THE COULOMB SCATTERING IN HOMOGENEOUS MAGNETIC FIELD

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Outline

1. Application of the adiabatic method for solving axis channeling problem for oppositive or similar charged ions in a homogeneous magnetic field or a transversal oscillator potential.
2. Effects of resonance transmission and total reflection of oppositive or similar charged ions in a transversal oscillator potential.
3. The estimation of the resonance photoionization cross-section and laser-induced recombination rate of hydrogen atom in homogeneous magnetic filed.
4. The quanlitative estimation of an enhancement coefficient in a vicinity of the pair impact point of ions in presence of a transversal oscillator potential.

1. Statement of the problem

The Schrödinger equation [1] for a wave function $\hat{\Psi}(\Omega) = \Psi(r,\eta)\exp(\imath m\varphi)/\sqrt{2\pi}$ of a hydrogen atom with a charge q in an axially symmetric homogeneous magnetic field $\vec{B} = [B_x = 0, B_y = 0, B_z = B]$ writing in spherical coordinates $\Omega = (r, \eta = \cos\theta, \varphi)$ is reduced to the 2D equation for a partial component $\Psi(r,\eta) \equiv \Psi^{m\sigma}(r,\eta) = \sigma\Psi^{m\sigma}(r,-\eta)$ at fixed values of the magnetic quantum number $m = 0, \pm 1, \dots$ and z-parity $\sigma = \pm 1$

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

Here we use the atomic units $(a.u.)$ $\hbar = m_e = e = 1$ and put the mass of the nucleus to be infinite, and $\epsilon = 2E$, E is an energy (expressed in Rydbergs, $1\,Ry = (1/2)\,a.u.$) of a state $|m\sigma\rangle$.
A similar equation with the reduced charge, $q = \mu q_1 q_2$, and reduced mass, $\mu = m_1 m_2/\left(m_1 + m_2\right)$, of pair ions is described axis channeling of the similar charged particles possess equal charge-to-mass ratios, $q_1/m_1 = q_2/m_2$, such that the motion of the center of mass is separated in transversal oscillator potential[2] with frequency γ.

[1] O. Chuluunbaatar *et al.*, J. Phys. A **40**, 11485 (2007).
[2] O. Chuluunbaatar, et al. Phys. At. Nucl., **72**, 768 (2009).

Parametric basis functions

The operator $\hat{A}(p)$ is defined by

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

where $p = \gamma r^2/2$ is the confinement potential induced by the magnetic field, $\gamma = B/B_0$, $B_0 \cong 2.35 \times 10^5\, T$, is a dimensionless parameter determining the field B.

Let us consider a formal adiabatic expansion of the partial solution $\Psi_i^{Em\sigma}(r,\eta)$ of Eq. (1) in terms of one-dimensional basis functions $\{\Phi_j^{m\sigma}(\eta;r)\}_{j=1}^{j_{\max}}$

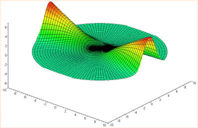
$$\Psi_i^{Em\sigma}(r,\eta) = \sum_{j=1}^{j_{\max}} \Phi_j^{m\sigma}(\eta;r)\chi_j^{(m\sigma i)}(E,r). \qquad (2)$$

The radial wave functions $\chi^{(i)}(r) \equiv \chi^{(m\sigma i)}(E,r)$, $(\chi^{(i)}(r))^T = (\chi_1^{(i)}(r), \ldots, \chi_{j_{\max}}^{(i)}(r))$ are unknown.

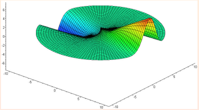
The orthonormal basis wave functions
$\Phi(r,\eta) \equiv \Phi^{m\sigma}(\eta;r) = \sigma\Phi^{m\sigma}(-\eta;r)$ and the potential curves
$E_j(r)$ (in Ry) are the solutions of the parametric eigenvalue problem

$$\hat{A}(p)\Phi_j(\eta;r) = E_j(r)\Phi_j(\eta;r). \tag{3}$$

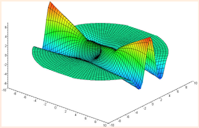
The solutions of this problem with shifted eigenvalues
$\check{E}_j(r) = E_j(r) - 2pm$ corresponded to the angular oblate spheroidal functions [3].



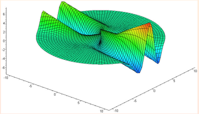
$\Phi_1^{\sigma=0,m=0}$



$\Phi_1^{\sigma=1,m=0}$



$\Phi_2^{\sigma=0,m=0}$



$\Phi_2^{\sigma=1,m=0}$

[3] M. Abramovits, and I.A. Stegun, Handbook of Mathematical Functions (New York: Dover, 1972)

System of radial equations

By using the expansion (2) we reduce of the problem (1) to a boundary problem for a set of $j_{\max}$ coupled second-order ordinary differential equations that determine the radial wave functions $\chi^{(i)}(r)$ of the expansion (2) on the finite interval $r \in [0, r_{\max}]$

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

with the boundary conditions

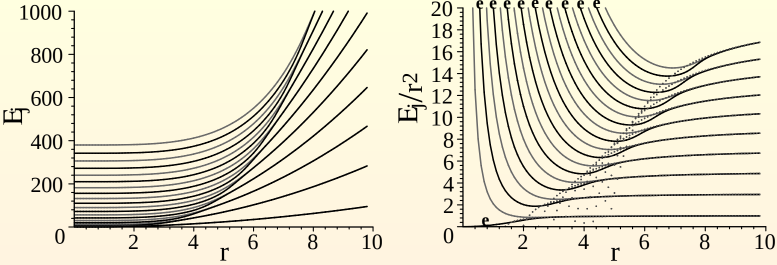
$$\lim_{r\to 0} r^2\left(\frac{d\chi^{(i)}(r)}{dr} - \mathbf{Q}(r)\chi^{(i)}(r)\right) = 0. \qquad (5)$$

Here $\mathbf{I}$, $\mathbf{U}(r)$ and $\mathbf{Q}(r)$ are $j_{\max} \times j_{\max}$ matrices with the elements evaluated as

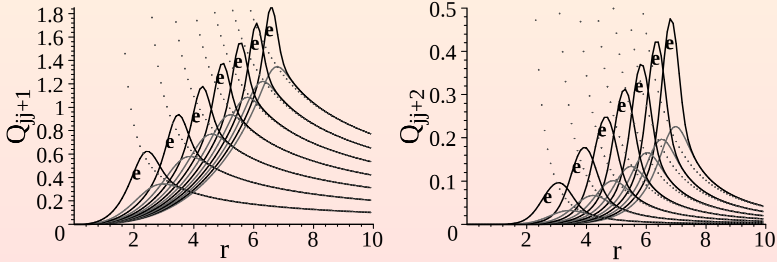
$$U_{ij}(r) = \frac{E_i(r) + E_j(r) + 4qr}{2}\delta_{ij} + r^2 H_{ij}(r), \; I_{ij} = \delta_{ij},$$
$$H_{ij}(r) = H_{ji}(r) = \int_{-1}^{1} \frac{\partial \Phi_i(\eta; r)}{\partial r} \frac{\partial \Phi_j(\eta; r)}{\partial r} d\eta, \tag{6}$$
$$Q_{ij}(r) = -Q_{ji}(r) = -\int_{-1}^{1} \Phi_i(\eta; r) \frac{\partial \Phi_j(\eta; r)}{\partial r} d\eta.$$

The calculations of the eigenfunctions $\Phi_j(\eta; r)$, potential curves $E_i(r)$ and radial coupling matrix elements $H_{ij}(r)$ and $Q_{ij}(r)$ have been performed by means of the program POTHMF [4] or the program ODPEVP [5]

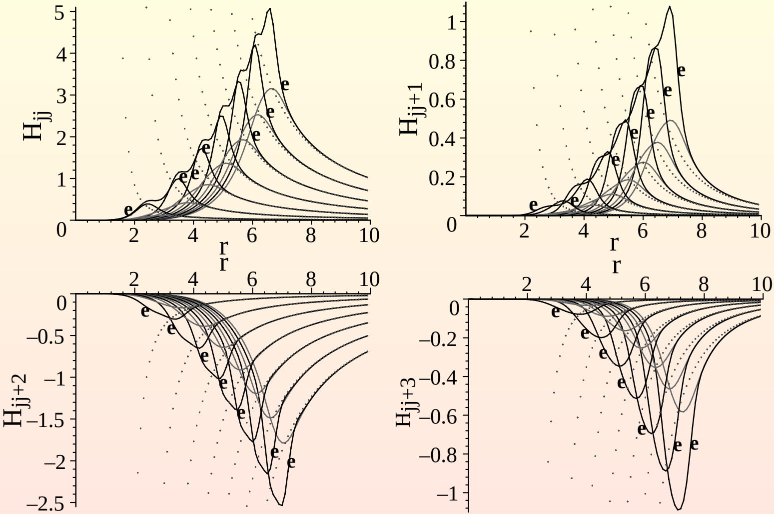
[4] O. Chuluunbaatar *et al.*, Comput. Phys. Commun. **178**, 301 (2008)
[5] O. Chuluunbaatar *et al.*, Comput. Phys. Commun., **180**, 1358 (2009).



The behavior of potential curves $E_j(r)$, $j = 1, 2, \ldots$ at $m = 0$ and $\gamma = 1$ for some first even $j = (l - |m|)/2 + 1$ (marked by 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

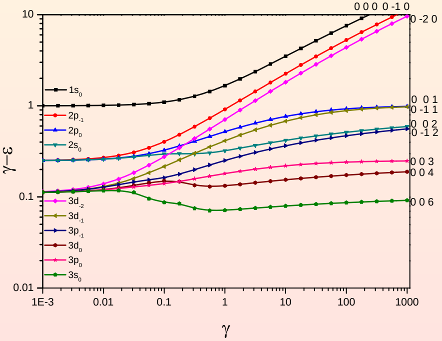


Some potentials H_{ij} for even (marked by symbol "e") and odd parity at $m = 0$ and $\gamma = 1$. The dotted lines are asymptotics of potentials at large r.

The discrete spectrum solutions

The discrete spectrum solutions $\chi^{(i)}(r)$ obey the first-type boundary condition, $\chi^{(i)}(r_{\max}) = 0$, to calculate unknown energies $E \equiv E_{m\sigma i\mathrm{v}}$, $\mathrm{v} = \overline{0, \mathrm{v}_{\max}}$, and corresponding $\Psi^{m\sigma}_{i\mathrm{v}}(r,\eta) \equiv \Psi^{Em\sigma}_{i}(r,\eta)$ of Eqs. (2) at $i = 1$ by the program KANTBP [6]. The orthogonality/normalization condition for $\hat{\Psi}^{m\sigma}_{i\mathrm{v}}(\Omega)$ is

$$\left\langle \hat{\Psi}^{m\sigma}_{i\mathrm{v}}(\Omega) \middle| \hat{\Psi}^{m'\sigma'}_{i'\mathrm{v}'}(\Omega) \right\rangle = \delta_{\mathrm{v}\mathrm{v}'}\delta_{mm'}\delta_{\sigma\sigma'}\delta_{ii'}. \qquad (7)$$



The binding energy $\mathcal{E}_i = \gamma - \epsilon_i$ (in Ry) vs γ of first ten states at $m \le 0$.
Correspondence rule: $(N, l, m) \to (N_\rho, m, N_z)$

[6] O. Chuluunbaatar *et al.*, Comput. Phys. Commun. **177**, 649 (2007)

Table of correspondence rule: $(N, l, m) \longrightarrow (N_\rho, m, N_z)$

$\gamma \to 0$ $\gamma \to \infty$

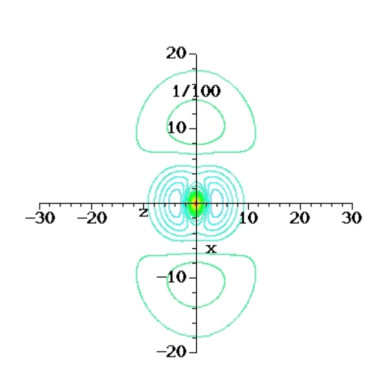
N	l	m	σ	N_η	N_r	N_ρ	N_z	m	ϵ^{th}	j
1	0	0	1	0	0	0	0	0	γ	1
2	0	0	1	0	1	0	2	0	γ	1
2	1	−1	1	0	0	0	0	−1	γ	1
2	1	0	−1	1	0	0	1	0	γ	1
2	1	1	1	0	0	1	0	1	3γ	2
3	0	0	1	0	2	0	6	0	γ	1
3	1	−1	1	0	1	0	2	−1	γ	1
3	1	0	−1	1	1	0	3	0	γ	1
3	1	1	1	0	1	1	2	1	3γ	2
3	2	−2	1	0	0	0	0	−2	γ	1
3	2	−1	−1	1	0	0	1	−1	γ	1
3	2	0	1	2	0	0	4	0	γ	1
3	2	1	−1	1	0	1	1	1	3γ	2
3	2	2	1	0	0	2	0	2	5γ	3

$$N_z = 2\left[\frac{N_r}{2}\right] + \begin{cases} 2\left[\frac{N-|m|+1}{2}\right]\left[\frac{N-|m|}{2}\right], & \sigma = +1, \\ 2\left[\frac{N-|m|}{2}\right]\left[\frac{N-|m|-1}{2}\right] + 1, & \sigma = -1, \end{cases}$$

$$N_\rho = \frac{|m| + m}{2},$$

$$\epsilon_{N_\rho |m| N_z} = \epsilon_{N_\rho, -|m|, N_z} + 2|m|.$$

$3s_0$ rotational state vs γ:
$1/100 < \gamma < 99/100 \sim 1$



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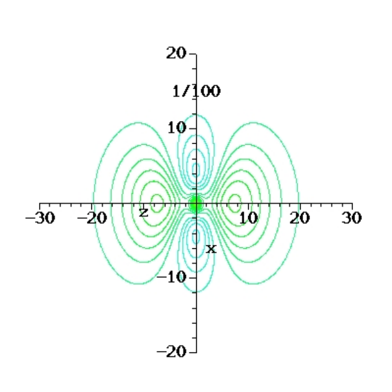


The asymptotic expansion of 2D-function in Kantorovich form at $r \to 0$

$$\psi_{i_o}^{(\mathrm{as})}(\eta, r) = \sum_{i=1}^{j_{\max}} \sum_{k=0}^{k_{\max}} \sum_{p=0}^{k_{\max}-k} \sum_{j=1}^{j_{\max}} r^{\mu_i + k} \phi_j^{(k-p)}(\eta) \tilde{\chi}_{ji}^{(p)\mathrm{reg}} C_{i i_o}$$

$$= \sum_{i=1}^{j_{\max}} \sum_{k=0}^{k_{\max}} \sum_{p=0}^{k_{\max}-k} \sum_{j=1}^{j_{\max}} \sum_{s=\max(-l,-2k+2p)}^{2k-2p} r^{\mu_i + k} P_{l+s}^{|m|}(\eta) b_{sj}^{(k-p)} \tilde{\chi}_{ji}^{(p)\mathrm{reg}} C_{i i_o}$$

where $P_{l+s}^{|m|}(\eta)$ is Legendre polynomials,
$l = 2i + |m| + (-\sigma + |\sigma|)/2$, $\mu_i = l$. The recurrence relations for evaluation coefficients $b_{sj}^{(k-p)}$ and $\tilde{\chi}_{ji}^{(p)\mathrm{reg}}$ is given in [7] and constant $C_{i i_o}$ calculated by program KANTBP 2.0[8] This expansion is satisfy to the Kato condition and corresponds to expansion for Coulomb function at $\gamma = 0$.

[7] O. Chuluunbaatar, , et al. Physics of Atomic Nuclei. **72**, pp. 768–778 (2009).
[8] O. Chuluunbaatar, , et al. Comput. Phys. Commun. 179 (2008) 685

The above asymptotic of Kantorovich expansion is equivalent of Galerkin expansion over basis of Legendre polynomials:

$$\psi_{i_o}^{(\mathrm{as})}(\eta, r) = \sum_{i=1}^{j_{\max}} \sum_{k=0}^{k_{\max}} \sum_{s=\max(-l,-2k+2p)}^{2k-2p} r^{\mu_i+k} P_{l+s}^{|m|}(\eta) g_{si}^{(k_{\max}-k)} C_{ii_o}$$

for

$$g_{si}^{(k_{\max}-k)} = \sum_{p=0}^{k_{\max}-k} \sum_{j=1}^{j_{\max}} b_{sj}^{(k-p)} \tilde{\chi}_{ji}^{(p)\mathrm{reg}}.$$

This expansion will be correspond to one given in[9]

[9] V.V. Pupyshev. Generalization of Fock and Kato expansions for systems of three quantum particles. Physics of Elementary Particles and Atomic Nuclei V. 40, N 4, p. 763-892 (2009)

The continuous spectrum solutions

The continuous spectrum solutions $\chi^{(i)}(r)$ obey the third-type boundary condition at fixed energy $\epsilon = 2E$ above the first threshold $E_j(\infty) \equiv \epsilon^{th}_{mj}(\gamma) = \gamma(2j - 1 + m + |m|)$ with $j = 1$

$$\frac{d\chi(r)}{dr} = \mathrm{R}\chi(r), \qquad r = r_{\max}, \tag{8}$$

where $\mathbf{R}$ is a non-symmetrical $j_{\max} \times j_{\max}$ matrix which is calculated by the program KANTBP[10]. The orthogonality/normalization condition for $\hat{\Psi}_i^{Em\sigma}(\Omega)$ is

$$\left\langle \hat{\Psi}_i^{Em\sigma}(\Omega) \middle| \hat{\Psi}_{i'}^{E'm'\sigma'}(\Omega) \right\rangle = \delta(E - E')\delta_{mm'}\delta_{\sigma\sigma'}\delta_{ii'}. \tag{9}$$

[10] O. Chuluunbaatar *et al.*, Comput. Phys. Commun. **179**, 685 (2008)

Asymptotic expansion of 2D-function in Kantorovich form:

$$\Psi_i^{m\sigma,as}(\eta,r) = (2\gamma)^{1/2} y^{|m|/2} \exp(-\frac{y}{2}) \left(1 - \frac{y}{2\gamma r^2}\right)^{|m|/2}$$
$$\times \sum_{k=0}^{k_{\max}} \sum_{k'=0}^{k_{\max}-2k} \left(\frac{1}{2\gamma}\right)^k r^{1-2k-k'}$$
$$\times \sum_{j=1}^{j_{max}} \sum_{s=\max(-k,1-j)}^{k} c_{s,j-1}^{(2k)} L_{j-1+s}^{(|m|)}(y)$$
$$\times \left(R_0(p_{i_o},r)\phi_{ji_o}^{(k')} + \frac{dR_0(p_{i_o},r)}{dr}\psi_{ji_o}^{(k')}\right).$$

where $R_0(p_{i_o},r)$ are Coulomb functions, $L_{j-1+s}^{(|m|)}(y)$ are Laguerre polynomials, $y = 2p(1-|\eta|)$, $p = \gamma r^2/2$, $\eta = \cos\theta$, $|\eta| \in [1-\eta_1, 1]$, $\eta_1 = o(p^{-1/2-\epsilon})$, $0 < \epsilon < 1/2$.
The recurrence relations for evaluation coefficients $c_{s,j-1}^{(2k)}$ and $\phi_{ji_o}^{(k')}$ is given in [11] and in the threshold case of $p_{i_o}. = 0$ in [12]

[11] O. Chuluunbaatar, J. Phys. **A 40**, pp. 11485–11524 (2007)
[12] S.I.Vinitsky et al, LNCS **5743**, pp. 334–349 (2009).

Correspondence between asymptotic expansions in spherical and cylindrical coordinates

For $k_{\max} = 1$ in terms of asymptotic functions $\langle \rho | j \rangle = \tilde{\Phi}_j^m(\rho)$, of the two-dimensional oscillator, we have

$$\phi^{(1)}_{j_1 i_o} = 0,$$

$$\psi^{(1)}_{j_1 i_o} = -\frac{1}{2}\langle j_1 | \rho^2 | i_o \rangle = \frac{\sqrt{n_o}\,\sqrt{n_o + |m|}}{\gamma}\delta_{j_1, i_o - 1} + \frac{\sqrt{n_o + 1}\sqrt{n_o + |m| + 1}}{\gamma}\delta_{j_1, i_o + 1}, \quad (10)$$

$$\phi^{(1)}_{i_o i_o} = 0, \quad (11)$$

$$\psi^{(1)}_{i_o i_o} = -\frac{1}{2}\langle i_o | \rho^2 | i_o \rangle = -\frac{2n_o + |m| + 1}{\gamma}.$$

In view of orthogonality $\langle j|i_o\rangle = \delta_{ji_o}$ completeness conditions $\sum_j |\langle\rho'|j\rangle\langle j|\rho\rangle = \delta(\rho' - \rho)$ and relation $|z| = r(1 - \rho^2/(2r^2)) + O(r^{-2})$, Asymptotic of total wave function at $p_{i_o}\rho^2/(2r) \ll 1$ takes form:

$$\begin{aligned}
\Psi^{m\hat{v}}(r,\eta) &= r\sum_j |j\rangle\left[\langle j|i_o\rangle - \frac{1}{2r}\langle j|\rho^2|i_o\rangle\frac{d}{dr}\right]R_0(p_{i_o},r) \\
&= r\sum_j |j\rangle\langle j|\left[|i_o\rangle - \frac{1}{2r}\rho^2|i_o\rangle\frac{d}{dr}\right]R(p_{i_o},r) \qquad (12) \\
&\approx r\,\langle\rho|i_o\rangle R_0\left(p_{i_o}, r\left(1 - \frac{\rho^2}{2r^2}\right)\right) \approx \frac{1}{2}\Phi^m_{i_0}(\rho)X^{(+)}_{i_oi_o}(|z|)\exp(\imath\,\delta^c_{i_o}),
\end{aligned}$$

where $\delta^c_{i_o}$ is Coulomb phase shift and $X^{(\pm)}_{n'n}(z)$ is required asymptotic

$$X^{(\pm)}_{n'n}(z) = p_{n'}^{-1/2}\exp\left(\pm\imath p_{n'}z \mp \imath\frac{q}{p_{n'}}\frac{z}{|z|}\ln(2p_{n'}|z|)\right)\delta_{n'n}.$$

"standing-wave" solutions

We express the corresponding eigenfunction $\Psi_i^{Em\sigma}(r,\eta)$ in open channels, $i=\overline{1,N_o}$, $N_o=\max_{2E\geq\epsilon_{mj}^{th}} j<j_{\max}$, of the continuous spectrum with the energy $\epsilon=2E$ in the form of Eq. (2), where $\hat{\chi}^{(m\sigma)}(E,r)\equiv\{\chi^{(i_o)}(r)\}_{i_o=1}^{N_o}$ is now the radial part of the eigenchannel or "incoming" wave function.

The eigenchannel wave function $\hat{\chi}^{(m\sigma)}(E,r)$ is expressed as

$$\hat{\chi}^{(m\sigma)}(E,r)=(2/\pi)^{1/2}\chi^{(p)}(r)\mathbf{C}\cos\delta. \quad (13)$$

The function $\chi^{(p)}(r)$ is a numerical solution of Eq. (4) that satisfies the "standing-wave" boundary conditions (8) and has the standard asymptotic form

$$\chi^{(p)}(r)=\chi^{s}(r)+\chi^{c}(r)\,\mathbf{K},\quad \mathbf{K}\,\mathbf{C}=\mathbf{C}\tan\delta. \quad (14)$$

reaction matrix

Here $\mathbf{K} \equiv \mathbf{K}_\sigma$ is the numerical short-range reaction matrix with the eigenvalue $\tan\delta$ and the orthogonal matrix $\mathbf{C}^T\mathbf{C} = \mathbf{I}_{oo}$ of the corresponding eigenvectors $\mathbf{C}$, where $\mathbf{I}_{oo}$ is the unit $N_o \times N_o$ matrix. The regular $\chi^s(r) = 2\,\Im(\chi(r))$ and irregular $\chi^c(r) = 2\,\Re(\chi(r))$ asymptotic functions are expressed via the fundemential asymptotic solution $\chi(r)$ with leading terms at $r \rightarrow \infty$

$$\chi_{ji_o}(r) = \frac{\exp(\imath\, p_{i_o} r + \imath\,\zeta \ln(2p_{i_o} r) + \imath\,\delta^c_{i_o})}{2r\sqrt{p_{i_o}}}\delta_{ji_o}, \qquad (15)$$

where $p_{i_o} = \sqrt{2E - \epsilon^{th}_{i_o}} > 0$ is the relative momentum in the channel i_o, $\zeta \equiv \zeta_{i_o} = -q/p_{i_o}$ is a Zommerfeld-type parameter, $\delta^c_{i_o} = \arg\Gamma(1 - \imath\zeta)$ is the known Coulomb phase shift[13].

[13] M. Abramovits, and I.A. Stegun, Handbook of Mathematical Functions (New York: Dover, 1972)

Using $\mathbf{R}$-matrix calculus , we obtain the equation expressing the reaction matrix $\mathbf{K}$ via the matrix $\mathbf{R}$ at $r = r_{\max}$

$$\mathbf{K} = -\mathbf{X}^{-1}(r_{\max})\mathbf{Y}(r_{\max}), \tag{16}$$

where $\mathbf{X}(r)$ and $\mathbf{Y}(r)$ are square $N_o \times N_o$ matrices depended on the open-open matrix (channels)

$$\mathbf{X}(r) = \left(\frac{d\chi^c(r)}{dr} - \mathbf{R}\chi^c(r)\right)_{oo}, \tag{17}$$
$$\mathbf{Y}(r) = \left(\frac{d\chi^s(r)}{dr} - \mathbf{R}\chi^s(r)\right)_{oo},$$

“incoming” wave function

The radial part of the “incoming” wave function $\hat{\chi}^{(m\sigma)}(E,r) = (2/\pi)^{1/2}\chi^{-}(r)$ is expressed via the numerical “standing” wave function and the short-range reaction matrix $\mathbf{K}$ by the relation

$$\chi^{-}(r) = \imath\chi^{(p)}(r)(\mathbf{I}_{oo} + \imath\,\mathbf{K})^{-1}, \tag{18}$$

and has the asymptotic form

$$\hat{\chi}^{(m\sigma)}(E,r) = (2/\pi)^{1/2}(\chi(r) - \chi^{*}(r)\mathbf{S}^{\dagger}). \tag{19}$$

Here $\mathbf{S} \equiv \mathbf{S}_{\sigma}$ is the short-range scattering matrix, $\mathbf{S}^{\dagger}\mathbf{S} = \mathbf{S}\mathbf{S}^{\dagger} = \mathbf{I}_{oo}$, expressed via the calculated $\mathbf{K}$ matrix

$$\mathbf{S} = (\mathbf{I}_{oo} + \imath\,\mathbf{K})(\mathbf{I}_{oo} - \imath\,\mathbf{K})^{-1}. \tag{20}$$

“incident wave + ingoing wave”

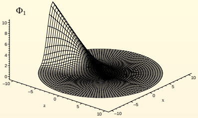
The ionization wave function $\Psi^{(-)}_{Em\hat{v}}(r,\eta) \equiv \Psi^{(-)}_{Em\rightleftarrows}(r,\eta)$ has the asymptotic form reverse to the common scattering problem, namely, “incident wave + ingoing wave”

$$\Psi^{(-)}_{Em\hat{v}}(r,\eta) = \frac{\Psi^{Em,+1}(r,\eta) \pm \Psi^{Em,-1}(r,\eta)}{\sqrt{2}} \exp(-\imath\delta^c). \qquad (21)$$

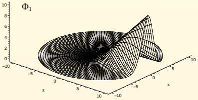
The function $\Psi^{(-)}_{Em\hat{v}}(r,\eta)$ corresponds to the function $|E\hat{v}mN_\rho\rangle$ defined in cylindrical coordinates (ρ, z, φ)

$$|E\hat{v}mN_\rho\rangle = \frac{\exp(\imath m\varphi)}{2\pi} \sum_{n'=1}^{j_{\max}} \Phi_{n'}(\rho)\chi^{(-)}_{Em\hat{v}n'n}(z). \qquad (22)$$

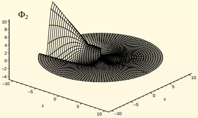
Here $N_\rho = n - 1$, $\hat{v} = \leftrightarrows$ denotes the initial direction of the particle motion along the z axis, $\Phi_{n'}(\rho)$ is the eigenfunction of the two-dimensional oscillator that corresponds to $\Phi_{n'}(\rho) \rightarrow \lim_{r\rightarrow\infty} r^{-1}\Phi^{m\hat{v}}_j(r,\eta)$:
$\Phi^{m\hat{v}}_j(r,\eta) = (\Phi^{m,+1}_j(r,\eta) \pm \Phi^{m,-1}_j(r,\eta))/\sqrt{2}$ at $r \rightarrow \infty$.



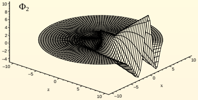
$\Phi_1^{m=0,\rightarrow}$



$\Phi_1^{m=0,\leftarrow}$

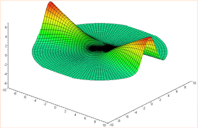


$\Phi_2^{m=0,\rightarrow}$

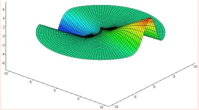


$\Phi_2^{m=0,\leftarrow}$

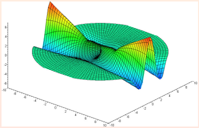
$$\Phi_j^{m\leftrightarrows}(r,\eta) = (\Phi_j^{m,+1}(r,\eta) \pm \Phi_j^{m,-1}(r,\eta))/\sqrt{2}$$



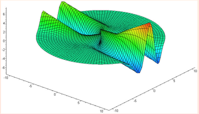
$\Phi_1^{\sigma=0,m=0}$



$\Phi_1^{\sigma=1,m=0}$



$\Phi_2^{\sigma=0,m=0}$



$\Phi_2^{\sigma=1,m=0}$

Asymptotics

At $z \to \pm\infty$ the function $\chi^{(-)}_{Em\hat{v}n'n}(z)$ has the following asymptotics:

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

where the matrix elements of $\mathbf{X}^{(\pm)}(z)$ are

$$X^{(\pm)}_{n'n}(z) = \exp\left(\pm \imath p_{n'} z \pm \imath \zeta_{n'} \frac{z}{|z|} \ln(2p_{n'}|z|)\right) \frac{\delta_{n'n}}{\sqrt{p_{n'}}}, \tag{24}$$

transmission and reflection amplitude matrices

$\hat{\mathrm{T}}$ and $\hat{\mathrm{R}}$ are the transmission and reflection amplitude matrices, $\hat{\mathrm{T}}^\dagger\hat{\mathrm{T}} + \hat{\mathrm{R}}^\dagger\hat{\mathrm{R}} = \mathbf{I}_{oo}$. It is easy to show that $\hat{\mathrm{T}}$ and $\hat{\mathrm{R}}$ may be expressed in terms of the long-range scattering matrices $\check{\mathbf{S}}_{\sigma} = \exp(\imath\delta^c)\,\mathbf{S}_{\sigma}\,\exp(\imath\delta^c)$ as

$$\hat{\mathrm{T}} = 2^{-1}(-\check{\mathrm{S}}_{+1} + \check{\mathrm{S}}_{-1}), \quad \hat{\mathrm{R}} = 2^{-1}(-\check{\mathrm{S}}_{+1} - \check{\mathrm{S}}_{-1}). \qquad (25)$$

The asymptotics of "incident+ingoing" wave function has the form

$$\begin{pmatrix} \Psi^{(-)}_{Em\rightarrow}(r,\eta_+) & \Psi^{(-)}_{Em\leftarrow}(r,\eta_+) \\ \Psi^{(-)}_{Em\rightarrow}(r,\eta_-) & \Psi^{(-)}_{Em\leftarrow}(r,\eta_-) \end{pmatrix} \rightarrow \sqrt{\frac{2}{\pi}} \begin{pmatrix} \Phi^{m\leftarrow}(\eta_+;r) & 0 \\ 0 & \Phi^{m\rightarrow}(\eta_-;r) \end{pmatrix}^T$$

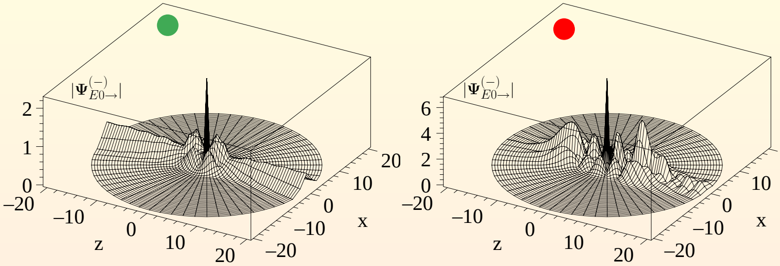
$$\times \left[\begin{pmatrix} \check{\chi}(r) & 0 \\ 0 & \check{\chi}(r) \end{pmatrix} + \begin{pmatrix} 0 & \check{\chi}^*(r) \\ \check{\chi}^*(r) & 0 \end{pmatrix} \hat{\mathrm{S}}^\dagger \right], \qquad (26)$$

where $\eta_\pm = \pm|\eta|$, $|\eta| \sim 1$ and $\hat{\mathrm{S}}^\dagger = \hat{\mathrm{S}}^{-1}$ inverse scattering matrix

$$\hat{\mathrm{S}}^\dagger = \begin{pmatrix} \hat{\mathrm{T}}^\dagger & \hat{\mathrm{R}}^\dagger \\ \hat{\mathrm{R}}^\dagger & \hat{\mathrm{T}}^\dagger \end{pmatrix}, \qquad \hat{\mathrm{S}}\hat{\mathrm{S}}^\dagger = \mathbf{I} \qquad (27)$$

Note that the transition operator $\hat{\mathcal{T}} = \hat{\mathrm{S}} - 1$ satisfy to $\hat{\mathcal{T}}\hat{\mathcal{T}}^\dagger = -2\Re\hat{\mathcal{T}}$

2a. Effects of resonance transmission and total reflection of oppositive charged ions in a transversal oscillator potential

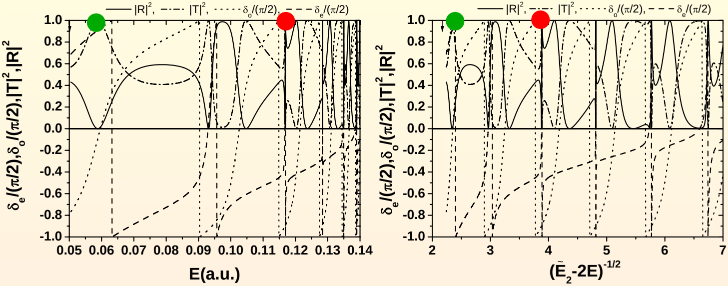


(a) (b)

Fig. 1 Profiles $|\boldsymbol{\Psi}^{(-)}_{\boldsymbol{Em}\rightarrow}|$ of the total wave functions of the continuous spectrum in the $\boldsymbol{zx}$ plane with $\boldsymbol{q=-1}$, $\boldsymbol{m=0}$, $\boldsymbol{\gamma=0.1}$ and the energies $\boldsymbol{E=0.05885\,a.u.}$ (a) and $\boldsymbol{E=0.11692\,a.u.}$ (b), demonstrating resonance transmission and total reflection, respectively.

Profiles of the wave function (21) for $\boldsymbol{q=-1}$, $\boldsymbol{m=0}$, $\boldsymbol{\gamma=0.1}$ and $\boldsymbol{j_{\max}=10}$ are shown in Fig. 1 at two fixed values of energy $\boldsymbol{E}$, corresponding to resonance transmission $|\hat{\mathbf{T}}|^2=\sin^2(\delta_e-\delta_o)=1$ and total reflection $|\hat{\mathbf{R}}|^2=\cos^2(\delta_e-\delta_o)=1$.

Transmission and reflection coefficients



(a) (b)

Fig. 2. Transmission $|\hat{\mathbf{T}}|^2$ and reflection $|\hat{\mathbf{R}}|^2$ coefficients, even δ_e and odd δ_o phase shifts versus the energy E (a) and $(\tilde{E}_2 - 2E)^{-1/2}$ (b) for $\gamma = 0.1$ and the final state with $\sigma = -1$, $q = -1$, $m = 0$. The arrow marks the first Landau threshold $E_1 = \gamma/2$.

Transmission and reflection coefficients are explicitly shown in Fig. 2 together with even δ_e and odd δ_o phase shifts versus the energy E (Fig. 2a) and $(\tilde{E}_2 - 2E)^{-1/2}$ (Fig.2b), where $\tilde{E}_2 = \epsilon^{th}_{m2}(\gamma)$ is second threshold shift. The quasi-stationary states imbedded in the continuum correspond to the short-range phase shifts $\delta_{o(e)} = n_{o(e)}\pi + \pi/2$ at $(\tilde{E}_2 - 2E)^{-1/2} = n_{o(e)} + \Delta_{n_{o(e)}}$.

Nonmonotonic behavior of $|\hat{\mathbf{T}}|$ and $|\hat{\mathbf{R}}|$ is seen to include the cases of resonance transmission and total reflection, related to the existence of these quasistationary states.

3.Photoionization cross-section

Therefore the cross-section $\sigma^d_{Nlm}(\omega)$ of photoionization by the light linearly polarized along axis z reads as

$$\sigma^d_{Nlm}(\omega) = 4\pi^2\alpha\omega\sum_{i=1}^{N_o}\left|D^{m\sigma\sigma'}_{i,N,l}(E)\right|^2 a_0^2, \qquad (28)$$

where α is the fine-structure constant, a_0 is the Bohr radius, $D^{m\sigma\sigma'}_{i,N,l}(E) \equiv D^{m\sigma\sigma'}_{i,i',\mathrm{v}'}(E)$ are the dipole moment matrix elements

$$D^{m\sigma\sigma'}_{i,i',\mathrm{v}'}(E) = \left\langle \Psi_i^{Em\sigma=\mp1}(r,\eta)\middle| r\eta \middle| \Psi_{i'\mathrm{v}'}^{m\sigma'=\pm1}(r,\eta)\right\rangle. \qquad (29)$$

In the above expressions $\omega = E - E_{Nlm}$ is the frequency of radiation, $E_{Nlm} \equiv E_{m\sigma' i'\mathrm{v}'}$ is the energy of the initial bound state $|Nlm\rangle = \Psi^{m\sigma'}_{i'\mathrm{v}'}(r,\eta)$ below half of the first true threshold shift $\epsilon^{th}_{m1}(\gamma)/2$ at $i'=1$. The continuous spectrum solution $\chi^{(p)}(r)$ having the asymptotic form of a "standing" wave and the reaction matrix $\mathbf{K}$ required for using Eq. (13) or (19), as well as the discrete spectrum solution $\chi(r)$ and the eigenvalue $E_{m\sigma' i'=1\mathrm{v}'}$, can be calculated using the program KANTBP .

photoionization cross-section

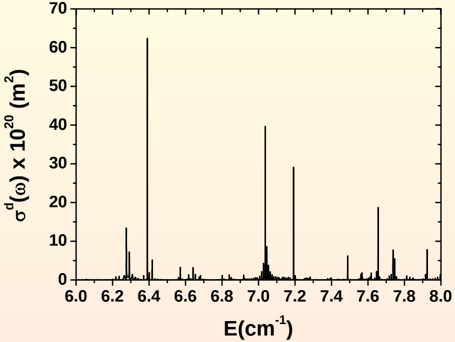


Fig. 3 Cross-section of photoionization from the state $3s_0$ versus the energy $\boldsymbol{E}$ for $\gamma = \mathbf{2.595 \times 10^{-5}}$ and the final state with $\boldsymbol{\sigma = -1}$, $\boldsymbol{q = -1}$, $\boldsymbol{m = 0}$.

Fig. 3 clarifies the behavior of the cross-section of photoionization by the light, linearly polarized along the axis z, from the rotational state $3s_0$ at $\boldsymbol{B_0 = 6.1\,T}$ $(\gamma = \mathbf{2.595 \times 10^{-5}})$ in the energy interval $\boldsymbol{E = 6.0 - 8.0\,cm^{-1}}$ at $\boldsymbol{j_{\max} = 35}$. The cross-sections have been calculated with the energy step $\mathbf{5 \times 10^{-4}}\,\boldsymbol{cm^{-1}}$ in all the region except the vicinity of peaks, where the step was $\mathbf{5 \times 10^{-6}}\,\boldsymbol{cm^{-1}}$.

laser-stimulated recombination rate

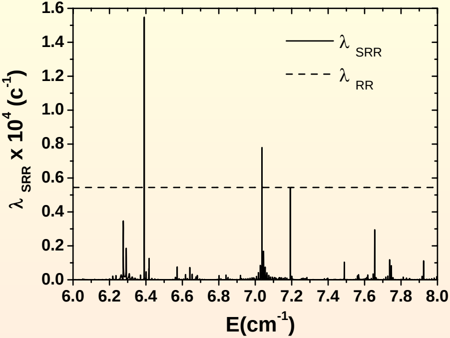


Fig. 4 Laser-stimulated radiative recombination rate into the bound state $N' = 3, l' = 0, m' = 0$ versus the energy E of the initially free positron.

Fig. 4 shows the dependence of the laser-stimulated recombination rate λ_{SRR} per one antiproton upon the initial energy $E = E_{Nlm} + \omega$ of the positron. For comparison the horizontal dashed line displays the rate λ_{RR} of the spontaneous radiative recombination into all the states with $N = 3$, which at the intensity considered is equal to the rate of the laser-stimulated recombination without the magnetic field [14] One can see narrow resonances for which the rate of recombination into the state with fixed $l = 0$, $m = 0$ in the magnetic field is appreciably higher than the rate of recombination into all nine states with different l and m possible for $N = 3$ without the magnetic field.

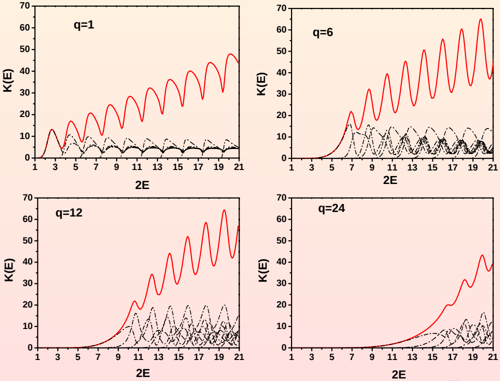
[14] M.V. Ryabinina and L.A. Melnikov, Nucl. Instr. Meth. Phys. Res. B **214**, 35 (2004).

4. Model of axis channeling of similar charged ions

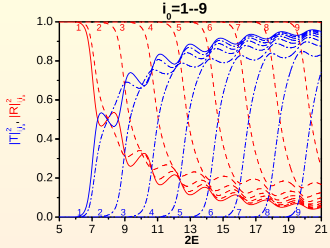
Enhancement coefficient $K(E)$ of a nuclear reaction rate of channeling ions is ratio of probability density of wave function in a vicinity of pair collision point $r = 0$ of ions with/without an additional transversal potential:

$$K(E) = \frac{|C\,(2E)\,|^2}{|C_0\,(2E)\,|^2} = \sum_{i=1}^{N_o} \frac{|C_i\,(2E)\,|^2}{|C_0\,(2E)\,|^2},$$

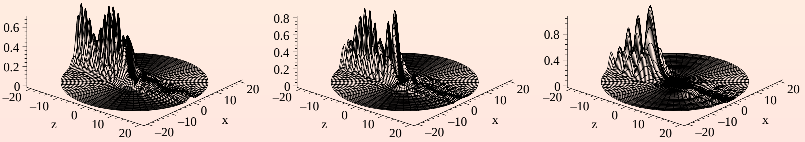
where $C_i\,(2E) = \Psi_{1i}(r = 0)$ is numerical values of solutions at $\gamma = 1$; $C_0\,(2E) = \Psi_{11}(r = 0)$ is Coulomb function, $N_o \leq 10$.



2b. Reflection and transmission coefficients at $q = 6$



$$|\mathbf{R}|^2 = \begin{pmatrix} 0.967329 & 0.004785 & -0.000094 \\ 0.004785 & 0.990368 & 0.000074 \\ -0.000094 & 0.000074 & 0.999999 \end{pmatrix} \quad \text{at} \quad 2E = 6.552$$



Resonance effects of practically full reflection and transition of similar charged ions in a channel of crystal characterized by transversal oscillator potential are predicted firstly and upper estimation of enhancement coefficient of a nuclear reaction rate of channeling ions are obtained.

These results may be interpreted as a resonance mechanism of anomalous repulsion Coulomb scattering on a nonspherical barrier. Such mechanism can be explained in the framework of a diagonal approximation of Eq. (4) in that is reduced to effective equations in each open channel i_o=1,...,10:

$$-\frac{1}{r^2}\frac{d}{dr}\frac{r^2}{\mu_{i_oi_o}(r)}\frac{d}{dr}\chi^{\rm eff}_{i_oi_o}(r)+\frac{\mu'_{i_oi_o}(r)}{\mu^2_{i_oi_o}(r)}\chi^{\rm eff}_{i_oi_o}(r) \quad (30)$$

$$+[U^{\rm eff}_{i_oi_o}(q,r)-(2E-1)]\chi^{\rm eff}_{i_oi_o}(r,E,q,\gamma)=0,$$

where $\mu^{-1}_{i_oi_o}(r)=(1+W_{i_oi_o}(r))$ is the effective mass and $U^{\rm eff}_{i_oi_o}(q,r)$ are the effective potentials[15].

[15] Chuluunbaatar O. et al J. Phys. A 2007, V. 40, P. 11485

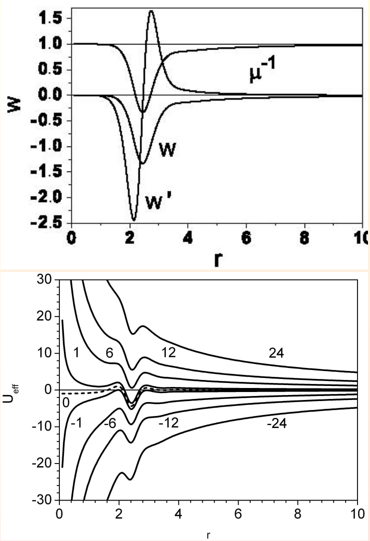
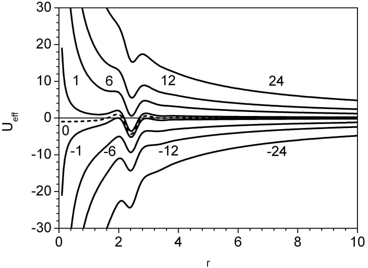


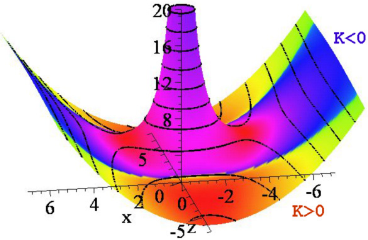
Fig. 5. The effective mass correction W_{11}, its derivative W'_{11} and the inverse effective mass μ^{-1} and effective potentials $U_{eff} \equiv U^{\text{eff}}_{11}(q,r)$ for *q=-24,-12,-6,-1,0,1,6,12,24* at $\mu = 1$, $\gamma = 1$ and $m = 0$ for the first even state $i_o = 1$.

The dashed line is values of effective potential $U_{eff} \equiv U^{\text{eff}}_{11}(q,r)$ for *q=0* that describes in spherical coordinates the exact-solvable problem for scattering of electron in homogenous magnetic field $\gamma = 1$ in cylindrical coordinates.[16]

[16] Landau, L.D.; Lifshits, E.M. 1977. Quantum Mechanics, N.Y.: Pergamon Press.

One can see that for charges $q = 1,\ 6,\ 12,\ 24$ and for $\gamma = 1$ the barrier energies are:





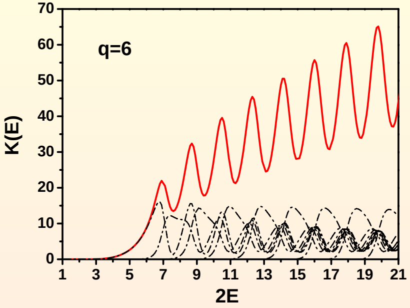
$$U^{\text{eff}}_{11}(q = 1, r \approx 2.95) = 1.27$$
$$\approx 2U_0 - 1 = 0.89,$$
$$\varepsilon^{th}_{1} = 2(1 - 1) + 1 = 1;$$

$$U^{\text{eff}}_{11}(q = 6, r \approx 2.90) = 4.72$$
$$\approx 2U_0 - 1 = 5.24,$$
$$\varepsilon^{th}_{3} = 2(3 - 1) + 1 = 5$$

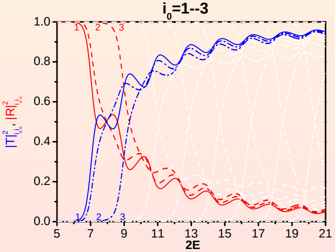
$$U^{\text{eff}}_{11}(q = 12, r \approx 2.85) = 8.90$$
$$\approx 2U_0 - 1 = 8.90,$$
$$\varepsilon^{th}_{5} = 2(5 - 1) + 1 = 9$$

$$U^{\text{eff}}_{11}(q = 24, r \approx 2.80) = 17.4$$
$$\approx 2U_0 - 1 = 14.7,$$
$$\varepsilon^{th}_{8} = 2(8 - 1) + 1 = 15$$

that approximately correspond to relative energy of open channel with the numbers $i_o = N^{sp}_o \approx \max(1, U_0 = 3(q/(2\sqrt{\gamma}))^{2/3}/2 = 1, 3, 5, 8$.



$$
\begin{aligned}
p_1^2 = E - \epsilon_1^{th} &= 5.52 \\
> 2U_0 - 1 &= 5.24 \\
> U_{11}^{\mathrm{eff}}(q=6, r \approx 2.9) &= 4.72 \\
> \varepsilon_{\mathbf{3}}^{th} - 1 &= 4.
\end{aligned}
$$



$$i_o = N_0^{sp} = 3$$

Conclusions

1. We demonstrate the efficiency of the proposed approach and program packages POTHMF [17], ODPEVP[18], KANTBP [19], KANTBP 2.0[20] in calculations of:
   i) photoionization and laser-induced recombination of a (anti)hydrogen atom in the magnetic field
   ii) the effects of resonance transmission and total reflection of oppositely and similarly charged particles in the magnetic field or transversal oscillator potential.
2. Further applications of the method may be associated with calculations of laser-induced recombination of antihydrogen in magnetic traps [21], channeling of light nuclei in thin doped films [22] and potential scattering with confinement potentials [23], photo-absorbtion in quantum well [24] and three-body problems [25].

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[17] O. Chuluunbaatar *et al.*, Comput. Phys. Commun. **178**, 301 (2008)
[18] O. Chuluunbaatar *et al.*, Comput. Phys. Commun., **180**, 1358 (2009).
[19] O. Chuluunbaatar *et al.*, Comput. Phys. Commun. **177**, 649 (2007)
[20] O. Chuluunbaatar, et al. Comput. Phys. Commun. **179**, 685 (2008)
[21] V.V. Serov *et al.*, Opt. & Spectr. **102**, 557 (2007).
[22] Yu.N. Demkov and J.D. Meyer, Eur. Phys. J. B **42**, 361 (2004).
[23] J.I. Kim, et al. Phys. Rev. Lett. **97**, 193203 (2006)
[24] S.I.Vinitsky et al, LNCS **5743**, 334 (2009)
[25] O. Chuluunbaatar et al, J. Phys. **B 39**, 243 (2006)