ELEMENTARY PARTICLES AND FIELDS Theory

Channeling Problem for Charged Particles Produced by Confining Environment*

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Abstract—Channeling problem produced by confining environment that leads to resonance scattering of charged particles via quasistationary states imbedded in the continuum is examined. Nonmonotonic dependence of physical parameters on collision energy and/or confining environment due to resonance transmission and total reflection effects is confirmed that can increase the rate of recombination processes. The reduction of the model for two identical charged ions to a boundary problem is considered together with the asymptotic behavior of the solution in the vicinity of pair-collision point and the results of R -matrix calculations. Tentative estimations of the enhancement factor and the total reflection effect are discussed.

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1. INTRODUCTION

The interaction of channelled particles is considered as one of the possible ways to solve the problem of synthesis of light elements and study the interactions of nuclei at low energies [1–3]. It is supposed [3], that the effect of superfocusing beam channelling can essentially change the behavior of a nuclear reaction cross section as a function of the energy of colliding particles and the parameters of the crystal lattice. To estimate the cross section it is necessary to calculate the wave function of the continuous spectrum describing the interaction of channelled particles in a vicinity of the point of their pair impact, rather than the reflection and transmission coefficients within the framework of the model [4]. One of the known approaches to solve such type of problems has been proposed in [5, 6]. It was also applied to calculate the quasistationary states, providing the full reflection and resonant transmission of electrons and protons in a homogeneous magnetic field at resonant energies [7]. Here this approach is applied to the scattering of similarly charged particles channelled in a crystal in the framework of the model of [4]. We calculate the wave function of the continuous spectrum and estimate the dependence of the reaction enhancement coefficient on the energy by calculating a ratio of the probability density in the vicinity of the pair-collision

point in the presence of an additional confining potential and without it.

The paper is organized as follows. In Section 2 the axis channelling model of two identical charged ions is briefly described. In Section 3 the nonrelativistic problem of an ion in the Coulomb field and the uniform magnetic field is recalled. In Section 4 the details of the R-matrix-calculation scheme of the continuous spectrum problem on a finite interval with the thirdtype boundary conditions are described together with the brief analysis of an example of quasistationary states. In Section 5 the asymptotic expansions of the continuous spectrum solutions in open channels at small values of the radial variable (i.e., in the vicinity of the pair-collision point) are presented. In Section 6 preliminary estimations of the enhancement factor are discussed. In Conclusion the prospects of further application of the proposed approach and the expected results are discussed.

2. THE CHANNELLING MODEL OF TWO IDENTICAL CHARGED IONS

The nonrelativistic model of two positive ions labelled by $i = 1, 2$ with the effective masses m_i and charges q_i under the axis channelling condition with the energy E_t in the laboratory frame is described by the 6D equation

$$
(H_t - E_t)\Psi_t(\mathbf{r}_1, \mathbf{r}_2) = 0,
$$
 (1)

$$
H_t = -\frac{1}{2m_1} \Delta_{\mathbf{r}_1}^{(3)} - \frac{1}{2m_2} \Delta_{\mathbf{r}_2}^{(3)} + U_1(\mathbf{r}_1) \qquad (2)
$$

$$
+ U_2(\mathbf{r}_2) + U_{12}(\mathbf{r}_1 - \mathbf{r}_2),
$$

[∗]The text was submitted by the authors in English.

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where \mathbf{r}_i are the position vectors of ions in R^3 , $\Delta_{\mathbf{r}_i}^{(3)}$ are the Laplace operators in R^3 , $U_i(\mathbf{r}_i)$ is the energy of interaction between the particles and the crystal and $U_{12}({\bf r}_1 - {\bf r}_2) = q_1 q_2 / |{\bf r}_1 - {\bf r}_2|$ is their mutual Coulomb interaction energy in atomic units.

The potentials of interaction between the particles and the crystals are approximated by the $\sum_{s} U_i(|\mathbf{r}_i - R_s|)$, where \mathbf{R}_s are position of crystal known continuous potentials [8] of the form $U_i(\mathbf{r}_i) \equiv$ atomic chains formed a channel, and their expansions in powers of the distance from channelling axis coincided with the axis Z of a laboratory frame. Their leading approximation yield 2D harmonic oscillators $U_i(\mathbf{r}_i) = m_i \omega_i^2 \rho_i^2 / 2$ with frequencies $\omega_1 \neq \omega_2$ with respect to the transverse variables ρ_i : $\mathbf{r}_i = (z_i, \rho_i, \tilde{\varphi}_i) \in$ R^3 , where $\omega_i^2 = 2\alpha_i q_i/m_i$, and $\alpha_i \approx \alpha$ are constants of particle–crystal interaction.

The motion of a system of two particles with total mass $M = m_1 + m_2$ and reduced mass $\mu =$ $m_1m_2/(m_1 + m_2)$ in Jacobi variables $\mathbf{R} = (m_1\mathbf{r}_1 + m_2)$ $(m_2\mathbf{r}_2)/(m_1 + m_2)$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is averaged in the plane-wave approximation with the momentum K_Z along the axis Z, which yields the $5D$ equation [4]

$$
(H - E)\Psi(\mathbf{R}_{\perp}, \mathbf{r}) = 0,\t\t(3)
$$

$$
\Psi(\mathbf{R}_{\perp}, \mathbf{r}) = \Psi_t(\mathbf{R}, \mathbf{r}) \exp(iK_Z Z),
$$

\n
$$
H = -\frac{1}{2M} \Delta_{\mathbf{R}_{\perp}}^{(2)} - \frac{1}{2\mu} \Delta_{\mathbf{r}}^{(3)}
$$

\n
$$
+ U(\mathbf{R}_{\perp}, \mathbf{r}_{\perp}) + U_{12}(\mathbf{r}),
$$
\n(4)

where $E = E_t - K_Z^2/2M$ is the energy, $\mathbf{R}_{\perp} =$ (X_{\perp}, Y_{\perp}) and $\mathbf{r}_{\perp} = (x_{\perp}, y_{\perp})$ are transverse components of radius-vectors of the center-of-mass and relative motion of ions, $\Delta^{(2)}_{\mathbf{R}_\perp}$ is the Laplace operator in the transversal space R^2 and $U(\mathbf{R}_{\perp}, \mathbf{r}_{\perp})$ is the effective potential of the system of two particles

$$
U(\mathbf{R}_{\perp}, \mathbf{r}_{\perp}) = \frac{m_1 \omega_1^2 + m_2 \omega_2^2}{2} \mathbf{R}_{\perp}^2 + \mu (\omega_1^2 - \omega_2^2) \mathbf{r}_{\perp} \mathbf{R}_{\perp} + \frac{\mu^2}{2} \left(\frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2} \right) \mathbf{r}_{\perp}^2.
$$

Under the condition $\omega_1^2 - \omega_2^2 = 0$, namely, $q_1 m_2$ – $q_2m_1 = 0$, the variables can be separated: $\Psi(\mathbf{R}_{\perp}, \mathbf{r}) = \Psi_{\perp}(\mathbf{R}_{\perp}) \Psi_{\text{int}}(\mathbf{r})$, so that the 5D problem is split into the $2D$ equation describing the center-ofmass motion with the energy $E_{a_{\perp}}$,

$$
\left(-\frac{1}{2\mu}\Delta_{\mathbf{R}_{\perp}}^{(2)} + \frac{m_1\omega_1^2 + m_2\omega_2^2}{2}\mathbf{R}_{\perp}^2\right) \qquad (5)
$$

$$
\times \Psi_{\perp}(\mathbf{R}_{\perp}) = E_{a_{\perp}}\Psi_{\perp}(\mathbf{R}_{\perp}),
$$

and the 3D equation that describes the relative motion,

$$
\left(-\frac{1}{2\mu}\Delta_{\mathbf{r}}^{(3)} + \frac{\mu^2}{2}\left(\frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2}\right)\mathbf{r}_\perp^2 + U_{12}(\mathbf{r})\right) (6)
$$

$$
\times \Psi_{\text{int}}(\mathbf{r}) = E_{\text{int}}\Psi_{\text{int}}(\mathbf{r}),
$$

where $E_{\text{int}} = E - E_{a}$ is the energy in the center-ofmass frame. Note, that in accordance with the Kohn theorem [9], the generalization of the above model onto a similar n -particle system is also possible. Such setting of the problem can be also used if the frequencies ω_i are considered as phenomenological parameters induced by a certain environment like artificial waveguides and if $U_{12}({\bf r})$ is the screening Coulomb potential for the scattering model of neutral atoms with confining potentials [10, 11].

We can rewrite Eq. (6) in the explicit form with respect to Coulomb interaction

$$
\left(-\Delta_{\mathbf{r}}^{(3)} + \frac{2Z}{r} + \frac{\gamma^2}{4}\mathbf{r}_{\perp}^2\right)\Psi_{\text{int}}\left(\mathbf{r}\right) = \epsilon\Psi_{\text{int}}\left(\mathbf{r}\right),\quad(7)
$$

where $Z = \mu q_1 q_2$ is the reduced charge, $\gamma^2 = 8\mu \alpha \tilde{q}$, $\tilde{q} = (q_1 m_2^2 + q_2 m_1^2) / (m_1 + m_2)^2$, is the interaction constant, and $\epsilon = 2\mu E_{\text{int}}$ is the reduced energy. Further, we use the scale transformation $r \to \sqrt{\gamma}r$, $Z \to$ $Z/\sqrt{\gamma}$, $E_{\text{int}} \rightarrow E_{\text{int}}/\gamma$:

$$
\left(-\Delta_{\mathbf{r}}^{(3)} + \frac{2\hat{Z}}{r} + \frac{1}{4}\mathbf{r}_{\perp}^{2}\right)\Psi_{\text{int}}\left(\mathbf{r}\right) = \hat{\epsilon}\Psi_{\text{int}}\left(\mathbf{r}\right),\quad(8)
$$

where $\hat{Z} = Z/\sqrt{\gamma}$ and $\hat{\epsilon} = \epsilon/\gamma$.

3. AN ION IN COULOMB AND UNIFORM MAGNETIC FIELDS

Equation (8) is similar to the Schrödinger equation describing the motion of a particle with mass m_1 and charge q_1 in Coulomb field of the particle with the infinite mass m_2 and charge q_2 , and in an axially symmetric magnetic field $\mathbf{B} = (0, 0, B =$ γB_0), $B_0 = 2.35 \times 10^5$ T [6]. In spherical coordinates $(r, \eta = \cos \theta, \varphi)$ the later can be written in atomic units for the wave function $\Psi(r, \eta, \phi) =$ $\Psi_m(r,\eta)\exp{(im\varphi)}/(2\pi)^{1/2}$ as the 2D equation for the fixed magnetic quantum number m in the region $\Omega = \{0 < r < \infty, -1 < \eta < 1\}$:

$$
\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hat{A}^{(0)}(\eta;r)}{r^2} + \frac{2Z}{r} - \epsilon\right) \quad (9)
$$

$$
\times \Psi_m(r,\eta) = 0.
$$

The operator $\hat{A}^{(0)}(\eta;r) = A^{(0)}(\eta;r) - (\text{sign}q_1)\gamma mr^2$, where $(signq_1) = -(+)$, for example, for electron (positron), and $A^{(0)}(r, \eta)$ is given by

$$
A^{(0)}(\eta;r) = -\frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} + \frac{m^2}{1 - \eta^2}
$$
 (10)

$$
+ \left(\frac{\gamma r^2}{\rho}\right)^2 (1 - \eta^2).
$$

Here,
$$
Z = m_1q_1q_2
$$
 is the reduced charge and $\epsilon = 2m_1E$ is the reduced energy. Thus, Eq. (8) with
proper definitions for Z, ϵ , and γ formally corresponds
to Eq. (9) if we put $\hat{A}^{(0)}(\eta; r) = A^{(0)}(\eta; r)$, i.e., if we
omit γmr^2 . The wave function satisfies the following
boundary conditions in each $m\sigma$ subspace (σ is
z parity $\Psi_m(r, -\eta) = \sigma \Psi_m(r, \eta)$) of the full Hilbert
space:

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

$$
\Psi_m(r, \pm 1) = 0, \quad \text{if} \quad m \neq 0,
$$

$$
\frac{\partial \Psi_m(r, \eta)}{\partial \eta}\Big|_{\eta = 0} = 0, \quad \text{if} \quad \sigma = +1,
$$

$$
\Psi_m(r, 0) = 0, \quad \text{if} \quad \sigma = -1.
$$

We consider the Kantorovich expansion of the partial solution $\Psi_i^{m\sigma}(r,\eta)$ using the set of onedimensional parametric basis functions $\phi_i(\eta; r) \equiv$ $\phi_j^{m\sigma}(\eta;r)$:

$$
\Psi_i^{m\sigma}(r,\eta) = \sum_{j=1}^{j_{\text{max}}} \phi_j^{m\sigma}(\eta;r)\chi_j^{(i)}(r). \qquad (11)
$$

The matrix-valued functions $\boldsymbol{\chi}(r) \equiv \{\boldsymbol{\chi}^{(i)}(r)\}_{i=1}^{j_{\text{max}}}$ composed from vector functions $(\boldsymbol{\chi}^{(i)})^T =$ $(\chi_1^{(i)}(r),\ldots,\chi_{j_{\text{max}}}^{(i)}(r))$ are unknown. The vector angular functions $(\phi(\eta; r))^T = (\phi_1(\eta; r), \dots,$ $\phi_{j_{\text{max}}}(\eta; r)$) form an orthonormal basis for each value of the radius r which is treated here as a parameter. The *angular oblate spheroidal functions* $\phi_i(\eta; r) \in$ $\mathcal{F}_r \sim L_2([-1,1])$ and the corresponding *potential curves* $E_i(r)$ (in Ry = 1/2 a.u.) are determined as the solutions of the following one-dimensional parametric eigenvalue problem:

$$
\hat{A}^{(0)}(\eta;r)\phi_j(\eta;r) = E_j(r)\phi_j(\eta;r),
$$

$$
\int_{-1}^{1} \phi_i(\eta;r)\phi_j(\eta;r)d\eta = \delta_{ij}.
$$

By substituting expansion (11) into the above boundary-value problem (9) – (11) , we arrive at an eigenvalue problem for a system of j_{max} ordinary second-order differential equations that determines the coefficients (radial wave functions) at the fixed energy ϵ $(\chi^{(i)}(r))^T = (\chi_1^{(i)}(r), \chi_2^{(i)}(r), \ldots, \chi_{j_{\text{max}}}^{(i)}(r))$ in the expansion (11):

$$
\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\mathbf{U}(r)}{r^2} + \mathbf{Q}(r)\frac{d}{dr}\right] \qquad (12)
$$

$$
+\frac{1}{r^2}\frac{dr^2\mathbf{Q}(r)}{dr}\right)\chi^{(i)}(r) = \epsilon_i\mathbf{I}\chi^{(i)}(r),
$$

Here, **I**, $\mathbf{U}(r)$, and $\mathbf{Q}(r)$ are finite $j_{\text{max}} \times j_{\text{max}}$ matrices whose elements are given by the relations

$$
U_{ij}(r) = \frac{E_i(r) + E_j(r) + 4Zr}{2} \delta_{ij} + r^2 H_{ij}(r), \quad (13)
$$

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

$$
Q_{ij}(r) = -\int_{-1}^{1} \phi_i(\eta; r) \frac{\partial \phi_j(\eta; r)}{\partial r} d\eta.
$$

The continuum wave function $\Psi(r, \theta)$ satisfies the boundary condition of the third type:

$$
\frac{d\Phi(r)}{dr} = \mathbf{R}(r)\Phi(r),\tag{14}
$$

$$
\mathbf{R}(r) \equiv \frac{d\Phi(r)}{dr} \Phi^{-1}(r),
$$

at fixed values of the energy ϵ and the radial variable $r = r_{\text{min}} > 0$ and $r = r_{\text{max}} \gg 1$, where $\Phi(r) =$ $\{\boldsymbol{\chi}^{(i)}(r)\}_{i=1}^{N_o}$ is an unknown $j_{\text{max}} \times N_o$ matrix and $N_o = \max_{2E \geq \epsilon^\text{th}_j} j < j_\text{max}$ is the number of open channels with Landau threshold $\epsilon_{mj}^{th}(\gamma) =$ $\lim_{r \to \infty} r^{-2} E_j(r) = \gamma(2j - 1 + |m| - (\text{sign}q_1)m).$

4. THE CONTINUOUS SPECTRUM PROBLEM

The continuous spectrum solutions $\chi^{(i)}(r)$ obey the third-type boundary condition at fixed energy $\epsilon =$ $2E$ above the first Landau threshold $\epsilon_{mj}^{\text{th}}(\gamma)$ with $j=1$ 1:

$$
\frac{d\mathbf{\chi}(r)}{dr} = \mathbf{R}\mathbf{\chi}(r), \quad r = r_{\text{max}}, \tag{15}
$$

where **R** is a nonsymmetric $j_{\text{max}} \times j_{\text{max}}$ matrix which was calculated using the program KANTBP [5]. The orthogonality/normalization condition for $\hat{\Psi}_i^{Em\sigma}(\Omega)$ at $m = m'$ is

$$
\langle \hat{\Psi}_i^{Em\sigma}(\Omega) | \hat{\Psi}_{i'}^{E'm'\sigma'}(\Omega) \rangle
$$
\n
$$
= \delta(E - E') \delta_{mm'} \delta_{\sigma\sigma'} \delta_{ii'}.
$$
\n(16)

We express the corresponding eigenfunction $\Psi_i^{Em\sigma}(r,\eta)$ of the continuous spectrum with the energy $\epsilon = 2E$ in open channels $i = \overline{1, N_o}$ in the form of Eq. (11), 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" and "outgoing" wave function. The eigenchannel wave function $\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r)$ is expressed as

$$
\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = (2/\pi)^{1/2} \boldsymbol{\chi}^{(p)}(r) \mathbf{Ccos} \boldsymbol{\delta}.
$$
 (17)

The function $\chi^{(p)}(r)$ is a numerical solution of Eq. (12) that satisfies the "standing-wave" boundary conditions (15) and has the standard asymptotic form [5]

$$
\chi^{(p)}(r) = \chi^s(r) + \chi^c(r)\mathbf{K},\tag{18}
$$

$KC = Ctan_δ$.

Here, $\mathbf{K} \equiv \mathbf{K}_{\sigma}$ is the symmetric numerical *shortrange reaction matrix* with the diagonal eigenvalue matrix $\tan\delta \equiv \{\delta_{ij} \tan \delta_j\}_{ij=1}^{N_o}$ depending on the *short-range even/odd phase shift vector* δ \equiv $\boldsymbol{\delta}_{\sigma} = \{\delta^{\sigma}_j\}_{j=1}^{N_o},$ and the orthogonal matrix $\mathbf{C}^T\mathbf{C} = \mathbf{I}_{oo}$ of the corresponding eigenvectors C , where I_{oo} is the unit $N_o \times N_o$ matrix. Note, that in Eq. (17), $\cos\delta$ is a diagonal matrix defined in the same terms. The regular $\chi^s(r) = 2\Im(\chi(r))$ and irregular $\chi^c(r) =$ $2\Re(\chi(r))$ asymptotic functions are expressed via the fundamental asymptotic solution $\chi(r)$ with the leading terms at $r \to \infty$:

$$
\chi_{ji_o}(r) = \frac{\exp(ip_{i_o}r + i\zeta \ln(2p_{i_o}r) + i\delta_{i_o}^c)}{2r\sqrt{p_{i_o}}}\delta_{ji_o},
$$
 (19)

where p_{i_o} is the relative momentum in the channel $i_o, \zeta \equiv \zeta_{i_o} = Z/p_{i_o}$ is a Sommerfeld-type parameter, $\delta_{i_o}^c = \arg \Gamma(1 - i \zeta)$ is the known Coulomb phase shift [12]. Using the **R**-matrix calculus [5], we obtain the equation expressing the reaction matrix **K** via the matrix **R** at $r = r_{\text{max}}$

$$
\mathbf{K} = -\mathbf{X}^{-1}(r_{\text{max}})\mathbf{Y}(r_{\text{max}}),\tag{20}
$$

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

$$
\mathbf{X}(r) = \left(\frac{d\mathbf{\chi}^c(r)}{dr} - \mathbf{R}\mathbf{\chi}^c(r)\right)_{oo},\qquad(21)
$$

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$$
\mathbf{Y}(r) = \left(\frac{d\mathbf{\chi}^s(r)}{dr} - \mathbf{R}\mathbf{\chi}^s(r)\right)_{oo}.
$$

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

$$
\chi^{-}(r) = i\chi^{(p)}(r)(\mathbf{I}_{oo} + i\mathbf{K})^{-1},
$$
\n
$$
\chi^{+}(r) = -i\chi^{(p)}(r)(\mathbf{I}_{oo} - i\mathbf{K})^{-1},
$$
\n(22)

and have the asymptotic forms

$$
\hat{\boldsymbol{\chi}}^{(m\sigma)}(E,r) = (2/\pi)^{1/2}(\boldsymbol{\chi}(r) - \boldsymbol{\chi}^*(r)\mathbf{S}^\dagger), \quad (23)
$$

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

Here, $S \equiv S_{\sigma}$ is the symmetric unitary short-range scattering matrix, $S^{\dagger}S = SS^{\dagger} = I_{oo}$, which can be expressed via the calculated **K** matrix as

$$
\mathbf{S} = (\mathbf{I}_{oo} + \imath \mathbf{K})(\mathbf{I}_{oo} - \imath \mathbf{K})^{-1}.
$$
 (24)

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

$$
\Psi_{Em\hat{v}}^{(-)}(r,\eta) = 2^{-1/2} (\Psi^{Em,+1}(r,\eta)) \qquad (25)
$$

$$
\pm \Psi^{Em,-1}(r,\eta)) \exp(-i\delta^c).
$$

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

$$
|E\hat{v}mN_{\rho}\rangle = \frac{\exp(im\varphi)}{2\pi} \sum_{n'=1}^{j_{\text{max}}} \Phi_{n'}(\rho)\chi_{Em\hat{v}n'n}^{(-)}(z).
$$
\n(26)

Here, $N_\rho = n - 1$, \hat{v} denotes the initial direction of the particle motion along the *z* axis, $\Phi_{n'}(\rho)$ is the eigenfunction of a two-dimensional oscillator that corresponds to $\Phi_j^{m\hat{v}}(r,\eta)=(\Phi_j^{m,+1}(r,\eta) \pm \pi)$ $\Phi_j^{m,-1}(r,\eta)/\sqrt{2}$ at $r \to \infty$. At $z \to \pm \infty$ the function $\chi^{(-)}_{Em\hat{v}n'n}(z)$ has the following asymptotic form:

$$
\chi_{E\hat{v}}^{(-)}(z) \tag{27}
$$

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

Fig. 1. Profiles of total wave functions (25) of the continuous spectrum in the z , x plane with $Z = -1$, $m = 0$, and $\gamma = 0.1$. The states with the energy $E = 0.05885$ a.u. (left) correspond to the resonance transmission, while those with the energy $E = 0.11692$ a.u. (right) correspond to the total reflection.

Fig. 2. Transmission $|\hat{\mathbf{T}}|^2$ (dash-dotted curve) and reflection $|\hat{\mathbf{R}}|^2$ (solid curve) coefficients (29), even δ_e (dashed curve) and odd δ _o (dotted curve) short-range phase shifts (18) versus $(\tilde{E}_2 - 2E)^{-1/2}$ for $Z = -1$, $m = 0$, $\gamma=0.1$. Here, the position of the first threshold $2E=$ $E_1 = \gamma = 0.1$ corresponds to $(E_2 - 2E)^{-1/2} \approx 2.23$.

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

$$
X_{n'n}^{(\pm)}(z)
$$
\n
$$
= \exp\left(\pm i p_{n'} z \pm i \zeta_{n'} \frac{z}{|z|} \ln(2p_{n'}|z|)\right) \frac{\delta_{n'n}}{\sqrt{p_{n'}}},
$$
\n(28)

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

$$
\hat{\mathbf{T}} = 2^{-1}(-\check{\mathbf{S}}_{+1} + \check{\mathbf{S}}_{-1}),
$$

\n
$$
\hat{\mathbf{R}} = 2^{-1}(-\check{\mathbf{S}}_{+1} - \check{\mathbf{S}}_{-1}).
$$
\n(29)

Note, that the scattering wave function $\mathbf{\Psi}_{Em\hat{v}}^{(+)}(r,\eta)$

is defined by the formula $\Psi_{Em\rightleftarrows}^{(+)}(r,\eta) =$ $\left(\Psi_{Em\rightarrow}^{(-)}(r,\eta)\right)^*$ having the asymptotic form "incident wave + outgoing wave". For recombination the above wave function should be renormalized to one particle per unit length in the incident wave by factor $\sqrt{p_{i_o}}$ in each partial wave functions.

The continuous spectrum solution $\chi^{(p)}(r)$ having the asymptotic form of a "standing" wave and the reaction matrix \bf{K} from (18) were calculated using the program KANTBP [5]. As an example, the profiles of the wave function (25) using Eq. (22) for $Z = -1$, $m = 0, \gamma = 0.1, j_{\text{max}} = 10$, and $N_o = 1$ are shown in Fig. 1 at two fixed values of energy E , corresponding to resonance transmission $|\hat{\mathbf{T}}|^2 = \sin^2(\delta_e - \delta_o) =$ 1 and total reflection $|\hat{\mathbf{R}}|^2 = \cos^2(\delta_e - \delta_o) = 1$. One can see that the probability density of the wave function around a point of pair impact in the case of reflection is greater than in the case of transmission. Here, $\delta_e \equiv \delta_1^{+1}$ and $\delta_o \equiv \delta_1^{-1}$ are the *short-range phase shifts* for even and odd states from Eq. (18), respectively. The transmission and reflection coefficients are explicitly shown in Fig. 2 together with the even δ_e and odd δ _o phase shifts versus the inverse square root of energy $(\tilde{E}_2 - 2E)^{-1/2}$ relative to the second threshold shift $\tilde{E}_2 = \epsilon^{\text{th}}_{m2}(\gamma)$. The countable series of quasistationary states imbedded in the continuum corresponds to the *short-range phase shifts* $\delta_{o(e)} =$ $n_{o(e)}\pi + \pi/2$ at $(\tilde{E}_2 - 2E)^{-1/2} = n_{o(e)} + \Delta_{n_{o(e)}}$ (the first $n_{o(e)} = 1-6$ of them are presented in Fig. 2). 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.

One can fit the obtained numerical results for a finite number of quasistationary states using the appropriate analytic parametrization [13] to extrapolate them from above the i_o th threshold to below the $(i_o +$

1)th threshold and, as a result, to estimate the countable set of quasistationary states between the thresholds. Such a procedure provides a considerable reduction of the computer facilities required and allows one to select the appropriate energy subregions for further numerical calculations aimed at the determination of the resonance frequencies of photoionization and the induced or spontaneous recombination [14].

5. ASYMPTOTIC SOLUTION AT SMALL VALUES OF THE RADIAL VARIABLE

Let us suppose that the set of linearly independent solutions $\tilde{\mathbf{\Phi}}_{\rm reg}(r)=\{\tilde{\boldsymbol{\chi}}_{\rm reg}^{(i)}(r)\}_{i=1}^{j_{\rm max}},$ where $\tilde{\boldsymbol{\chi}}_{\rm reg}^{(i)}(r)=$ $(\tilde{\chi}_{1i}^{\text{reg}}(r), \ldots, \tilde{\chi}_{j_{\text{max}}}^{\text{reg}})$ $\int_{j_{\rm max} i}^{\rm reg} (r))^T$, is constructed. Using a linear combination of these regular solutions, $\tilde{\boldsymbol{\chi}}_{\mathrm{reg}}^{(i)}(r),$ we can find the required matrix solution $\Phi(r)$ at $r = r_{\min} > 0$:

$$
\Phi(r) = \tilde{\Phi}_{reg}(r) \mathbf{C},
$$
\n
$$
\chi_{ji_o}(r) = \sum_{i=1}^{j_{\text{max}}} \tilde{\chi}_{ji}^{reg}(r) C_{ii_o},
$$
\n(30)

where **C** is an unknown nonzero constant $j_{\text{max}} \times N_o$ matrix. Using the identity $CC^{-1} = I$, the **R**(*r*) matrix at $r = r_{\text{min}}$ can be easily found via the known set of linear independent regular solutions $\mathbf{\Phi}_{reg}(r)$:

$$
\mathbf{R}(r) \equiv \frac{d\tilde{\mathbf{\Phi}}_{\text{reg}}(r)}{dr} \tilde{\mathbf{\Phi}}_{\text{reg}}^{-1}(r),
$$
(31)

$$
R_{ji}(r) = \sum_{i'=1}^{j_{\text{max}}} \frac{d\tilde{\chi}_{ji'}^{\text{reg}}(r)}{dr} (\tilde{\chi}^{\text{reg}}(r))_{i'i}^{-1}.
$$

After the numerical calculation of the solution $\Phi(r)$ = $\pmb{\Phi}^h(r)$ in the nodes of the finite-element grid Ω^h_r within the interval $[r_{\min},r_{\max}]$, taking Eqs. (14)–(31) into account, the matrix **C** can be evaluated using the formula at $j = 1, \ldots, j_{\text{max}}$ and $i_o = 1, \ldots, N_o$:

$$
\mathbf{C} = \tilde{\mathbf{\Phi}}_{\text{reg}}^{-1}(r_{\text{min}}) \mathbf{\Phi}(r_{\text{min}}),
$$
(32)

$$
C_{ji_o} = \sum_{i=1}^{j_{\text{max}}} (\tilde{\chi}_{\text{reg}}^{-1})_{ji}(r_{\text{min}}) \chi_{ii_o}(r_{\text{min}}).
$$

The matrix **C** is applied to the analysis of the matrix solution $\Phi(r)$ in the vicinity of $r = 0$. For example, a $\tilde{\mathbf{c}}$ constant matrix **C** keeps the ratio $\tilde{\mathbf{\Phi}}_{\text{reg}}^{-1}(0)\mathbf{\Phi}(0)$ finite and nonzero even if $\Phi(0) \equiv 0$ or is very close to zero. To extract the required matrix **C** in this case, one can use the known asymptotic form of the regular solutions at r_{min} . The value r_{min} is defined in the asymptotic domain of the $\Phi_{reg}(r)$. As a result, we obtain the total wave function in each open channel $r \leq r_{\min}$:

$$
\psi_{i_o}(\eta, r) = \sum_{j=1}^{j_{\text{max}}} \sum_{i=1}^{j_{\text{max}}} \phi_j^{m\sigma}(\eta; r) \chi_{ji}^{\text{reg}}(r) C_{ii_o}.
$$

At small r we find the asymptotic solutions of the problem (12) – (14) as an expansion in powers of r and Legendre polynomials $P_{l+s}^{|m|}(\eta;r)$ with $l = 2(j-1)$ + $|m| + (1 - \sigma)/2$:

$$
E_j(r) = E_j^{(0)} + E_j^{(2)}r^2 + \sum_{k=1}^{k_{\text{max}}/4} r^{4k} E_j^{(4k)},
$$
(33)

$$
\phi_j(\eta; r) = \phi_j^{(0)}(\eta; r) + \sum_{k=1}^{k_{\text{max}}} r^{4k} \phi_j^{(k)}(\eta; r),
$$

$$
\phi_j^{(k)}(\eta; r) = \sum_{s=-2k}^{2k} P_{l+s}^{|m|}(\eta; r) b_{sj}^{(k)}.
$$

The substitution of Eq. (33) into Eq. (12) leads to the recursive relations for the unknowns $b_{sj}^{(k)}$ for $s\neq 0$ and $E_j^{(4k)}$:

$$
(s^{2} + (2l+1)s)b_{sj}^{(k)}
$$
 (34)
=
$$
-\sum_{s'= -2}^{2} v_{s;s'}^{(1)} b_{s-s'j}^{(k-1)} + \sum_{p=0}^{k-1} E_{j}^{(4k-4p)} b_{sj}^{(p)},
$$

where the matrix elements are defined by the relations with the notation $t = l + s$:

$$
v_{-2;t}^{(k)} = \delta_{1k} \frac{1}{4(2|m| + 2t - 1)}
$$

\n
$$
\times \sqrt{\frac{(t - 1)t(2|m| + t - 1)(2|m| + t)}{(2|m| + 2t - 3)(2|m| + 2t + 1)}},
$$

\n
$$
v_{0;t}^{(k)} = \delta_{1k} \frac{2(t^2 + t + 2|m|t + 2|m|^2 + |m| - 1)}{(2|m| + 2t - 1)(2|m| + 2t + 3)},
$$

\n
$$
v_{2;t}^{(k)} = \delta_{1k} \frac{1}{4(2|m| + 2t + 3)}
$$

\n
$$
\times \sqrt{\frac{(t + 1)(t + 2)(2|m| + t + 1)(2|m| + t + 2)}{(2|m| + 2t + 1)(2|m| + 2t + 5)}}
$$

These equations were solved at given initial data $E_j^{(0)}=l(l+1)$ and $b_{sj}^{(0)}=\delta_{s0}.$ The coefficients $b_{0j}^{(k)}$ at $s = 0$ were calculated from the normalization condition (12):

$$
b_{0j}^{(k)} = -\sum_{p=0}^{k} \sum_{s'=-2k}^{2k} \sum_{s=-2k}^{2k} b_{sj}^{(k-p)} \langle s | s' \rangle b_{s'j}^{(p)}.
$$
 (35)

Thus, the asymptotic expansions of the matrix elements take the form

$$
H_{jj'}(r) = \sum_{k=1}^{k_{\text{max}}/4} r^{4k-2} \bar{H}_{jj'}^{(4k-2)},
$$

\n
$$
Q_{jj'}(r) = \sum_{k=1}^{k_{\text{max}}/4} r^{4k-1} \bar{Q}_{jj'}^{(4k-1)},
$$

\n
$$
\bar{H}_{jj'}^{(4k-2)} = \sum_{p=0}^{k} \sum_{s'=-2k}^{2k} \sum_{s=-2k}^{2k} b_{sj}^{(k-p)}
$$

\n
$$
\times 16p(k-p)\delta_{s+js'+j'}b_{s'j'}^{(p)},
$$

$$
\bar{Q}_{jj'}^{(4k-1)} = \sum_{p=0}^{k} \sum_{s'=-2k}^{2k} \sum_{s=-2k}^{2k} b_{sj}^{(k-p)} \times 4(k-p) \delta_{s+js'+j'} b_{s'j'}^{(p)}.
$$

The calculation was performed using the algorithm implemented in MAPLE up to $k_{\text{max}} = 16$. Below we display the first few coefficients of the matrix elements with $l = 2(j - 1) + |m| + (1 - \sigma)/2$:

$$
\begin{aligned}\n\bar{E}_j^{(0)} &= l(l+1), & \bar{E}_j^{(2)} &= \gamma m, \\
\bar{E}_j^{(4)} &= \frac{\gamma^2 (l^2 + l - 1 + |m|^2)}{2(2l-1)(2l+3)},\n\end{aligned}
$$

$$
\bar{Q}_{jj-2}^{(3)} = -\frac{\gamma^2 (l+|m|)^{1/2} (l-|m|)^{1/2} (l-1-|m|)^{1/2} (l-1+|m|)^{1/2}}{2(2l-3)^{1/2} (2l+1)^{1/2} (2l-1)^2}.
$$

At small r we find the asymptotic solutions of the problem (12) – (14) in the form of an expansion in powers of r:

$$
\tilde{\chi}_{ji}(r) = \sum_{k=0}^{k_{\text{max}}} \tilde{\chi}_{ji}^{(k)} r^{\mu_i + k}, \quad \tilde{\chi}_{ji}^{(0)} = \delta_{ji}, \quad (36)
$$

where μ_0 is the unknown characteristic parameter. The substitution of Eq. (36) into Eq. (12) leads to the recursive relations for the unknowns $\tilde{\chi}^{(k)}_{ji}$ with $l' = 2(j - 1) + |m| + (1 - \sigma)/2, l = 2(i - 1) + |m| +$ $(1 - \sigma)/2$:

$$
-(l'+1+\mu_i+k)(\mu_i-l'+k)\tilde{\chi}_{ji}^{(k)}\qquad(37)
$$

$$
= 2Z\tilde{\chi}_{ji}^{(k-1)} - (m\gamma - \epsilon)\tilde{\chi}_{ji}^{(k-2)} - \sum_{s=4}^{k} \bar{E}_j^{(s)} \tilde{\chi}_{ji}^{(k-s)} - \sum_{s=4}^{k-2} \bar{H}_{jj}^{(s)} \tilde{\chi}_{ji}^{(k-s-2)}
$$

$$
-\sum_{s=3}^{k-1} \sum_{j'=\max(1,i-[s/4]),j'\neq j}^{\min(j_{\max},i+[s/4])} (2l+2k-s)\bar{Q}_{jj'}^{(s)}\tilde{\chi}_{j'i}^{(k-s-1)}
$$

$$
-\sum_{s=4}^{k-2} \sum_{j'=\max(1,i-[s/4]), j' \neq j}^{\min(j_{\max},i+[s/4])} \bar{H}_{jj'}^{(s)} \tilde{\chi}_{j'i}^{(k-s-2)}.
$$

As follows from Eq. (37) at $k = 0$, the conventional characteristic equation yields two roots for the unknown μ_i : $\mu_i = -l' - 1$ and $\mu_i = l'$. The value $\mu_i =$ −l − 1 corresponds to irregular unbound solutions and is not considered here. The value $\mu_i = l'$ corresponds to the required regular and bound solutions and is the one we have used in our calculations. In this case (37) the coefficients of the asymptotic expansion of the regular solution (36) are

$$
\tilde{\chi}_{ii}^{(0)} = 1, \quad \tilde{\chi}_{ii}^{(1)} = \frac{Z}{l+1},\tag{38}
$$

$$
\tilde{\chi}_{ii}^{(2)} = -\frac{-2Z^2 + (\epsilon - m\gamma)(l+1)}{2(l+1)(2l+3)},
$$

$$
\tilde{\chi}_{ii}^{(3)} = -\frac{Z(-2Z^2 + (\epsilon - m\gamma)(3l+4))}{6(l+1)(l+2)(2l+3)},
$$

$$
\tilde{\chi}_{i-1i}^{(4)} = \frac{\bar{Q}_{i-1i}^{(3)}(2l+5)}{6(2l+3)},
$$

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Fig. 3. (*a*) Effective potential 2U in the z, x plane; (*b*) the full enhancement coefficient (solid line) and partial enhancement coefficients in each open channel ($i = 1-5$) versus the threshold energy 2E, for the effective charge $Z = +6$ and $\gamma = 1$ (in scaled variables).

$$
\tilde{\chi}_{ii}^{(4)} = \frac{\bar{E}_i^{(4)}}{4(2l+5)} + \frac{(\epsilon - m\gamma)^2}{8(2l+3)(2l+5)} + \frac{Z^4 - Z^2(\epsilon - m\gamma)(3l+5)}{6(l+1)(l+2)(2l+3)(2l+5)},
$$

$$
\tilde{\chi}_{i+1i}^{(4)} = \frac{\bar{Q}_{i+1i}^{(3)}(2l+5)}{2(2l+7)}.
$$

χ˜

As a result, we get the required expansion of 2D-solution in the Kantorovich form:

$$
\psi_{i_o}^{\rm (as)}(\eta,r)
$$

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

$$
\phi_j^{(k-p)}(\eta) = \sum_{s=\text{max}(-l,-2k+2p)}^{2k-2p} P_{l+s}^{|m|}(\eta) b_{sj}^{(k-p)},
$$

where $l = 2(i - 1) + |m| + (1 - \sigma)/2$, $\mu_i = l$. The above asymptotic form of the Kantorovich expansion is equivalent to the Galerkin one over the basis of Legendre polynomials:

$$
\psi_{i_o}^{(\text{as})}(\eta, r)
$$
\n
$$
= \sum_{i=1}^{j_{\text{max}}} \sum_{k=0}^{k_{\text{max}}} \sum_{s=\text{max}(-l, -2k+2p)}^{2k-2p} f_s^{(k)}(r, \eta) g_{si}^{(k_{\text{max}}-k)} C_{ii_o},
$$
\n
$$
f_s^{(k)}(r, \eta) = r^{\mu_i+k} P_{l+s}^{|m|}(\eta),
$$
\n
$$
g_{si}^{(k_{\text{max}}-k)} = \sum_{p=0}^{k_{\text{max}}-k} \sum_{j=1}^{j_{\text{max}}} b_{sj}^{(k-p)} \tilde{\chi}_{ji}^{(p) \text{reg}}.
$$

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Moreover, using the substitution $r = (\rho^2 + z^2)^{1/2}$ and $\eta = z(\rho^2 + z^2)^{-1/2}$, one gets the asymptotic series for the regular solution in the Galerkin form in cylindrical coordinates (ρ, z) over the homogeneous polynomials of the degree $(\mu_i + k)$ with respect to the variables (ρ, z) :

$$
f_s^{(k)}(\rho, z) = (\rho^2 + z^2)^{(\mu_i + k)/2} P_{l+s}^{|m|} (z(\rho^2 + z^2)^{-1/2}).
$$

Note, that one can also derive the above asymptotic expansion in Galerkin form with the help of the direct calculation scheme [15]. The above asymptotic expansions can be applied to set the third-type boundary condition around the point of pair impact in different calculation schemes.

6. PRELIMINARY ESTIMATIONS OF THE ENHANCEMENT COEFFICIENT

The solution of the channelling problem (8) with the help of calculation schemes described in Sections 4 and 5 was found using the programs KANTBP 2.0 and POTHMF at various values of the scaled energy E and the effective charge Z. As a result, the values of the enhancement coefficient have been calculated by means of the formula $\left|C\left(2E\right)/C_0\left(2E\right)\right|^2=$ $\sum_{i=1}^{N_o} |C_i (2E) / C_0 (2E)|^2$, where $C_i (2E) =$ $=\chi_{1i}(r=0)$ are the numerical values of the solution at the point of pair impact from Eq. (12) and $C_0(2E) = \chi_{11}(r=0)$ is the Coulomb function with the effective charge Z at the energy $2E - 1$.

Figure 3 illustrates the estimations of the total enhancement coefficient and the enhancement coefficients in each open channel $(1–5)$ as functions of the energy $2E$, related to the zero energy of free threshold, at the effective charge $Z = 6$ for even components of

Fig. 4. Profiles of total wave functions $|\Psi_{i_0;EO}^{(-)}|$ of the continuous spectrum in the z, x plane for the first, second, and third $(a-c)$ open channels at $2E = 6.552$, $Z = +6$, $\gamma = 1$ (in scaled variables).

Fig. 5. Profiles of total wave functions $|\Psi_{i_o;E0\leftarrow}^{(-)}|$ in the *z*, *x* plane of the continuous spectrum of first, second, third, and fourth $(a-d)$ open channels at $2E = 7.70$, $Z = +6$, $\gamma = 1$ (in scaled variables).

the solution at $m = 0$. The maximum of the total enhancement coefficient is achieved at the value $2E =$ 6.9, between the third and the fourth channel at passing the minimum of the barrier $2U_0 = 6.24$, where

 $2U_0 = 2U(\rho, z) = 2Z/(\rho^2 + z^2)^{1/2} + (1/4)\rho^2$ at the saddle point with coordinates $z=0$ and $\rho=\rho_0$ under the condition $\partial U(\rho,z)/\partial \rho|_{\rho} = 0$ (see Fig. 3*b*). The reflection is practically total, indeed, at $2E = 6.552$

Fig. 6. Asymptotic behavior of the total wave functions $|\Psi_{i_0;EO}^{(-)}|$ of the continuous spectrum in the z, x plane for the first, second, and third $(a-c)$ open channels at $2E = 6.552$, $Z = +6$, $\gamma = 1$ (in scaled variables).

the matrix of reflections coefficients is

 $|\hat{\mathbf{R}}|^2 =$ $\sqrt{2}$ $\overline{\mathcal{L}}$ 0.967329 0.004785 −0.000094 0.004785 0.990368 0.000074 −0.000094 0.000074 0.999999 \setminus $\vert \cdot \vert$ first local minimum of the total enhancement coefficient appears with increasing energy above the forth threshold energy to $2E = 7.70$, where the diagonal elements of the transition coefficient matrix increases to approximately ~ 0.5 in the first and the second channels:

.

Similar to the case of attraction (see Fig. 1), the

$$
|\hat{\mathbf{R}}|^2 = \begin{pmatrix} 0.473201 & 0.235919 & 0.043577 & -4 \times 10^{-7} \\ 0.235919 & 0.555215 & -0.003336 & 1 \times 10^{-7} \\ 0.043577 & -0.003336 & 0.995355 & 4 \times 10^{-8} \\ -4 \times 10^{-7} & 1 \times 10^{-7} & 4 \times 10^{-8} & 1.00000 \end{pmatrix}
$$

Such a behavior is a consequence of the effects of superstrong focusing, corresponding to astrophysical magnetic fields. At interaction of particles in the channel the competition of two processes occur: the defocusing due to Coulomb interactions and the focusing due to the oscillator interaction [3], effectively lowering the dimension of the problem. Hence, there exists a region of energy, where the probability density at the point of pair impact has a maximum for quasistationary states of the continuous spectrum. For example, the first component of the *short-range even phase-shift vector* $\delta \equiv$ $\boldsymbol{\delta_e} = \{\delta^e_j\}_{j=1}^{N_o=3} = (-1.5707, 0.7717, 0.5343)^T$ of the even state equals $-\pi/2$ at $2E = 6.552$ (see Fig. 3). Figures 4–6 present the partial ionization wave functions $|\Psi_{i_o;E0\leftarrow}^{(-)}|$ and their asymptotic behavior versus the coordinates (x, z) in the plane $y = 0$.

To study the interaction of channelled particles at real values of an effective charge, Z, for example, for identical particles with masses and charges of a deuterium nucleus, it is necessary to set an effective charge, $Z \sim 100$, and to solve the problem with a large number of open channels, $N_o \sim U_0 \sim$ $3(Z/2)^{2/3}/2$, that requires significant computer resource.

7. CONCLUSIONS

In the present paper the optimal conditions have been determined under which it is possible to solve the problem of interaction of channelled particles. Tentative estimations of the enhancement factor were obtained without additional short-range nuclear potentials. The dependence of the enhancement factor upon the energy is nonmonotonic, which is a manifestation of two potentials, the defocucing Coulomb potential of interaction between identical charged particles and the focusing oscillator potential, responsible for the interaction of particles with the crystal, supporting the quasistationary states in the continuous spectrum and providing the practically total reflection. In the framework of the proposed approach one can obtain improved estimations of the enchancement factor taking into account the known parametrizations of the R matrix of nuclear reactions at an appropriate point $r_{\min} = r_0$ in the vicinity of the pair impact point.

The presented approach and the programs that allow one to study the threshold peculiarities of photoionization and recombination of particles with the opposite-sign charges (positrons, antiprotons) in a magneto-optical trap [16], the optical absorption in quantum wells [17], and the channelling of similarly charged particles in thin doped films [3] or neutral atoms and molecules in artificial waveguides or surfaces [10, 11].

The application of the total reflection effect to oppositely charged particles in a homogeneous magnetic field can give a new mechanism of jumps in a magneto-optical trap [16, 18] after each pair collision without any additional external confinement in the longitudinal direction under the resonance conditions (the temperature and the axial magnetic field parameter γ or the frequency and the polarization of the additional laser field [14, 19]), provided that the collision integral in the Boltzmann equation will be properly taken into account [20, 21].

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REFERENCES

- 1. Vit. M. Bystritskiı˘ et al., Phys. At. Nucl. **64**, 855 (2001).
- 2. F. Raiola et al., Eur. Phys. A **13**, 377 (2002); J. Phys. G **31**, 1141 (2005).
- 3. Yu. N. Demkov and J. D. Meyer, Eur. Phys. J. B **42**, 361 (2004).
- 4. P. M. Krassovitskiy and N. Zh. Takibaev, Bull. Russ. Acad. Sci., Phys. Ser. **70**, 815 (2006).
- 5. O. Chuluunbaatar et al., Comput. Phys. Commun. **177**, 649 (2007); **179**, 685 (2008).
- 6. O. Chuluunbaatar et al., Comput. Phys. Commun. **178**, 301 (2008); Phys. At. Nucl. **71**, 844 (2008).
- 7. O. Chuluunbaatar et al., Phys. Rev. A **77**, 034702 (2008).
- 8. A. H. Sorencen, Nucl. Instrum. Methods Phys. Res. B **119**, 1 (1996).
- 9. W. Kohn, Phys. Rev. **123**, 1242 (1961).
- 10. V. S. Melezhik, J. I. Kim, and P. Schmelcher, Phys. Rev. A **76**, 053611 (2007).
- 11. F. M. Pen'kov, Phys. Rev. A **62**, 044701 (2000).
- 12. M. Abramowits and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
- 13. A. I. Baz, Ya. B. Zeldovich, and A. M. Perelomov, *Scattering, Reactions and Decays in Nonrelativistic Quantum Mechanics* (Nauka, Moscow, 1971) [in Russian].
- 14. V. V. Serov, V. L. Derbov, and S. I. Vinitsky, Opt. Spectrosc. **102**, 557 (2007).
- 15. V. V. Pupyshev, Theor. Math. Phys. **136**, 970 (2003); **156**, 1058 (2008).
- 16. M. C. Fujiwara et al., Phys. Rev. Lett. **101**, 053401 (2008).
- 17. E. M. Kazaryan, A. A. Kostanyan, and H. A. Sarkisyan, Physica E **28**, 423 (2005).
- 18. A. Yu. Voronin and P. Froelich, J. Phys. B **38**, L301 (2005)
- 19. M. V. Ryabinina and L. A. Melnikov, Nucl. Instrum. Methods Phys. Res. B **214**, 35 (2004).
- 20. V. L. Saveliev and K. Nanbu, Phys. Rev. E **65**, 051205 (2002).
- 21. D. Benedetto, F. Castella, R. Esposito, and M. Pulvirenti, Commun. Math. Phys. **277**, 1 (2008).