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The Cross Section of Reaction of Two Charged Particles in a Channel of a Crystal

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Abstract—The problem of interaction of two channeling similarly charged particles in the center-of-mass system has been reduced to the Schrödinger equation in spherical coordinates with an additional oscillator potential. Preliminary estimations have been obtained and nonmonotonic behavior of the multiplication factor of nuclear reactions on the collision energy is established.

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INTRODUCTION

The interaction of channeling particles is considered as a possible solution to the problem of synthesis of light elements and interaction of low-energy nuclei [1, 2]. It is suggested that the effect of focusing of a channeling beam can significantly change the behavior of the nuclear reaction cross section, depending on the energy of colliding particles and lattice parameters. To estimate the cross section, it is necessary to calculate the wave function of the continuous spectrum, which describes the interaction of channeling particles at the point of their pair collision rather than only the reflectances and transmittances within the model [3, 4]. One of known approaches to solving such problems was proposed in [5, 6] and applied in [7] to calculate the quasi-stationary states, providing total reflection and resonant transmission of electrons and protons in a uniform magnetic field at resonant energies [7].

In this study, the approach of [5–7] is used to solve the problem of scattering of channeling similarly charged particles in a crystal within the model [3, 4] in order to calculate the wave function of continuous spectrum and estimate the energy dependence on the nuclear reaction multiplication factor: the ratio of the probability densities of the wave functions at the point of pair collision with an additional confinement potential and without it.

STATEMENT OF THE PROBLEM

We use the model of two similarly charged particles in the channeling mode, which are described by the Schrödinger equation

$$\left(-\frac{1}{2M}\Delta_{\mathbf{R}} - \frac{1}{2\mu}\Delta_{\mathbf{r}} + U_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) + U_1(\mathbf{r}_1) + U(\mathbf{r}_2)\right) \times \Psi(\mathbf{r}_1, \mathbf{r}_2) = E_G\Psi(\mathbf{r}_1, \mathbf{r}_2), \quad (1)$$

where $\mathbf{r}_1$, and $\mathbf{r}_2$ are the radius vectors of the particles with masses m_1 and m_2 and charges z_1 and z_2, respectively; M and μ are the total and reduced masses of the two particles and R and r are the Jacobian radius vectors. The potentials $U_1(\mathbf{r}_1)$, $U_2(\mathbf{r}_2)$, and $U_{12}(|\mathbf{r}_1 - \mathbf{r}_2|)$ determine the interaction of particles with the crystal and their Coulomb interaction in atomic units. Approximation of the interaction potential of the particles and crystal by a continuous potential, its expansion in a series in powers of distance from the channeling axis (ρ), and consideration of only the main term [8], provided that the ratios of charges and masses of the interacting particles are equal, make it possible to separate the part corresponding to the center-of-mass motion in Eq. (1) [3, 4]. Then, the wave function directly describing the interaction between the particles obeys the 3D Schrödinger equation in atomic units:

$$\left(-\frac{1}{2\mu}\Delta_{\mathbf{r}} + U_{12}(|\mathbf{r}|) + \alpha'\rho^2\right)\psi(\mathbf{r}) = E_{int}\psi(\mathbf{r}). \quad (2)$$

Here, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $\alpha' = \alpha(m_2^2 z_1 + m_1^2 z_2)/(m_1 + m_2)^2$, α is the expansion parameter of the particle–crystal interaction potential, and $U_{12}(|\mathbf{r}|) = z_1 z_2/r$ is the Coulomb potential of particle interaction.

In Eq. (2), we can perform partial separation of variables, specifically, separate the dependence on the angle φ in cylindrical (z, ρ, φ) or spherical (r, θ, φ) coordinates (the distance from the channeling axis coincides with the coordinate ρ).

Numerical analysis showed that the scattering problem for Eq. (2) can be solved in the cylindrical coordinate system in the range $\Omega = (0 \le \rho \le \rho_{\max}, 0 \le |z| \le z_{\max})$ if the solution must be calculated in the asymptotic region $\Omega_{\text{as}} = \left(\rho, z | \frac{\rho}{|z|} \ll 1\right)$; however, in the range

$\Omega\backslash\Omega_{as}$, the solution to the problem is unstable. In [4], this problem was solved using a matrix sweep with discretization of the initial equation according to the Numerov method. The transmittances and reflectances were obtained by direct sweep for the corresponding scattering problem on specified grids of energy values. However, the reverse sweep, successfully reconstructing the wave function in the larger part of Ω, fails to yield a solution in the region $\Omega_0 = |z^2 + \rho^2| < 1$, because it is necessary to take into account a large number of rapidly oscillating functions in this region. With due regard to the fact that the wave function in Ω_0 is determined by the dominant spherically symmetric Coulomb potential, one can obtain an estimate for the steps Δz and $\Delta\rho$ of the crowding grid Ω:

$$\frac{(l_{\max} + l_z)\sqrt{(\Delta z)^2 + (\Delta\rho)^2}}{2\pi} \ll \sqrt{z^2 + \rho^2}, \qquad (3)$$

where $l_{\max}$ and l_z are, respectively, the maximum angular momentum (taken into account) and its conserved projection on the z axis. The alternative method [5–7], which makes it possible to solve the problem in spherical coordinates and takes into account the cylindrical symmetry in the asymptotic region Ω_{as}, is described below.

KANTOROVICH METHOD

Equation (2) in spherical coordinates, at a fixed magnetic quantum number m and z parity, can be written as

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{A^{(0)}(r,\theta)}{r^2} + \frac{2Z}{r} - 2E\right)\Psi(r,\theta) = 0, \qquad (4)$$

where the operator $A^{(0)}(r, \theta)$, dependent on the parameter r, has the form

$$A^{(0)}(r,\theta) = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{m^2}{\sin^2\theta} + \frac{1}{4}\gamma^2 r^4\sin^2\theta. \qquad (5)$$

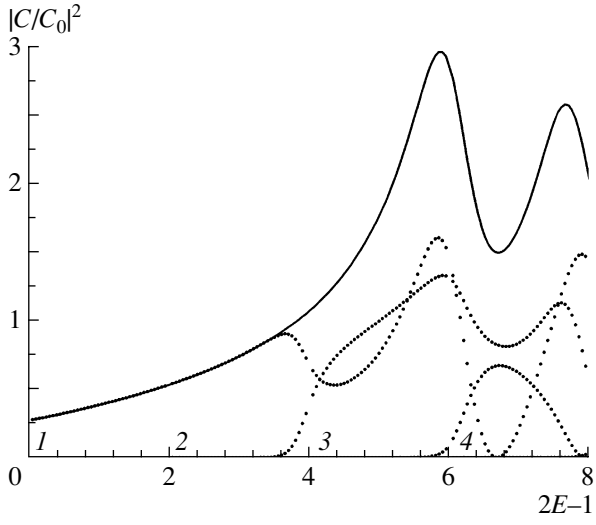
Here, the quantities $\gamma^2 = 8\mu\alpha'$, $Z = \mu z_1 z_2$ and $E = \mu E_{int}$ are determined from Eq. (2). Furthermore, we use the scale transformation $r \to \sqrt{\gamma}r$, $Z \to Z/\sqrt{\gamma}$, and $E \to E/\gamma$. The solution to Eq. (4) is sought in the form of a Kantorovich expansion of the function $\Psi(r, \theta)$ in angular oblate spheroidal functions $\Phi_i(r, \theta)$ of the operator $A^{(0)}(r, \theta)$, which are calculated using the POTHMF program on the specified grid $r \in \Omega_r$ of radial variables [6]. The expansion coefficients $\chi_{ij}(r)$ of the function $\Psi(r, \theta)$ satisfy the system of N differential equations

$$\left(-\frac{1}{r^2}\mathbf{I}\frac{d}{dr}r^2\frac{d}{dr} + \mathbf{V}(r) + \frac{2Z}{r} + \mathbf{Q}(r)\frac{d}{dr} + \frac{1}{r^2}\frac{dr^2\mathbf{Q}(r)}{dr} - 2E\mathbf{I}\right)\chi(r) = 0, \qquad (6)$$

where $\mathbf{I}$ is the unit matrix; $\mathbf{V}$ and $\mathbf{Q}$ are matrices with a dimension of $N \times N$, calculated on the specified grid $r \in \Omega_r$ using the POTHMF program [6]; and $\chi(r) = \{\chi_i(r)\}_{i=1}^{N_0}$ is a rectangular $N \times N_0$ matrix, composed of columns $\chi_i(r) = \{\chi_{ji}(r)\}_{j=1}^{N}$ (N_0 is the number of open channels with the energy $2E > E_i(\infty) = 2i–1 + |m| > 0$, $i = 1, \ldots, N_0$). The boundary-value problems of continuous spectrum for the system of N equations (6) with N_0 open channels are solved using the KANTBP program [5], which implements the finite-element method of high accuracy on the grid Ω_r, including the vicinity of $r = 0$.

PRELIMINARY ESTIMATIONS OF THE MULTIPLICATION FACTOR

Using the KANTBP and POTHMF programs at different energies E and effective charges Z, we calculated the multiplication factors $|C(2E)/C_0(2E)|^2 = \sum_{i=1}^{N_0}|C_i(2E)/C_0(2E)|^2$, where $C_i(2E) = \chi_{1i}(r = 0)$ are the numerical values of solutions to Eq. (6) at the pair impact point and $C_0(2E) = \chi_{11}(r = 0)$ is the Coulomb function with the effective charge Z at energy $2E - 1$.



Dependence of the total multiplication factor (solid line) and the multiplication factor in each open channel (*1–4*, dotted lines) on the doubled energy $2E$, counted from the first threshold $E_1 = 1$, i.e. $2E - 1$ at the effective charge $Z = 6$. The doubled barrier height is $2U_0 = 6.24$.

Figure shows the estimate of the total multiplication factor and the multiplication factors in each open channel (1–4) as functions of the energy $2E - 1$, counted from the first threshold, at the effective charge $Z = 6$ for the even solution component at $m = 0$. The maximum total multiplication factor is obtained at $2E - 1 = 5.9$, between the third and fourth channels at transmission through the barrier $2U_0 = 6.24$ and almost total reflection. Such behavior is a consequence of superstrong focusing effects, accompanying astrophysical magnetic fields. The interaction of particles in a channel involves two competing processes: defocusing (Coulomb interaction) and focusing (oscillator interaction, effectively decreasing the dimension of the problem); therefore, there is the energy range where the probability density of the wave function at the pair collision point has a maximum for quasi-stationary continuous-spectrum states. To study the interaction of channeling particles at real values of the effective charge Z, for example, for identical particles with the mass and charge of deuteron nucleus, it is necessary to set the effective charge $Z \approx 100$ and solve the problem with a large number of open channels $N_0 \approx U_0 = 3(Z/2)^{2/3}$, which requires significant computational resources.

CONCLUSIONS

We have determined the optimal conditions under which the problem of interaction of channeling particles can be solved. Preliminary estimates of the multiplication factor are obtained. The energy dependence of the multiplication factor is nonmonotonic, which is explained by the presence of two potentials: defocusing Coulomb potential (interaction between similarly charged particles) and focusing oscillator potential (interaction of particles with the crystal). These potentials maintain quasi-stationary continuous-spectrum states and provide almost total reflection.

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