 0$ ,  $|R|^2 = 1$ ).

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Squared modulus of the matrix element  $\check{T}_{11}$ , multiplied by 7/4, odd phase shift  $\delta_o$  multiplied by  $14/\pi$  and cross-section  $\sigma^d(\omega)$  (72) of photoionization from the initial state 1s<sub>0</sub> versus the energy E (a) and  $(\check{E}_2 - 2E)^{-1/2}$  (b) for the final scattering state with  $\sigma = -1$ , Z = 1, m = 0 and  $\gamma = 1 \times 10^{-1}$ .

The finite element grids of  $\hat{r} = \sqrt{\gamma}r$  have been chosen as 0 (200) 3 (200) 20 (200) 100 for the discrete spectrum and 0 (200) 3 (200) 20 (200) 100 (1000) 1000 for the continuous one. The numbers in parentheses are the numbers of finite elements of the order k = 4 in each interval. The number of nodes in the grids is 2400 and 6401, so that the maximum number of unknowns in Eqs. (49) is 24000 and 64010, respectively.

2.2.4.  $\hat{\mathbf{S}}$ -matrix

The  $\hat{S}$ -matrix may be composed of the transmission and reflection amplitudes<sup>7</sup>

$$\hat{\mathbf{S}} = \begin{pmatrix} \hat{\mathbf{T}} & \hat{\mathbf{R}} \\ \hat{\mathbf{R}} & \hat{\mathbf{T}} \end{pmatrix}, \qquad \mathbf{S}^{\dagger}\mathbf{S} = \mathbf{S}\mathbf{S}^{\dagger} = \mathbf{I}_{oo}.$$
(28)

This matrix is unitary, since  $\hat{\mathbf{T}}^{\dagger}\hat{\mathbf{T}} + \hat{\mathbf{R}}^{\dagger}\hat{\mathbf{R}} = \mathbf{I}_{oo}$  and  $\hat{\mathbf{R}}^{\dagger}\hat{\mathbf{T}} + \hat{\mathbf{T}}^{\dagger}\hat{\mathbf{R}} = \mathbf{0}$ . To calculate the ionization it is convenient to use the function renormalized to  $\delta(E'-E)$ , i.e., divided by  $\sqrt{2\pi}$ 

$$E\hat{v}mN_{\rho}\rangle = \frac{\exp(\imath m\varphi)}{2\pi} \sum_{n'=1}^{\jmath_{\max}} \tilde{\Phi}_{n'}(\rho)\tilde{\chi}^{(-)}_{Em\hat{v}n'n}(z)$$
<sup>(29)</sup>

or

$$|E\hat{v}mN_{\rho}\rangle = \frac{\exp(im\varphi)}{2\pi} \sum_{n'=1}^{j\max} \hat{\Phi}_{n'}(\rho;z)\hat{\chi}_{Em\hat{v}n'n}^{(-)}(z),$$
(30)

where  $N_{\rho} = n - 1$ .

 <sup>&</sup>lt;sup>7</sup>V.V. Kostrykin , A.A. Kvitsinsky and S.P. Merkuriev J. Phys. A 28. 3493 (1995)
 O. Chuluunbaatar et al, Proc. SPIE 6537 (2007)

2.2.5. Photoionization cross section

The expression for the cross section of ionization by the light linearly polarized along the axis z is

$$\sigma^{ion} = 4\pi^2 \alpha \omega \sum_{N_\rho=0}^{N_o-1} \sum_{\hat{v}} |\langle E\hat{v}mN_\rho | z | Nlm \rangle|^2 a_0^2.$$
(31)

In the above expressions  $\omega = E - E_{Nlm}$  is the frequency of radiation,  $E_{Nlm}$  is the energy of the initial bound state  $|Nlm\rangle$  specified by the spherical quantum numbers N, l, m,  $\alpha$  is the fine-structure constant,  $a_0$  is the Bohr radius.

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

$$\sigma^{ion} = 4\pi^2 \alpha \omega \sum_{N_{\rho}=0}^{N_{o}-1} \sum_{\hat{v}} |\langle E\hat{v}m \pm 1N_{\rho}|\vec{e}_{\pm}\vec{r}|Nlm\rangle|^2 a_0^2,$$
(32)

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



energy for  $\gamma = 1 \times 10^{-1}$ , and for the final state with  $\sigma = -1$ , Z = 1, m = 0. The arrows indicate the successive Landau thresholds  $E_j = 1/2\epsilon_{mj}^{th}$ .

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2.2.6. The rate of recombination induced by the light

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

$$|vmN_{\rho}\rangle = \sqrt{p_n} \frac{\exp(\imath m\varphi)}{\sqrt{2\pi}} \sum_{n'=1}^{j\max} \tilde{\Phi}_{n'}(\rho) \tilde{\chi}^{(+)}_{Em\hat{v}n'n}(z)$$
(33)

or

$$|vmN_{\rho}\rangle = \sqrt{p_n} \frac{\exp(im\varphi)}{\sqrt{2\pi}} \sum_{n'=1}^{j_{\max}} \hat{\Phi}_{n'}(\rho; z) \hat{\chi}_{Em\hat{v}n'n}^{(+)}(z),$$
(34)

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where  $v = \hat{v}p_n$  and  $N_{\rho} = n - 1$ .

The expression for the rate of recombination induced by the light linearly polarized along the axis z for the particle, initially moving in the channel  $N_\rho$  with the velocity v has the form

$$\lambda_{N\rho}^{rec}(v) = 4\pi^2 \alpha I \sum_{l=0}^{N-1} \sum_{m=-l}^{0} |\langle Nlm|z|vmN_{\rho}\rangle|^2 \delta(E - E_{Nlm} - \omega) a_0^2,$$
(35)

I being the intensity of the incident light.

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

$$\lambda_{N_{\rho}}^{rec}(v) = 4\pi^2 \alpha I \sum_{l=0}^{N-1} \sum_{m=-l}^{0} |\langle Nlm \pm 1 | \vec{e_{\pm}} \vec{r} | vmN_{\rho} \rangle|^2 \delta(E - E_{Nlm} - \omega) a_0^2,$$
(36)

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

3. Statement of the problem in spherical coordinates

In spherical coordinates  $(r, \theta, \phi)$  the Eq. (2) can be rewritten as follows<sup>8</sup>

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\hat{A}(p) - \frac{2Z}{r}\right)\Psi(r,\eta) = \epsilon\Psi(r,\eta),\tag{37}$$

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

$$\hat{A}(p) = -\frac{\partial}{\partial \eta} (1-\eta^2) \frac{\partial}{\partial \eta} + \frac{m^2}{1-\eta^2} + 2pm + p^2 (1-\eta^2),$$
(38)

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and  $p = \gamma r^2/2$ , and  $\Psi(r, \eta) \equiv \Psi^{m\sigma}(r, \eta) = \sigma \Psi^{m\sigma}(r, -\eta)$ . The sign of *z*-parity,  $\sigma = (-1)^{N_\eta}$ , is defined by the number of nodes  $N_\eta$  of the solution  $\Psi(r, \eta)$  with respect to the variable  $\eta$ . We will also use the scaled radial variable  $\hat{r} = r\sqrt{\gamma}$ , the effective charge  $\hat{Z} = Z/\sqrt{\gamma}$ , and the scaled energy  $\hat{\epsilon} = \epsilon/\gamma$  or  $\hat{E} = E/\gamma$ .

Practically it means replacing  $\gamma$  with 1 and multiplying Z by  $1/\sqrt{\gamma}$  and  $\epsilon$  or E by  $1/\gamma$  in all equations above.

<sup>&</sup>lt;sup>8</sup>M.S. Kaschiev, S.I. Vinitsky and F.R. Vukajlovic Phys. Rev. A 22 557 (1980)

#### Boundary conditions

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

$$\lim_{\eta \to \pm 1} (1 - \eta^2) \frac{\partial \Psi(r, \eta)}{\partial \eta} = 0, \quad \text{for} \quad m = 0,$$
(39)

$$\Psi(r, \pm 1) = 0, \text{ for } m \neq 0,$$
 (40)

$$\lim_{r \to 0} r^2 \frac{\partial \Psi(r, \eta)}{\partial r} = 0.$$
(41)

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

$$\lim_{r \to \infty} r^2 \Psi(r, \eta) = 0 \quad \to \quad \Psi(r_{\max}, \eta) = 0.$$
(42)

In the Fano-Lee R-matrix theory<sup>9</sup> the wave function of the continuum  $\Psi(r,\eta)$  obeys the boundary condition of the third type at fixed values of the energy  $\epsilon$  and the radial variable  $r=r_{\rm max}$ 

$$\frac{\partial \Psi(r,\eta)}{\partial r} - \mu \Psi(r,\eta) = 0.$$
(43)

Here the parameters  $\mu \equiv \mu(r_{\max}, \epsilon)$ , determined by the variational principle, play the role of eigenvalues of the logarithmic normal derivative matrix of the solution of the boundary problem (37)–(41), (43).

<sup>&</sup>lt;sup>9</sup>U. Fano and C.M.Lee, Phys. Rev. Lett. 31, 1573 (1973); C.M.Lee Phys. Rev. A 10, 584 (1974)

## 3.1. Kantorovich expansion<sup>10</sup>

Consider a formal expansion of the partial solution  $\Psi_i^{Em\sigma}(r,\eta)$  of Eqs. (37)–(41) with the conditions (42), (43), corresponding to the eigenstate  $|m\sigma i\rangle$ , in terms of the finite set of one-dimensional basis functions  $\{\Phi_j^{m\sigma}(\eta; r)\}_{j=1}^{j_{max}}$ 

$$\Psi_i^{Em\sigma}(r,\eta) = \sum_{j=1}^{j_{\text{max}}} \Phi_j^{m\sigma}(\eta;r)\chi_j^{(m\sigma i)}(E,r).$$
(44)

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In Eq. (44) the functions

$$\boldsymbol{\chi}^{(i)}(r) \equiv \boldsymbol{\chi}^{(m\sigma i)}(E, r), \qquad (\boldsymbol{\chi}^{(i)}(r))^T = (\chi_1^{(i)}(r), \dots, \chi_{j_{\max}}^{(i)}(r))$$

are unknown, and the surface functions

$$\boldsymbol{\Phi}(\eta;r) \equiv \boldsymbol{\Phi}^{m\sigma}(\eta;r) = \sigma \boldsymbol{\Phi}^{m\sigma}(-\eta;r), \quad (\boldsymbol{\Phi}(\eta;r))^T = (\Phi_1(\eta;r), \dots, \Phi_{j_{\max}}(\eta;r))$$

form an orthonormal basis for each value of the radius r which is treated as a parameter.

<sup>&</sup>lt;sup>10</sup>M.G. Dimova, M.S. Kaschiev and S.I. Vinitsky, J. Phys. B 38 2337 (2005)

In the Kantorovich approach the wave functions  $\Phi_j(\eta; r)$  and the potential curves  $E_j(r)$  (in Ry) are determined as the solutions of the following one-dimensional parametric eigenvalue problem for oblate angular spheroidal functions <sup>11</sup>

$$\hat{A}(p)\Phi_j(\eta;r) = E_j(r)\Phi_j(\eta;r),$$
(45)

with the boundary conditions

$$\lim_{\eta \to \pm 1} (1 - \eta^2) \frac{\partial \Phi_j(\eta; r)}{\partial \eta} = 0, \quad \text{for} \quad m = 0$$
(46)

$$\Phi_j(\pm 1; r) = 0, \quad \text{for} \quad m \neq 0.$$
 (47)

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Since the operator in the left-hand side of Eq. (45) is self-adjoint, its eigenfunctions are orthonormal

$$\left\langle \Phi_i(\eta; r) \middle| \Phi_j(\eta; r) \right\rangle_{\eta} = \int_{-1}^1 \Phi_i(\eta; r) \Phi_j(\eta; r) d\eta = \delta_{ij}.$$
 (48)

<sup>&</sup>lt;sup>11</sup>M. Abramovits and I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1965



Profiles of the even  $\Phi_i \equiv \Phi^{m\sigma=+1}(\eta;r)$  and odd  $\Phi_i \equiv \Phi^{m\sigma=-1}(\eta;r)$  basis functions for i=1,2



Profiles of the left  $\Phi_i \equiv \Phi^{min}(\eta; r) = (\Phi^{mo} - \gamma(\eta; r) - \Phi^{mo} - \gamma(\eta; r))/\sqrt{2}$  and right  $\Phi_i \equiv \Phi^{m\leftarrow}(\eta; r) = (\Phi^{m\sigma=+1}(\eta; r) + \Phi^{m\sigma=-1}(\eta; r))/\sqrt{2}$  basis functions for i = 1, 2

3.1.1. Boundary problems for a set of the radial equations

From here we transform the solution of the problem (37) into the solution of an eigenvalue problem for a set of  $j_{\text{max}}$  ordinary second-order differential equations that determines the energy  $\epsilon$  and the coefficients (radial wave functions)  $\chi^{(i)}(r)$  of the expansion (44)

$$\left(-\mathbf{I}\frac{1}{r^{2}}\frac{d}{dr}r^{2}\frac{d}{dr}+\frac{\mathbf{U}(r)}{r^{2}}+\mathbf{Q}(r)\frac{d}{dr}+\frac{1}{r^{2}}\frac{dr^{2}\mathbf{Q}(r)}{dr}\right)\boldsymbol{\chi}^{(i)}(r)=\epsilon_{i}\mathbf{I}\boldsymbol{\chi}^{(i)}(r),\quad(49)$$
$$\lim_{r\to0}r^{2}\left(\frac{d\boldsymbol{\chi}^{(i)}(r)}{dr}-\mathbf{Q}(r)\boldsymbol{\chi}^{(i)}(r)\right)=0.\quad(50)$$

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

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

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

$$Q_{ij}(r) = -Q_{ji}(r) = -\int_{-1}^{1} \Phi_i(\eta; r) \frac{\partial \Phi_j(\eta; r)}{\partial r} d\eta.$$
(51)

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The calculations of the above matrix elements and there asymptotic forms were performed using the combined codes EIGENF, MATRM and MATRA implemented in MAPLE 8 and FORTRAN<sup>12</sup>.

<sup>&</sup>lt;sup>12</sup>O. Chuluunbaatar et al, submitted to Comput. Phys. Commun. (2007)

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

$$\lim_{r \to \infty} r^2 \boldsymbol{\chi}^{(i)}(r) = 0 \quad \to \quad \boldsymbol{\chi}^{(i)}(r_{\max}) = 0, \tag{52}$$

$$\int_0^{r_{\max}} r^2 \left( \boldsymbol{\chi}^{(i)}(r) \right)^T \boldsymbol{\chi}^{(j)}(r) dr = \delta_{ij}.$$
(53)

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

$$\frac{d\boldsymbol{\chi}(r)}{dr} = \mathbf{R}\boldsymbol{\chi}(r), \quad \mathbf{R} = \mathcal{R} + \mathbf{Q}.$$
(54)

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Here the nonsymmetric matrix  ${\bf R}$  is determined via symmetric matrix  ${\cal R}$  that is calculated using the method of  $^{13}.$ 

<sup>13</sup>O. Chuluunbaatar et al, Proc. SPIE 6165, 66 (2006)

3.2. four steps of Kantorovich method

Thus, within the framework of the Kantorovich approach the original problem is reduced to the following steps:

- Calculation of the potential curves  $E_j(r)$  and eigenfunctions  $\Phi_j(\theta; r)$  of the spectral problem (45)–(48) for a given set of  $r \in \omega_r$  at fixed values m and  $\gamma = 1$ .
- Calculation of the derivatives  $\partial \Phi(\theta; r) / \partial r$  and computation of the corresponding integrals (see (51)) necessary for obtaining the elements of the radial coupling matrices  $\mathbf{U}(r)$  and  $\mathbf{Q}(r)$ .
- Calculation of the scaled energies  $\hat{\epsilon}$  and the radial wave functions  $\chi^{(i)}(r)$  as solutions of the one-dimensional eigenvalue problem (49)–(51) with (53) at fixed  $m, \gamma = 1$  and the effective charge  $\hat{Z} = Z/\sqrt{\gamma}$ , examination of the convergence of these solutions depending on the number of channels  $j_{\rm max}$  and recalculation the scaled energies to the initial ones  $\epsilon = \hat{\epsilon}\gamma$  or  $E = \hat{E}\gamma$ .
- Calculation of the matrix R and the reaction matrix K (Eqs. (54), (65)) corresponding to the radial wave functions χ<sup>(i)</sup>(r) as the solutions of one-dimensional eigenvalue problem (49)–(51) with the boundary condition (54) at fixed m, the effective charge γ = 1, Ẑ = Z/√γ, and the scaled energy ê or Ê; examination of the convergence of the solutions depending on the number of channels j<sub>max</sub>.

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



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



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

4.1. Asymptotics of matrix elements of radial coupling at large r

At large r asymptotics of matrix elements by inverse power of r (i.e., without exponential terms) is of the analytical form <sup>14</sup> up to an finite order  $k_{\text{max}} = 8$ 

$$r^{-2}E_{j}(r) = E_{j}^{(0)} + \sum_{k=1}^{k_{\max}} r^{-2k}E_{j}^{(2k)}, \quad H_{jj'}(r) = \sum_{k=1}^{k_{\max}} r^{-2k}H_{jj'}^{(2k)},$$
$$Q_{jj'}(r) = \sum_{k=1}^{k_{\max}} r^{-2k+1}Q_{jj'}^{(2k-1)}, \quad r \gg \max(n_{l}, n_{r})\gamma/2.$$
(55)

Here

$$\begin{split} E_{j}^{(0)} &= \gamma(2n+|m|+m+1), \\ E_{j}^{(2)} &= -2n^{2}-2n-1-2|m|n-|m|, \\ H_{jj'}^{(2)} &= (2n^{2}+2n+2|m|n+|m|+1)\delta_{|n_{l}-n_{r}|,0} \\ &-\sqrt{n+1}\sqrt{n+|m|+1}\sqrt{n+2}\sqrt{n+|m|+2}\delta_{|n_{l}-n_{r}|,2}, \\ Q_{jj'}^{(1)} &= (n_{r}-n_{l})\sqrt{n+1}\sqrt{n+|m|+1}\delta_{|n_{l}-n_{r}|,1}, \end{split}$$
(56)

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In these formulas asymptotic quantum numbers  $n_l$ ,  $n_r$  denote transversal quantum numbers  $N_{\rho}$ ,  $N'_{\rho}$ , that connected with the unified numbers j, j' by the above mentioned formulas  $n_l = j - 1$ ,  $n_r = j' - 1$  and  $n = \min(n_l, n_r)$ .

<sup>&</sup>lt;sup>14</sup> for details, see A.A. Gusev et al, Lecture Notes in Computer Science 4194, 205 (2006)

4.2. Asymptotics of radial solution at large r  $% r_{max}$  At large  $r>r_{max}$  and  $rp_{i_{o}}\gg 1$  the

asymptotics of the regular solutions  $\chi_j^{(i_o)}(r) \equiv \chi_{ji_o}(r), j = 1, \ldots, j_{\max}$ ,  $i_o = 1, \ldots, N_o \leq j_{\max}$  of Eq. (49) are sought as expansions in powers of r up to an finite order  $k_{\max} = 16$  in the analytical form <sup>15</sup>

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

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

$$\phi_{i_oi_o}^{(0)} = 1, \quad \psi_{i_oi_o}^{(0)} = 0,$$

$$\phi_{i_o-1i_o}^{(1)} = 0, \quad \psi_{i_o-1i_o}^{(1)} = \frac{\sqrt{i_o - 1}\sqrt{i_o + |m| - 1}}{\gamma} = -\frac{1}{2}\langle i_o - 1|\rho^2|i_o\rangle,$$

$$\phi_{i_oi_o}^{(1)} = 0, \quad \psi_{i_oi_o}^{(1)} = -\frac{2i_o + |m| - 1}{\gamma} = -\frac{1}{2}\langle i_o|\rho^2|i_o\rangle$$
(57)
$$\phi_{i_o+1i_o}^{(1)} = 0, \quad \psi_{i_o+1i_o}^{(1)} = \frac{\sqrt{i_o}\sqrt{i_o + |m|}}{\gamma} = -\frac{1}{2}\langle i_o + 1|\rho^2|i_o\rangle,$$

where  $R(p_{i_o},r)=\imath\,F(p_{i_o},r)+G(p_{i_o},r);\;F(p_{i_o},r),\;G(p_{i_o},r)$  are the Coulomb regular, irregular functions  $^{16}.$ 

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 <sup>&</sup>lt;sup>15</sup>S.I. Vinitsky, V.P. Gerdt, A.A. Gusev, et al Programming and Computer Software 33 105–116 (2007)
 <sup>16</sup>M. Abramovits and I.A. Stegun Handbook of Mathematical Functions (New York: Dover, 1972)

4.3. Correspondence of asymptotic solutions in spherical coordinates to cylindrical ones Taking into account of orthogonality  $\langle j|i_o\rangle = \langle \tilde{\Phi}_j^m(\rho)|\tilde{\Phi}_{i_o}^m(\rho)\rangle = \delta_{ji_o}$  and completeness  $\sum_j |\tilde{\Phi}_j^m(\rho')\rangle \langle \tilde{\Phi}_j^m(\rho)| = \delta(\rho' - \rho)$  of basis functions, the asymptotic of the total wave function can be written in the form for the region  $p_{i_o}\rho^2/(2r) \ll 1$ 

$$\Psi^{m\hat{v}}(r,\eta) = r \sum_{j} |\tilde{\Phi}_{j}^{m}(\rho)\rangle \bigg[ \langle \tilde{\Phi}_{j}^{m}(\rho) | \tilde{\Phi}_{i_{o}}^{m}(\rho) \rangle - \frac{1}{2r} \langle \tilde{\Phi}_{j}^{m}(\rho) | \rho^{2} | \tilde{\Phi}_{i_{o}}^{m}(\rho) \rangle \frac{d}{dr} \bigg] \chi^{(as)}_{i_{o}i_{o}}(p_{i_{o}}, r) = r \sum_{j} |\tilde{\Phi}_{j}^{m}(\rho)\rangle \langle \tilde{\Phi}_{j}^{m}(\rho) | \bigg[ |\tilde{\Phi}_{i_{o}}^{m}(\rho)\rangle - \frac{1}{2r} \rho^{2} | \tilde{\Phi}_{i_{o}}^{m}(\rho) \rangle \frac{d}{dr} \bigg] \chi^{(as)}_{i_{o}i_{o}}(p_{i_{o}}, r)$$
(58)  
$$\approx r \tilde{\Phi}_{i_{o}}^{m}(\rho) \chi^{(as)}_{i_{o}i_{o}}(p_{i_{o}}, r(1 - \rho^{2}/(2r^{2}))) \approx \frac{1}{2} \tilde{\Phi}_{i_{o}}^{m}(\rho) X^{(+)}_{i_{o}i_{o}}(|z|) \exp(\imath \delta_{i_{o}}^{c}).$$

In last transformation we use  $|z| = r(1 - \rho^2/(2r^2)) + O(r^{-2})$  and definitions (15) and (22). Thus, we show that the matrix of coefficients (57), corresponds to an overlap matrix between asymptotic of fundamental solutions (2) in cylindrical coordinates  $z = r \cos \theta$ ,  $\rho = r \sin \theta$ , at large values of |z|, and asymptotics of basis functions of independent variable,  $\eta = \cos \theta$  at large values of r.

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5. The scattering states and the photoionization cross sections

We express the eigenfunction of the continuum spectrum  $\Psi_i^{E\,m\sigma}(r,\eta)$  with the energy  $\epsilon=2E$  describing the ejected electron above the first threshold  $\epsilon_{m\sigma1}^{th}(\gamma)=\epsilon_{m\sigma}^{th}(\gamma)=\gamma(|m|+m+1)$  as follows

$$\Psi_{i}^{Em\sigma}(r,\eta) = \sum_{j=1}^{j_{\max}} \Phi_{j}^{m\sigma}(\eta;r)\hat{\chi}_{ji}^{(m\sigma)}(E,r), \quad i = 1,\dots, N_{o},$$
(59)

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

$$\left\langle \Psi_{i}^{Em\sigma}(r,\eta) \middle| \Psi_{i'}^{E'm'\sigma'}(r,\eta) \right\rangle = \sum_{j=1}^{j_{\text{max}}} \int_{0}^{\infty} r^{2} dr \left( \hat{\chi}_{ji}^{(m\sigma)}(E,r) \right)^{*} \hat{\chi}_{ji'}^{(m'\sigma')}(E',r)$$
$$= \delta(E-E') \delta_{mm'} \delta_{\sigma\sigma'} \delta_{ii'}.$$
(60)

### 5.1. Eigenchannel function

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

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}} \boldsymbol{\chi}^{(p)}(r) \mathbf{C} \cos \boldsymbol{\delta}.$$
(61)

Here a numerical solution  $\chi^{(p)}(r)$  of the (49) that satisfies the "standing" wave boundary conditions (54) and has the standard asymptotic form  $^{17}$ 

$$\boldsymbol{\chi}^{(p)}(r) = \boldsymbol{\chi}^{s}(r) + \boldsymbol{\chi}^{c}(r) \mathbf{K}, \quad \mathbf{K} \mathbf{C} = \mathbf{C} \tan \delta, \quad \mathbf{C} \mathbf{C}^{T} = \mathbf{C}^{T} \mathbf{C} = \mathbf{I}_{oo}.$$
 (62)

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

$$\mathbf{Wr}(\mathbf{Q}(r);\boldsymbol{\chi}^{c}(r),\boldsymbol{\chi}^{s}(r)) = \mathbf{I}_{oo}.$$
(63)

<sup>&</sup>lt;sup>17</sup>O. Chuluunbaatar et al, submitted to CPC

5.2. reaction matrix

Using R-matrix calculation<sup>18</sup>, we obtain the equation for the reaction matrix K expressed via the matrix R at  $r = r_{max}$ 

$$\left(\mathbf{R}\boldsymbol{\chi}^{c}(r) - \frac{d\boldsymbol{\chi}^{c}(r)}{dr}\right)\mathbf{K} = \left(\frac{d\boldsymbol{\chi}^{s}(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^{s}(r)\right).$$
(64)

When some channels are closed, the matrices in Eq. (64) are rectangular. Therefore, we obtain the following expression for the reaction matrix  ${\bf K}$ 

$$\mathbf{K} = -\mathbf{X}^{-1}(r_{\max})\mathbf{Y}(r_{\max}),\tag{65}$$

where

$$\mathbf{X}(r) = \left(\frac{d\boldsymbol{\chi}^{c}(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^{c}(r)\right)_{oo}, \quad \mathbf{Y}(r) = \left(\frac{d\boldsymbol{\chi}^{s}(r)}{dr} - \mathbf{R}\boldsymbol{\chi}^{s}(r)\right)_{oo}, \quad (66)$$

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

<sup>&</sup>lt;sup>18</sup>O. Chuluunbaatar et al, Proc. SPIE 6165, 66 (2006)

5.3. "incoming" wave function

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

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}} \boldsymbol{\chi}^{-}(r) = \imath \sqrt{\frac{2}{\pi}} \boldsymbol{\chi}^{(p)}(r) (\mathbf{I}_{oo} + \imath \, \mathbf{K})^{-1},$$
(67)

and has the asymptotic form

$$\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = \sqrt{\frac{2}{\pi}} (\boldsymbol{\chi}(r) - \boldsymbol{\chi}^*(r) \mathbf{S}^{\dagger}),$$
(68)

where S is the short-range scattering matrix, depends on the scattering matrix  $\tilde{S}_{\sigma}$  (25) and Coulomb phase shift  $\delta^{c}$ ,

$$\mathbf{S} \equiv \mathbf{S}_{\sigma} = \exp(-\imath \boldsymbol{\delta}^c) \, \check{\mathbf{S}}_{\sigma} \, \exp(-\imath \boldsymbol{\delta}^c), \quad \mathbf{S}^{\dagger} \mathbf{S} = \mathbf{S} \mathbf{S}^{\dagger} = \mathbf{I}_{oo}, \tag{69}$$

$$\mathbf{K} = \imath (\mathbf{I}_{oo} + \mathbf{S})^{-1} (\mathbf{I}_{oo} - \mathbf{S}), \quad \mathbf{S} = (\mathbf{I}_{oo} + \imath \mathbf{K}) (\mathbf{I}_{oo} - \imath \mathbf{K})^{-1}.$$
(70)

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The total wave function having the asymptotic form "waves going into the center + outgoing wave",

$$\Psi_{Em\hat{\upsilon}}^{(-)}(r,\eta) \equiv \Psi_{Em\stackrel{\longrightarrow}{\leftarrow}}^{(-)}(r,\eta) = \frac{1}{\sqrt{2}} \left( \Psi^{Em\sigma=+1}(r,\eta) \pm \Psi^{Em\sigma=-1}(r,\eta) \right) \exp(-\imath \delta^c), \quad (71)$$

that corresponds to function (29).

#### 5.4. the photoionization cross section

In terms of the above definitions  $\sigma(\omega)$  by the light linearly polarized along the axis z (31) is expressed as

$$\sigma(\omega) = 4\pi^2 \alpha \omega \sum_{i=1}^{N_o} \left| D_{i,N_{|z|},N_\rho}^{m\sigma\sigma'}(E) \right|^2 a_0^2,$$
(72)

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

$$D_{i,N_{|z|},N_{\rho}}^{m\sigma\sigma'}(E) = \left\langle \Psi_{i}^{Em\sigma=\mp1}(r,\eta) \middle| r\eta \middle| \Psi_{N_{|z|},N_{\rho}}^{m\sigma'=\pm1}(r,\eta) \right\rangle$$
$$= \sum_{j=1}^{j_{\max}} \int_{0}^{r_{\max}} r^{2} dr \hat{\chi}_{ji}^{(m\sigma=\mp1)}(E,r) d_{j}^{(m\sigma\sigma')}(r),$$
(73)

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

$$d_{j}^{(m\sigma\sigma')}(r) = \sum_{j'=1}^{j_{\max}} \left\langle \Phi_{j}^{m\sigma=\mp 1}(\eta; r) \middle| r\eta \middle| \Phi_{j'}^{m\sigma'=\pm 1}(\eta; r) \right\rangle_{\eta} \chi_{j'}^{(m\sigma'=\pm 1)}(r).$$
(74)

In the above expressions  $\omega = E - E(N_{|z|}, N_{\rho}, \sigma', m)$  is the frequency of radiation,  $E_{Nlm} \equiv E(N_{|z|}, N_{\rho}, \sigma', m)$  is the energy of the initial bound state  $\Psi_{N_{|z|}, N_{\rho}}^{m\sigma'}(r, \eta)$ , and  $N_{|z|} = N_r = N - l - 1$ .

The continuum spectrum solution  $\chi^{(p)}(r)$  having asymptotic of "standing" wave conditions and reaction matrix K required for calculating (61) or (68), and discrete spectrum solution  $\chi(r)$  and eigenvalue E can be calculated with help of the program KANTBP<sup>19</sup>.

One can see that using (61) or (68) for calculation of absolute value in formula (72) yields the same result as well as, with function (71) performing summation by  $\hat{v}$  in accordance with formula (31).

Therefore, (61) is preferable for using real arithmetics.

For the light circularly polarized in the plane xOy the similar expression can be written for formula (32) using expression  $(\vec{e}_{\pm}\vec{r}) = \frac{r}{\sqrt{2}}\sqrt{1-\eta^2}\exp(\pm\imath\varphi)$ .

In the calculations we used the following values of the physical constants:

 $1 \, cm^{-1} = 4.55633 \times 10^{-6} \, a.u.$ , the Bohr radius  $a_0 = 5.29177 \times 10^{-11} m$  and the fine-structure constant  $\alpha = 7.29735 \times 10^{-3}$ .

<sup>&</sup>lt;sup>19</sup>O. Chuluunbaatar et al, submitted to CPC



Photoionization cross section from the states 3s (left) and 3d (right) versus the energy for  $B_0 = 6.10 T$  ( $\gamma = 2.595 \times 10^{-5}$ ) and for the final state with  $\sigma = -1$ , m = 0. In this case we increased  $j_{\rm max}$  up to 35, and the finite element grids were chosen as 0 (200) 0.03 (200) 0.2 (200) 1 and 0 (200) 0.03 (200) 0.2 (200) 1 (2000) 100 (4000) 1000. The number of nodes in these grids is 2400 and 26401, respectively. The corresponding maximum number of unknowns in Eqs. (49) is 84000 and 924035.

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

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N' = 3, l' = 0, m' = 0 versus the energy of the initially free positron.

## 6. Conclusions

- 1. A new efficient method of calculating both the discrete and the continuous spectrum wave functions of a hydrogen atom in a strong magnetic field is developed based on the Kantorovich approach to the parametric eigenvalue problems in spherical coordinates.
- 2. The two-dimensional spectral problem for the Schrödinger equation with fixed magnetic quantum number and parity is reduced to a one-dimensional spectral parametric problem for the angular variable and a finite set of ordinary second-order differential equations for the radial variable.
- 3. The rate of convergence is investigated firstly numerically and is illustrated with a number of typical examples.
- It is shown that the calculated photoionization cross-sections has the true threshold behavior and recombination cross-sections can be recalculated using presented relations.
- 5. The presented recurrence relations for calculation of the coefficients of asymptotic expansions of fundamental solutions of a set of the radial equations or the overlap matrix open the door in the study of threshold phenomena using the known asymptotic expansion of Coulomb functions <sup>20</sup>.

 <sup>&</sup>lt;sup>20</sup>V.V. Pupyshev, J. Phys. A 28 3305 (1995)
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- 6. The main goal of the elaborated approach consists in the following. The calculations on all steps of Kantorovich approach are realized with help of stable calculation schemes and with a prescribed accuracy.
- 7. The economy of computer recourses is achieved with help of calculated all needed asymptotics of set of adaptive basis functions, matrix elements of radial coupling and radial solutions in analytic form to reduce interval of integration of the corresponded boundary problems.
- 8. The approach developed provides a useful tool for calculations of threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps<sup>21</sup>, quantum dots in magnetic field <sup>22</sup>, channeling processes<sup>23</sup> and potential scattering with confinement potentials <sup>24</sup>.

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