Asymptotic Theory of Channeling in the Field of an Atomic Chain and an Atomic Plane 

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1. INTRODUCTION

The present theory of channeling is based on the assumption that the potential of a set of atoms forming a crystal can be replaced by the potential of a system of continuous atomic chains or planes. This approach, first proposed by Lindhard [1], can be regarded as a model approach. Its quantum-mechanical version [2, 3] predicts a number of effects associated with channeling. In particular, radiation which accompanies channeling has received considerable attention [4 - 6]. Although the model approach is widely used, it is not quite satisfactory since, strictly speaking, it is not an approximate method and, therefore, it cannot describe correctly finer effects which require extension beyond the average potential such as discreteness of the potential, boundary effects, interstitial atoms, vacancies, etc. The average potential in the aforementioned model approach is introduced artificially (as the zeroth Fourier component of the real potential) and longitudinal scattering disappears in this approach. It follows that the problem of scattering from a realistic potential bounded in space cannot be treated by this method.

It is our aim to study elastic scattering of fast particles from the potentials of an atomic chain and an atomic plane within the general scattering theory. It will be shown quite rigorously that the average potential of an atomic chain introduced by Lindhard [1] is obtained from the potentials of an atomic chain and an atomic plane. An analysis of this equation indicates that the density of the wave function for negatively charged particles depends logarithmically on the length of the atomic chain near the maximum and can be much greater than unity. For real single crystals, this effect is known as flux peaking effect[7].

2. SCATTERING FROM AN EXTENDED ATOMIC CHAIN

We shall consider scattering of fast charged particles from the potential of an atomic chain containing \(N_z\) atoms separated by the lattice period \(c\). To ensure that the opposite ends of the chain tend uniformly to \(+\infty\) and \(-\infty\) in the limit \(N_z \to \infty\), we shall choose the origin at \(z = N_z c/2\). The Fourier transform of the potential then remains the same for even and odd \(N_z\), and we shall quote the potential for an odd number of atoms

\[
U(r) = \sum_{j_z = -\frac{N_z}{2}}^{\frac{N_z}{2} - 1} U_{at}(r + n_z c j_z),
\]

\[
U(k) = U_{at}(k) \frac{\sin(N_z k z c/2)}{\sin(k c/2)}. \tag{2}
\]

Without loss of generality, we shall consider the scattering of nonrelativistic particles whose wave function satisfies the Lippmann -Schwinger equation (\(\hbar = 1\))

\[
\Psi(r) = e^{i pr} + \int dr' \frac{e^{ip|r-r'|}}{-4\pi |r-r'|} V(r') \Psi(r'), \tag{3}
\]

where \(V(r) = 2MU(r)\), and \(M\) is the particle mass. It is well known that the solution of the integral equation (3)
can be written formally as an infinite Born series

$$\Psi(r) = \sum_{n=0}^{\infty} \Psi^{(n)}(r)$$  (4)

with terms \(\Psi^{(0)} = e^{ipr}\),
\[
\Psi^{(n)}(r) = e^{ipr} \int dR_1 \ldots dR_n \frac{e^{ipR_1 \ldots pR_n}}{-4\pi R_1} \times V(r - R_1) \ldots -4\pi R_n V(r - R_1 - \ldots - R_n).
\]

An eikonal expression for the wave function is obtained from the expansion of \(\Psi^{(n)}(r)\) in powers of \(p_z \to \infty\) followed by summation of the first terms of this expansion [8]. An additional expansion in powers of \(L_z \to \infty\) was considered in [9] within the eikonal approximation, i.e., a double asymptotic expansion has been used (first expansion in powers of \(p_z \to \infty\) and then in powers of \(L_z \to \infty\)). However, the eikonal approximation is not uniform with respect to the length of the chain (asymptotic expansion of \(\Psi\) should yield a different result). In fact, the pole of the Green function (in the momentum space shifted by an amount equal to the particle momentum \(p\))

$$\frac{1}{k^2 + 2pk - i\delta},$$

i.e., the point \(k_z = -p_z + \sqrt{p_z^2 - k^2 - 2p_z^2 k^2 - i\delta}\) merges in the limit \(p_z \to \infty\) with a removable singularity of the component \(k_z = 0\) of the Fourier potential of the chain defined by Eq. (2) and the resulting nonuniform behavior in the asymptotic expansion of the integrals involved is due to merging of certain critical singularities [10, 11]. To obtain the wave function in the field of a chain with \(L_z \gtrsim p_z R^2\), it is necessary to derive an asymptotic expansion of \(\Psi^{(n)}(r)\) which is uniform over the length of the chain \(L_z\). The parabolic approximative of Leontovich and Fock [12] represents such expansion. For \(L_z \gg p_z R^2\), the parabolic approximation can be simplified. The simplification in question can be obtained directly from Eq. (5) by expanding with respect to \(L_z \to \infty\) and then with respect to \(p_z \to \infty\), and the results are quoted below. Omitting the intermediate steps, we can write the principal term for \(\Psi^{(1)}\) in the form

$$\Psi^{(1)}(r) = e^{ipr} \int dR_{1\bot} - \frac{i}{8}[H_0^{(1)}(p_{\bot} R_{1\bot})] e^{-i p_{\bot} R_{1\bot}} V_{\bot}(r_{\bot} - R_{1\bot}, 0),$$

Here, \(H_0^{(1)}(\rho)\) is a Hankel function of first kind; \(H_0(\beta, \rho)\) is an incomplete Hankel cylindrical function [13]. The quantity \(V_{\bot}(r_{\bot} - R_{1\bot}, 0)\) is the average potential of an atomic chain which is usually introduced to describe the channeling [1].

Since the integrand in Eq.(6) is independent of \(r_z\), we can introduce quite consistently in Eq. (5) analogous expansions in each of the integrals involved. We obtain

$$\Psi^{(n)}(r) = e^{ipr} \int dR_{1\bot} \ldots dR_{n\bot} \frac{e^{-ipR_{1\bot} \ldots pR_{n\bot}}}{-4\pi R_{1\bot}} \times V_{\bot}(r_{\bot} - R_{1\bot}, 0) \ldots \tilde{G}_{p_{\bot}}(R_{1\bot}) e^{ipR_{1\bot} \ldots pR_{n\bot}} V_{\bot}(r_{\bot} - R_{1\bot} - \ldots - R_{n\bot}, 0).$$

Summation of the terms in Eq. (7) yields the wave function in the field of an atomic chain

$$\Psi(r) = e^{ip_{\bot} r_{\bot}} \phi_{p_{\bot}}(r_{\bot}),$$

where \(\phi_{p_{\bot}}(r_{\bot})\) satisfies the following two-dimensional integral equation:

$$\phi_{p_{\bot}} = e^{ip_{\bot} r_{\bot}} \int dr_{\bot} \tilde{G}_{p_{\bot}}(r_{\bot} - r_{\bot}^\prime) V_{\bot}(r_{\bot}^\prime, 0) \phi_{p_{\bot}}(r_{\bot}^\prime).$$

The solution of the Fredholm Integral equation (10) of second kind can be written in the form

$$\phi_{p_{\bot}}(r_{\bot}) = e^{ip_{\bot} r_{\bot}} - \sum_{k=1}^{\infty} a_k \phi_{p_{\bot}}^{(k)}(r_{\bot}),$$

where \(\lambda_k\) and \(\phi^{(k)}\) are the eigenvalues and eigenfunctions of the homogeneous Fredholm equation of second kind

$$\phi^{(k)}_{p_{\bot}}(r_{\bot}) = \lambda_k \int dr_{\bot} \tilde{G}_{p_{\bot}}(r_{\bot} - r_{\bot}^\prime) V_{\bot}(r_{\bot}^\prime, 0) \phi^{(k)}_{p_{\bot}}(r_{\bot}^\prime),$$

and

$$a_k = \int dr_{\bot} e^{ip_{\bot} r_{\bot}} V_{\bot}(r_{\bot}, 0) \phi^{(k)}_{p_{\bot}}(r_{\bot}).$$

The spectral equation (12) determines the transverse eigenfunctions and transverse eigenenergies for channeling in the field of an isolated atomic chain. The eigenfunctions and eigenenergies depend not only on the longitudinal momentum of the particle \(p_z\), but also on the longitudinal length of the chain \(L_z\). For an axially symmetric chain, the propagator defined by Eq. (8) can be conveniently written in the form (\(\lambda = L_z/4p_z\))

$$-\frac{i}{8}[H_0^{(1)}(p_{\bot} R_{1\bot}) + H_0(\frac{2\lambda p_{\bot}}{r_{\bot} - r_{\bot}^\prime})],$$

$$p_{\bot} |r_{\bot} - r_{\bot}^\prime| = \sum_{m=-\infty}^{\infty} e^{im\varphi} \tilde{G}_{p_{\bot}}^m(r_{\bot}, r_{\bot}^\prime),$$

where \(\varphi\) is the angle between \(r_{\bot}\) and \(r_{\bot}^\prime\), and

$$\tilde{G}_{p_{\bot}}^m(r_{\bot}, r_{\bot}^\prime) = \frac{1}{2\pi} \int_0^\infty kdz J_m(k r_{\bot}) J_m(k r_{\bot}^\prime)$$

$$\times \frac{1 - e^{-i\frac{\pi}{2}(k^2 - p_z^2)}}{p_{\bot}^2 - k^2 + i\delta}. $$
The wave function \( \phi_{p \perp} \) can be now expanded in terms of the azimuthal momentum (\( \varphi_1 \) is the angle between \( r \perp \) and \( p \perp \))

\[
\phi_{p \perp}(r \perp) = \sum_{-\infty}^{\infty} i^m e^{im\varphi_1} \Psi_m(p \perp, r \perp) \tag{15}
\]

where \( \Psi_m(p \perp, r \perp) \) satisfies the following integral equation:

\[
\Psi_m(p \perp, r \perp) = J_m(p \perp r \perp) + 2\pi \int_0^\infty r \perp' dr \perp' \tilde{G}^m_{p \perp}(r \perp, r \perp') V(r \perp', 0) \Psi_m(p \perp, r \perp'). \tag{16}
\]

We shall consider two cases corresponding to two limiting values of the parameter \( \rho \cdot sh(\beta) \) for which the incomplete cylindrical function \( H_0(\beta, \rho) \) can be expanded in a series\[13\]. In the first case when the condition \( \rho \cdot sh(\beta) > 1 \) is satisfied and

\[
H_0(\beta, \rho) = H^{(1)}_0(\rho) + O((\rho \cdot sh(\beta))^{-1}),
\]

the kernel defined by Eq. (8) becomes a two-dimensional Green function \(-i/4)H^{(1)}_0(p \perp r \perp)\) and Eq. (10) reduces to the usual two-dimensional Lippmann-Schwinger equation independent of \( L_z \). In the second case when the inequality \( \rho \cdot sh(\beta) < 1 \) holds, we obtain \[13\]

\[
H_0(\beta, \rho) = \frac{2}{i\pi} \beta + O((\rho \cdot sh(\beta))).
\]

This case corresponds to the condition

\[
\frac{p^2_z L_z}{4p_z} - \frac{|r \perp - r \perp'|^2 p_z}{L_z} \ll 1,
\]

i.e., to small angles of incidence \( \theta_0 \ll 2/\sqrt{p_z L_z} \) and to small distances from the axis of the chain \( |r \perp - r \perp'| \ll \sqrt{L_z/p_z} \). It will be shown that Eq. (10) holds for angles of incidence \( \theta_0 \lesssim 1/p_z R \) and, therefore, for all points within the range of the potential of the chain \( |r \perp - r \perp'| \lesssim R \) the condition \( p \perp, |r \perp - r \perp'| < 1 \) is satisfied and the Hankel function \( H^{(1)}_0(p \perp |r \perp - r \perp'|) \) can be expanded in a series. The function \( \tilde{G}_{p \perp}(r \perp) \) then satisfies the following equation:

\[
\tilde{G}_{p \perp} \sim \frac{1}{4\pi} \ln \frac{|r \perp - r \perp'|^2 \gamma p_z}{L_z} - \frac{i}{8}, \quad \gamma = 1.78...
\tag{17}
\]

and Eq. (10) can be written in the form

\[
\phi_{p \perp} = e^{i p \perp r \perp} + \int dr \perp' \left[ \frac{1}{4\pi} \ln \frac{|r \perp - r \perp'|^2 \gamma p_z}{L_z} - \frac{i}{8} |V_\perp(r \perp', 0)|\phi_{p \perp}(r \perp') \right]. \tag{18}
\]

For a potential with azimuthal symmetry, Eqs. (16) and (17) yield the following equation for the wave function with a momentum \( m \):

\[
\Psi_m(p \perp, r \perp) = J_m(p \perp r \perp) + 2\pi \int_0^\infty r \perp' dr \perp' \tilde{G}^m_{p \perp}(r \perp, r \perp') V(r \perp', 0) \Psi_m(p \perp, r \perp'). \tag{19}
\]

\[\text{FIG. 1: Dependencies of the probability density of finding particles on the atomic chain axis on the magnitude of the potential } U_0 = 2Z_1 Z_2 e^2 \epsilon/c \text{ (in units of } [M^2 R^4]^{-1} \text{). Curves 1 and 8 correspond to scattering of negatively and positively charged particles for the following values of the parameter } \ln(L_z/\gamma p_z R^2): \text{ 1, 8 - 6.0; 2, 7 - 5.0; 3, 6 - 4.0; 4, 5 - 3.0.}\]

\[\text{FIG. 2: Dependencies of the distribution of the particle density on the distance from the axis of an extended chain in the case of the maximum defined by Eq. (23) for } \ln(L_z/\gamma p_z R^2) = 3.2; 1 \text{ negatively charged particles; 2) positively charged particles.}\]

\[
\tilde{G}^m_{p \perp}(r \perp, r \perp') = \begin{cases} 
-\frac{1}{4\pi m} p_\perp < r_\perp' >, & m > 0, \\
\frac{1}{4\pi} \ln \frac{\gamma p_z}{L_z} - \frac{i}{8}, & m = 0.
\end{cases}
\tag{20}
\]

We shall now determine the probability density that the particle lies on the axis of the chain \( r \perp = 0 \). For \( m = 0 \), Eq. (19) yields

\[
\Psi_0(0, 0) = 1 + \frac{1}{2} \int_0^\infty r \perp' dr \perp' \ln \frac{r_\perp'^2 \gamma p_z}{L_z} - \frac{i\pi}{2} |V_\perp(r \perp', 0)|\Psi_0(0, r \perp').
\]
and we obtain

\[ |\Psi_0(0,0)|^2 = \frac{1}{B + C}, \quad (21) \]

\[ B = [1 - \frac{1}{2} \int_0^\infty r'_\perp^2 dr'_\perp \ln \frac{r'_\perp^2 \gamma p_z}{L_z} V(r'_\perp,0)^2], \]

\[ C = \left[ \frac{\pi}{4} \int_0^\infty r'_\perp^4 dr'_\perp V(r'_\perp,0)^2 \right]. \]

For \( m > 0 \), we obtain the obvious result \( \Psi_m(0,0) = 0 \).

Using the Molière potential [14] as an atomic potential, we can easily evaluate (for the corresponding average potential [15]) the integrals which appear in Eq. (21) (see [16]). We then obtain

\[ |\Psi_0(0,0)|^2 = \frac{1}{B_1 + C_1}, \quad (22) \]

\[ B_1 = [1 - M \frac{2Z_1Z_2e^2R^2}{c} \sum_{i=1}^3 \alpha_i \beta_i^{-2} \ln \frac{R^2\gamma p_z}{\beta_i^2 L_z}], \]

\[ C_1 = \frac{\pi}{2} M \frac{2Z_1Z_2e^2R^2}{c} \sum_{i=1}^3 \alpha_i \beta_i^{-2}. \]

where \( Z_1 \) is the charge of an atom in the target and \( Z_2 \) is the charge of the incident particle; \( \alpha_i \) and \( \beta_i \) are the parameters of the Molière potential. It follows from Eq. (22) that the density of positively charged particles on the axis of an extended chain \( (L_z >> p_z R^2) \) is always lower than unity and the density of negatively charged particles can exceed unity.

We note that the proposed approximation holds for an arbitrary strength of the potential \( \U_0 = 2Z_1 Z_2 e^2 / c \). In particular, for \( \U_0 \equiv 0 \), we obtain \( |\Psi_0(0,0)|^2 = 1 \) which is the correct result in the absence of scatterers. The dependence of \( |\Psi_0(0,0)|^2 \) on \( \U_0 \) is shown in Fig. 1. The locations and magnitudes of the maxima of the curves in Fig. 1 can be easily determined from Eq. (22)

\[ U_{0\text{max}} = \frac{\sum_{i=1}^3 \alpha_i \beta_i^{-2} \ln \frac{R^2\gamma p_z}{\beta_i^2 L_z}}{M R^2 (\sum_{i=1}^3 \alpha_i \beta_i^{-2} \ln \frac{R^2\gamma p_z}{\beta_i^2 L_z})^2 + \frac{3}{2} (\frac{\beta_i}{\gamma p_z})^2 \sum_{i=1}^3 \alpha_i \beta_i^{-2})^2}, \quad (23) \]

\[ |\Psi_{0\text{max}}(0,0)|^2 = \frac{1}{B_1 + C_1}, \]

\[ B_1 = [1 - M R^2 U_{0\text{max}} \sum_{i=1}^3 \alpha_i \beta_i^{-2} \ln \frac{R^2\gamma p_z}{\beta_i^2 L_z}], \]

\[ C_1 = \left[ \frac{\pi}{2} M R^2 U_{0\text{max}} \sum_{i=1}^3 \alpha_i \beta_i^{-2} \right]^2. \]

For \( \ln (\gamma R^2 p_z / L_z) >> 1 \), the density of negatively charged particles on the axis of the chain is logarithmically large and independent of the magnitude of the potential

\[ |\Psi_{0\text{max}}(0,0)|^2 = (\frac{\pi}{2})^2 \frac{\gamma R^2}{\beta_i^2 L_z} \sum_{i=1}^3 \alpha_i \beta_i^{-2} \ln \frac{R^2\gamma p_z}{\beta_i^2 L_z}, \quad (24) \]

The radial distribution of charged particles across the potential of the chain, obtained in this case, is shown in Fig. 2. For real crystals, the density on the chain axis can increase only for low-energy electrons. For other negatively charged particles (\( \mu^- \), \( \pi^- \), \( \bar{\rho} \), etc.) which have large masses and for ultrarelativistic electrons \( e^- \) [when \( M \) in Eq. (3) is replaced by \( E \)], the quantity \( U_{0\text{max}} \) becomes negligibly small for \( \ln (L_z / \gamma p_z R^2) >> 1 \) (see Table 1 where the calculations are presented for \( \ln (L_z / \gamma p_z R^2) = 10 \)). To observe an appreciable increase in the density for \( \mu^- \), \( \pi^- \), and \( \bar{\rho} \), it would be necessary to use high-index crystallographic directions but the effect of neighboring atomic chains would then be important.

| Crystal | \( e^- \) | \( \mu^- \) | \( \pi^- \) | \( \bar{\rho} \) |
|---------|---------|---------|---------|---------|
| Be      | 2.6     | 0.013   | 0.009   | 0.0014  |
| C       | 3.4     | 0.016   | 0.012   | 0.0019  |
| Si      | 6.0     | 0.029   | 0.022   | 0.0033  |
| Ge      | 10.4    | 0.05    | 0.038   | 0.0057  |

We shall now derive expressions for the amplitude and total scattering cross section. The wave function defined by Eq. (9) is valid only in the region \( |\mathbf{r}_z| \leq L_z \) (see Sec. 3). It follows that it can be used to calculate the amplitude provided Eq. (9) is substituted in the expression

\[ f = -\frac{1}{4\pi} \int d\mathbf{r} e^{-ip\mathbf{r} \cdot \mathbf{V}(\mathbf{r})} \Psi(\mathbf{r}) \quad (25) \]

which requires the knowledge of the wave function only in the region of action of the potential. We stress that such situation is analogous to the situation in the eikonal approximation. The eikonal wave function is a good approximation only in the region of space \( |\mathbf{r}_z| << p_z R^2 \) (see [17]) and its asymptotic behavior for \( |\mathbf{r}_z| \rightarrow \infty \) cannot be used to calculate the scattering amplitude. Substituting Eq. (9) in Eq. (25), we obtain

\[ f = -\frac{1}{4\pi} \sin(N_z(p_i \mathbf{z} - p_f \mathbf{z} / 2)) \times \int d\mathbf{r}_\perp e^{-i\mathbf{p}_\perp \cdot \mathbf{r}_\perp} \mathbf{V}_\perp (\mathbf{r}_\perp, p_i - p_f) \mathbf{\Psi}_{i\perp}(\mathbf{r}_\perp), \quad (26) \]

where \( \mathbf{V}_\perp (\mathbf{r}_\perp, q) \) is the longitudinal component of the chain Fourier potential \( \mathbf{V}_\perp (\mathbf{r}_\perp, q) = \mathbf{V}_\perp (\mathbf{r}_\perp, q) / c \). Since the integral in Eq. (26) is a slowly varying function of
\( p_{iz} - p_{fz} \) compared with the function outside the integral, we can write the scattering amplitude in the form

\[
\begin{aligned}
f &= \frac{-1}{2\pi} \frac{1}{(p_{iz} - p_{fz})} \times \\
&\int \!\! dr_\perp e^{-ip_{iz}r_\perp} V(r_\perp, 0) \psi_{p\perp}(r_\perp).
\end{aligned}
\tag{27}
\]

For small angles of incidence \( \theta_0 \ll 1 \) and for small angles of particles leaving the crystal \( \theta_1 \ll 1 \) measured from the direction of the Oz axis, we obtain

\[
p_{iz} - p_{fz} = 2p \sin\left(\frac{\theta_0 + \theta_1}{2}\right) \sin\left(\frac{\theta_1 - \theta_0}{2}\right) \approx \frac{1}{2} p_z (\theta_1^2 - \theta_0^2)
\]

It follows that the amplitude defined by Eq. (27) and the differential scattering cross section \( d\sigma/d\Omega = |f|^2 \) have sharp maxima at \( \theta_0 = \theta_1 \). For angles of incidence \( \theta_0 \gg 2/\sqrt{p_z L_z} \), the polar width of the maximum for an extended potential \( L_z >> p_z R^2 \) is given by

\[
|\theta_1 - \theta_0|_{\text{eff}} \approx \frac{2}{p_z L_z} \theta_0.
\]

The spatial distribution of the amplitudes defined by Eq. (27) is then either ring- or doughnut-shaped, which is observed in experiments on hyperchanneling [18,19]. For \( \theta_0 \lesssim 1/\sqrt{p_z L_z} \), the ring is compressed and becomes a peak. For \( \theta_0 \ll 2/\sqrt{p_z L_z} \), the width of the peak is given by

\[
|\theta_1 - \theta_0|_{\text{eff}} \approx \frac{2}{p_z L_z}.
\]

Using the optical theorem \( \sigma = (4\pi/p)Im f(0) \), we obtain the following result for the total scattering cross section:

\[
\sigma = -\frac{L_z}{p} \int dr_\perp e^{-ip_{iz}r_\perp} V(r_\perp, 0) \psi_{p\perp}(r_\perp).
\tag{28}
\]

For small angles of incidence \( \theta_0 \ll 2/\sqrt{p_z L_z} \), the cross section can be approximated by

\[
\sigma = \frac{L_z}{8p} \left[ \left( \frac{1}{2} \frac{1}{2\pi} \int \!\! r_\perp dr_\perp V(r_\perp, 0) \ln \frac{\sqrt{2} p_z L_z}{2\pi} \right)^2 + \frac{1}{64} \right]^{-1}.
\tag{29}
\]

With an accuracy up to a coefficient depending on the form of the potential, Eq. (29) reduces to the results of model calculations [20,21]. For angles of incidence \( \theta_0 \ll 2/\sqrt{p_z L_z} \), the wave function \( \psi_{p\perp}(r_\perp) \) is determined by the two-dimensional Lippmann-Schwinger equation and the cross section defined by Eq. (28) is proportional to the two-dimensional scattering amplitude from a potential \( V_\perp(r_\perp, 0) \) which may be resonant for negatively charged particles [21].

### 3. Scattering from an Extended Atomic Plane

We shall now consider scattering from the potential of a rectangular atomic plane containing \( N_y \) atomic chains separated by a period \( b \) and each containing \( N_z \) atoms. For simplicity, we shall assume that \( N_y \) and \( N_z \) are odd numbers

\[
U(r_\perp) = \sum_{-(N_y-1)/2}^{(N_y-1)/2} \sum_{-(N_z-1)/2}^{(N_z-1)/2} U_{at}(r + n_x c j_z + n_y b j_y).
\]

\[
U(k) = U_{at}(k) \sin(N_z k_x \frac{z}{2}) \sin(N_y k_y \frac{b}{2}) \sin(k_z \frac{z}{2}) \sin(k_y \frac{b}{2}).
\tag{30}
\]

As in the case of the chain potential, the eikonal approximation is not valid for an extended plane potential \( L_z >> p_z R^2 \) and \( L_y >> p_y R^2 \). We shall, therefore, base our discussion on the approach developed in Sec. 1 for scattering from a chain and seek the expansion of Eq. (5) for \( L_z = N_z c \to \infty \) and \( L_y = N_y b \to \infty \), and then perform expansion for \( p_z \to \infty \) and \( p_y \to \infty \). The final result which holds subject to the additional condition \( p_y/p_z \to 0 \) has the form

\[
\Psi^{(1)}(r) = e^{ipr} \int_{-\infty}^{\infty} \!\! \!\! dR_x \left( -\frac{i}{2} \right) e^{ipz|z|/p_x} - i \left( \frac{\pi |z|}{2p_x} \right)^{1/2} \times \Phi_{1/2}(\beta, \rho)
\]

\[
\Phi_{1/2}(\beta, \rho) = \left( \frac{\pi}{2} \right) \sin((\beta - \rho)/2) \sin(N_z k_x \frac{z}{2}) \sin(N_y k_y \frac{b}{2}).
\tag{31}
\]

Here, \( \Phi_{1/2}(\beta, \rho) \) is the incomplete cylindrical function of fractional order [13] and \( V_{\perp}(r_x, 0, 0) = V_{at}(r_x, 0, 0)/cb \) is the average potential of an atomic plane. Since the integral in Eq. (31) is independent of \( r_y \) and \( r_z \), we can perform expansions in the multiple integral which determines the correction \( \Psi^{(n)} \) as in the case of an atomic chain, which yields

\[
\Psi^{(n)}(r) = e^{ipr} \int_{-\infty}^{\infty} \!\! \!\! dR_1 \cdots \int_{-\infty}^{\infty} \!\! \!\! dR_N \tilde{G}_{p_x}(r_x) e^{-ipz_1} \times V_\perp(r_x - R_1x, 0, 0) \cdots \tilde{G}_{p_x}(R_N x) e^{-ipz_N x} \times V_\perp(r_x - R_N x - \cdots - R_N x, 0, 0),
\tag{32}
\]

\[
\tilde{G}_{p_x}(R_x) = \left( -\frac{i}{2} \right) \frac{e^{ipz|z|/p_x}}{p_x} - i \left( \frac{\pi |z|}{2p_x} \right)^{1/2} \times \Phi_{1/2}(\beta, \rho) = \left( \frac{\pi}{2} \right) \sin((\beta - \rho)/2) \sin(N_z k_x \frac{z}{2}) \sin(N_y k_y \frac{b}{2}).
\tag{33}
\]

Summation of the series in Eq. (4) with the terms defined by Eq. (32) yields the following expression for the wave function in the field of a rectangular atomic plane:

\[
\Psi(r) = e^{ipz_1 + ipy_1} \phi_{p_x}(r_x).
\tag{34}
\]
where the transverse function $\phi_{p_x}(r_x)$ satisfies an integral equation
\[
\phi_{p_x}(r_x) = e^{ip_x r_x} + \int_{-\infty}^{\infty} dr'_x \tilde{G}_{p_x}(|r_x - r'_x|) \times V_{\perp} (r'_x, 0, 0) \phi_{p_x}(r'_x),
\] (35)
with the kernel $\tilde{G}_{p_x}(R_x)$ determined by Eq. (33).

The distribution of the probability density, the amplitude, and the scattering cross section in the field of an atomic plane can be obtained from Eq. (35) by the method described for the atomic chain.

4. DISCUSSION OF RESULTS

The conditions of validity of the present approximation can be obtained from the requirement that the terms which were neglected in the derivation of Eqs. (10) and (35) should be small compared with the terms retained, i.e.,
\[
|\Psi^{(0)}| >> |\Psi_m^{(n)}|, \quad |\Psi_1^{(n)}| >> |\Psi_m^{(n)}|, \quad m \geq 2,
\] (36)
where $\Psi_m^{(n)}$ are the terms in the asymptotic expansion of the wave function $\Psi^{(n)}$ of the Born series defined by Eq. (4). We can write $\Psi^{(1)}$ with an accuracy up to terms $O(1/p_z^2 + 1/p_z L_z + 1/L_z^2)$ for an atomic chain
\[
\Psi^{(1)} = \Psi_1^{(1)} + \Psi_2^{(1)} + \Psi_3^{(1)},
\] (37)
\[
\Psi_1^{(1)} = e^{ip_r r} \int dr_{\perp} \left(-\frac{i}{\hbar} \right) [H_0^{(1)}(p_{\perp} R_{\perp}) + H_0(\ln \frac{N_z c p_{\perp}}{2p_z R_{\perp}}, p_{\perp} R_{\perp})] e^{-ip_{\perp} R_{\perp}} V_{\perp}(r_{\perp} - R_{\perp}, 0),
\]
\[
\Psi_2^{(1)} = e^{ip_r r} \frac{r_z}{2\pi L_z} \int dr_{\perp} e^{ip_{\perp}(R_{\perp} - r_{\perp})^2} \times V_{\perp}(r_{\perp} - R_{\perp}, 0),
\]
\[
\Psi_3^{(1)} = e^{ip_r r} \sum_{n=1,1/2,...} \frac{(-1)^{(N_z - 1)n} c}{4\pi p_z n} e^{i2\pi n r_z} \times V_{\perp}(r_{\perp}, 0) \frac{2\pi n}{c}.
\]

(a) We shall now consider small angles of incidence $\theta_0 << 2/\sqrt{p_z L_z}$. The integrals in Eq. (37) can be easily estimated
\[
|\Psi_1^{(1)}| \simeq |\tilde{V}_{\perp} R_z \ln \frac{p_z \gamma R_z^2}{L_z} |, \quad |\Psi_2^{(1)}| \simeq |\tilde{V}_{\perp} R_z^2 \frac{r_z}{2\pi L_z} |,
\]
\[
|\Psi_3^{(1)}| \simeq |\tilde{V}_{\perp} \frac{c}{4\pi p_z} |.
\]
Comparing $|\Psi_1^{(1)}|$ with $|\Psi_2^{(1)}|$, we find that the wave function defined by Eq. (9) is valid in the region
\[
|r_z| << 2\pi L_z \ln \frac{L_z}{p_z \gamma R_z^2}.
\] (38)
i.e., for $L_z >> p_z R_z^2$, the wave function defined by Eq. (9) is valid virtually in the whole region of action of the chain potential and can be used in the calculation of the scattering amplitude as described above. Comparing $|\Psi_1^{(1)}|$ and $|\Psi_3^{(1)}|$, we obtain the following important criterion:
\[
|p_z R_z^2 \ln \frac{L_z}{p_z \gamma R_z^2} | >> \frac{c}{4\pi}
\] (39)
which indicates that the dynamic length of longitudinal coherence $p_z R_z^2$ should exceed the distance $c$ separating the atom under study from the preceding and following atoms. We then obtain physical averaging of the potential of an atomic chain.

(b) We shall now assume that the angle of incidence satisfies $\theta_0 \simeq 2/\sqrt{p_z L_z}$. We then obtain
\[
|\Psi_1^{(1)}| \simeq \frac{\tilde{V}_{\perp} R_z^2}{\sqrt{p_z L_z}} |, \quad |\Psi_2^{(1)}| \simeq \frac{n_z \tilde{V}_{\perp} R_z^2}{2\pi L_z}.
\]
The condition $|\Psi_1^{(1)}| >> |\Psi_2^{(1)}|$ yields the following restriction on the angle of incidence:
\[
\theta_0 << \frac{(2\pi)^2}{p_z R_z}.
\] (40)

To derive this inequality, we set $r_z \sim L_z$ to satisfy the requirement that the wave function defined by Eq. (9) should be valid in the whole range of action of the chain potential. Such restriction can be interpreted as follows. It is well known that angles $\theta_0 \simeq 1/p_z R_z$ are important in the scattering from an isolated atom. For coherent scattering from the whole chain, we require that the next atom should lie within the diffraction cone of the scattering from the preceding atom. This condition can be satisfied provided the axis of the chain lies within a conical diffraction surface. When it lies outside such a conical surface, noncoherent effects become important. Finally, the additional requirement $|\Psi_2^{(1)}|, |\Psi_3^{(1)}| << 1$ which follows from the first condition in Eq. (36) should be satisfied. Combining this requirement with the condition (40), we find that the Lindhard angle $\theta_L \sim \sqrt{U_z/E}$ lies in the range defined by Eq. (40), i.e., the average potential is applicable for particles above the barrier. We wish to stress that the condition (40) does not contradict our initial assumption (b) when the condition $\theta_0 \simeq 2/\sqrt{p_z L_z}$ is satisfied, since, for an extended potential $L_z >> p_z R_z^2$, the inequality $1/p_z R_z >> 1/\sqrt{p_z L_z}$ always holds.

The mathematical framework of the present approach is similar to the eikonal approximation, but our method is valid also in the opposite limiting case. It can be easily seen that the conditions derived above follow from the conditions of the eikonal approximation [22, 23] (where the expansion is with respect to $p_z$ rather than with respect to $p$) provided $p_z R_z^2$ is replaced by $L_z$. The eikonal approximation neglects the diffraction effects [17, 23].
the opposite limit discussed earlier, the diffraction effects become dominant since the diameter of the chain $R$ is much smaller than the dimensions of the Fresnel zone $\sqrt{L_z/p_z}$ and the scattering cross section related to diffraction $\sim L_z/p_z$ [see Eq. (29)] exceeds considerably the classical cross section $\sim R^2$. Naturally, such effects are observable only if the length determined by multiple scattering from potential fluctuations is much longer than the length of the chain.

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