Solution of quantum kinetic equation in the locally eikonal approximation

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A stationary quantum kinetic equation is derived for the density matrix of fast charged particles in an inhomogeneous medium (a crystal or an amorphous medium) in the approximation of slowly varying amplitudes. This equation is used to derive the mutual coherence function of the wave field for scattering in a plate of an amorphous material with a sharp boundary. The longitudinal coherence is determined by the mean free path of the particles in the medium. Equations are derived for the orientational dependence of the total reflection coefficient of a single crystal for electrons with energies on the order of a few tens of keV in the case of incoherent multiple scattering (the channeling pattern). The diffraction fine structure of the angular distribution of back-scattered particles near Bragg directions (the back-scattering pattern) is derived analytically in the two-wave approximation. The results are found to correspond to experimental data.

1. INTRODUCTION

The eikonal approximation is used in quantum mechanics whenever a particle moving through a region of space with a potential $U(\mathbf{r})$ undergoes a momentum change $\Delta\mathbf{p}$ which is small in comparison with its initial momentum $\mathbf{p}$. If the initial state of the particle is described by a plane wave, the small value of $\Delta\mathbf{p}$ allows us to seek a solution of the wave equation in the region with the potential in the form ($\hbar = 1$)

$$\Psi(\mathbf{r}) = \exp(i\mathbf{pr})F(\mathbf{p}, \mathbf{r}), \tag{1.1}$$

where $F(\mathbf{p},\mathbf{r})$ is a function which varies slowly in comparison with the exponential function, so that when (1.1) is substituted into the wave equation we can ignore the second derivatives of F with respect to the coordinates. If the incident wave is not a plane wave, i.e., if it is a superposition of plane waves,

$$(2\pi)^{-3}\int d^3p C(\mathbf{p})\exp(i\mathbf{pr}),$$

we should replace (1.1) by

$$\psi(\mathbf{r}) = \int \frac{d^3p}{(2\pi)^3} C(\mathbf{p})\exp(i\mathbf{pr})F(\mathbf{p},\mathbf{r})$$

$$\equiv \int \frac{d^3p}{(2\pi)^3} g(\mathbf{p},\mathbf{r})\exp(i\mathbf{pr}). \tag{1.2}$$

If the system contains other particles with coordinates Q, we write

$$\psi(\mathbf{r}, Q) = \int \frac{d^3p}{(2\pi)^3} g(\mathbf{p},\mathbf{r},Q)\exp(i\mathbf{pr}) \tag{1.3}$$

and the behavior of a particle can be described by the density matrix[1]

$$\rho(\mathbf{r},\mathbf{r}') = \sum_Q \psi(\mathbf{r},Q)\psi^*(\mathbf{r}',Q)$$

$$= \int \frac{d^3p\, d^3p'}{(2\pi)^6} \exp(i\mathbf{pr} - i\mathbf{p}'\mathbf{r}')W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}'), \tag{1.4}$$

where

$$W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}') = \sum_Q g(\mathbf{p},\mathbf{r},Q)g^*(\mathbf{p}',\mathbf{r}',Q). \tag{1.5}$$

As fast particles move through a medium there will often be situations in which the momentum of a particle changes only slightly in a small volume of a scattering medium, although the overall change in the momentum in a thick slab can be large. It is then obvious that the density matrix of the particle can be assumed to have the form in (1.4) in some small region in the medium. This assumption is the basis of the approximate method introduced below for solving the quantum kinetic equation; this method might quite naturally be called the "locally eikonal method."

If this method is to be applicable, the function $W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}')$, which might be called the "amplitude coherence function," must vary substantially only over distances large in comparison with the wavelength of the particle, p^{-1}, and also in comparison with the dimensions of an individual scatterer. Below we will be discussing the scattering of a particle in crystalline and amorphous media; the conditions for the applicability of (1.4) in these two cases are, respectively,

$$\left|\frac{\partial W}{\partial \mathbf{r}}\right| \ll pW,\ \varkappa W,\ GW; \quad \left|\frac{\partial W}{\partial \mathbf{r}'}\right| \ll p'W,\ \varkappa W,\ GW, \tag{1.6a}$$

$$\left|\frac{\partial W}{\partial \mathbf{r}}\right| \ll pW,\ \varkappa W; \quad \left|\frac{\partial W}{\partial \mathbf{r}'}\right| \ll p'W,\ \varkappa W, \tag{1.6b}$$

where $\varkappa = me^2Z^{1/3}$, and $\mathbf{G}$ is the first reciprocal-lattice vector of the crystal.

A quantum kinetic equation for the scattering of fast particles in an amorphous medium was first formulated by Migdal.[2,3] Kagan and Kononets[4] generalized this equation to the case of a crystalline medium. In the formulation of boundary conditions on these time-varying equations it was assumed that they correspond to the small-angle approximation in the nearly normal incidence of the particles on the surface of the medium. Under these conditions the time t is related to the penetration depth (z) in the medium by $z = vt$, where v is the velocity of the particles.[5,6] The small-angle approximation, however, cannot be used for thick slabs of a scattering medium. Furthermore, in that time-varying approach difficulties arise in solving the problem of the reflection of particles from the medium.

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A stationary quantum kinetic equation for the Wigner function[7,8] is sometimes used in radiation transport theory. It is valid under the condition

$$\rho(\mathbf{r},\mathbf{r}',t)=\Phi\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{r}-\mathbf{r}',t\right)\equiv\Phi(\mathbf{R},\rho,t),$$
$$\left|\frac{\partial\Phi}{\partial\mathbf{R}}\right|\ll\left|\frac{\partial\Phi}{\partial\rho}\right|. \tag{1.7}$$

The violation of condition (1.7) near the boundary of the medium and in the case of a periodic arrangement of scatterers severely limits the range of applicability of the equations of Refs. 7 and 8.

The locally eikonal approximation, (1.4), makes it possible to construct a stationary kinetic equation for $W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r})$ which holds near the boundaries of the medium and which incorporates both diffraction by a regular array of atoms and inelastic (incoherent) scattering accompanied by the excitation of the electron and phonon subsystems.

We illustrate the use of this method below by finding an analytic solution of the problem of the reflection of fast electrons from a thick single crystal for nearly normal incidence of particles on the surface.

We also derive an expression for the mutual coherence function of the wave field of the particles which pass through a plate of an amorphous medium. We show that in the case of a scattering medium with sharp boundaries the density matrix $\rho(\mathbf{r},\mathbf{r},t)$ does not satisfy condition (1.7). The longitudinal coherence is then determined by the mean free path of the particles in the medium, in contrast with the results of Refs. 7 and 8.

2. STATIONARY QUANTUM KINETIC EQUATION

We consider the motion of a fast electron in a crystal (the case of an amorphous medium corresponds to taking the limit of infinitely large thermal displacements[5,9]). The state of the electron is described by the one-particle density

$$\rho(\mathbf{r},\mathbf{r}',t)=\mathrm{Sp}_{\mathrm{cryst}}\,\rho(\mathbf{r},\mathbf{r}';j,l;\mu,\nu;t), \tag{2.1}$$

where the sum is over the electron (j,l) and phonon (μ,ν) states of the crystal. In radiation transport theory, the function in (2.1) is called the "mutual coherence function."[10] Noting that (1.6) holds well for electrons with energies on the order of a few tens of keV (Refs. 11 and 12), and ignoring Fresnel reflection from the surface potential barrier (which is important only for angles of incidence in the grazing range,[13,14] $\vartheta<5°$), we find for (2.1) the equation

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\frac{\partial}{\partial\mathbf{r}}+\frac{\mathbf{p}'}{m}\frac{\partial}{\partial\mathbf{r}'}\right)W(\mathbf{p},\mathbf{p}';j,l;\mu,\nu;\mathbf{r},\mathbf{r}',t)$$
$$+i(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'}+E_j-E_l)W(\mathbf{p},\mathbf{p}';j,l;\mu,\nu;\mathbf{r},\mathbf{r}',t) \tag{2.2}$$
$$=-i\int\frac{d^3q}{(2\pi)^3}$$
$$\left[\sum_{n,\zeta}\langle j,\mu|U(\mathbf{q})|n,\zeta\rangle W(\mathbf{p}-\mathbf{q},\mathbf{p}';n,l;\zeta,\nu;\mathbf{r},\mathbf{r}',t)\right.$$
$$\left.-\sum_{n,\zeta}\langle n,\zeta|U'(\mathbf{q})|l,\nu\rangle W(\mathbf{p},\mathbf{p}'+\mathbf{q};j,n;\mu,\zeta;\mathbf{r},\mathbf{r}',t)\right],$$

where $\varepsilon_{\mathbf{p}}=\mathbf{p}^2/2m$, and E_j is the energy of the electron subsystem of the crystal. The quantity $\langle j,\mu|U(\mathbf{q})|n,\zeta\rangle$ is the matrix element of the interaction potential of the electron and the crystal:

$$U(\mathbf{r})=-\sum_a\frac{Z_ae^2}{|\mathbf{r}-\mathbf{R}_a-\mathbf{u}_a|}$$
$$+\sum_{a,s}\frac{e^2}{|\mathbf{r}-\mathbf{R}_a-\mathbf{u}_a-\boldsymbol{\rho}_{as}|}+\sum_b\frac{e^2}{|\mathbf{r}-\mathbf{r}_b|}, \tag{2.3}$$

where Z_a is the atomic number of an atom of the medium, $\mathbf{R}_a$ is the equilibrium position of the atom, and $\mathbf{u}_a$ is its thermal displacement. The second and third terms in (2.3) describe the interaction of a fast incident particle with, respectively, inner-shell electrons, whose coordinates $\boldsymbol{\rho}_{as}$ are reckoned from the instantaneous position of the center of the atom, and weakly bound conduction electrons. In insulators and semiconductors, the third term in (2.3) is negligible. In metals we need to allow for dynamic screening in the interaction of the fast charged particle with the conduction electrons.

We will be examining the case in which the interaction with the conduction electrons can be ignored, and the potential of the crystal is described well by only the first two terms in (2.3). In substituting (2.3) into (2.2) we need to bear in mind that $U(\mathbf{q})$ and $U'(\mathbf{q})$ are nonzero when $\mathbf{r}$ and $\mathbf{r}$, respectively, lie inside the scattering medium, Ω. For $\mathbf{r},\mathbf{r}'\notin\Omega$ we have $U(\mathbf{q})=U'(\mathbf{q})\equiv0$.

The diagonal elements of (2.3) correspond to the average arrangement of the atoms, which leads to a coherent Bragg diffraction. The elements which may be referred to as the "fluctuating part of the potential,"

$$\langle j,\mu|\delta U(\mathbf{q})|n,\zeta\rangle=\langle j,\mu|U(\mathbf{q})|n,\zeta\rangle-\delta_{jn}\delta_{\mu\zeta}\,\mathrm{Sp}\,U(\mathbf{q})\rho_{\mathrm{cryst}}, \tag{2.4}$$

lead to electron and phonon excitations (inelastic processes).

To construct a closed kinetic equation for $W(\mathbf{p},\mathbf{p};\mathbf{r},\mathbf{r};t)$ we need to sum (2.2) over j and μ in accordance with (2.1) and (1.4). By virtue of (1.6), we can use a method proposed by Migdal[2] (see also Refs. 1 and 5) to calculate the terms on the right side which contain fluctuation matrix elements (2.4):

$$\langle j,\mu|\delta U(\mathbf{q})|n,\zeta\rangle W(\mathbf{p}-\mathbf{q},\mathbf{p}';n,j;\zeta,\mu;\mathbf{r},\mathbf{r}',t)$$
$$=-i\pi\delta(\varepsilon_{\mathbf{p}-\mathbf{q}}-\varepsilon_{\mathbf{p}'}+E_n-E_j) \tag{2.5}$$
$$\times\int\frac{d^3k}{(2\pi)^3}\sum_{l,\eta}\{\langle j,\mu|\delta U(\mathbf{q})|n,\zeta\rangle\langle n,\zeta|\delta U(\mathbf{k})|l,\eta\rangle$$
$$\times W(\mathbf{p}-\mathbf{k}-\mathbf{q},\mathbf{p}';l,j;\eta,\mu;\mathbf{r},\mathbf{r}',t)$$
$$-\langle j,\mu|\delta U(\mathbf{q})|n,\zeta\rangle\langle l,\eta|\delta U'(\mathbf{k})|j,\mu\rangle$$
$$\times W(\mathbf{p}-\mathbf{q},\mathbf{p}'+\mathbf{k};n,l;\zeta,\mu;\mathbf{r},\mathbf{r}',t)\}.$$

The terms with principal values of integrals which have been discarded in (2.5) are smaller by an order of magnitude and go beyond the accuracy of experiments.[15]

Substituting (2.5) into (2.2), ignoring the deviation of the state of the crystal from thermodynamic equilibrium,[1] and summing the diagonal elements in (2.2) over j and μ, we find

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\frac{\partial}{\partial \mathbf{r}}+\frac{\mathbf{p}'}{m}\frac{\partial}{\partial \mathbf{r}'}\right)W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}',t)$$

$$+i(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'})W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}',t)$$

$$=i\sum_{\mathbf{K}}\Lambda(\mathbf{K})\{\theta(\mathbf{r})W(\mathbf{p}-\mathbf{K},\mathbf{p}';\mathbf{r},\mathbf{r}',t)$$

$$-\theta(\mathbf{r}')W(\mathbf{p},\mathbf{p}'+\mathbf{K};\mathbf{r},\mathbf{r}',t)\}$$

$$+\pi\theta(\mathbf{r})\int\frac{d^3q}{(2\pi)^3}\Big[\theta(\mathbf{r}')\sum_{\mathbf{K},j}\sigma_j(\mathbf{K}-\mathbf{q},\mathbf{q})\delta(\varepsilon_{\mathbf{p}-\mathbf{q}}-\varepsilon_{\mathbf{p}'}-E_{j0}) \tag{2.6}$$

$$\times W(\mathbf{p}-\mathbf{q},\mathbf{p}'+\mathbf{K}-\mathbf{q};\mathbf{r},\mathbf{r}',t)$$

$$-\sum_{\mathbf{K},j}\sigma_j(\mathbf{q},\mathbf{K}-\mathbf{q})\delta(\varepsilon_{\mathbf{p}-\mathbf{q}}-\varepsilon_{\mathbf{p}'}+E_{j0})$$

$$\times W(\mathbf{p}-\mathbf{K},\mathbf{p}';\mathbf{r},\mathbf{r}';t)\Big]$$

$$+\pi\theta(\mathbf{r}')\int\frac{d^3q}{(2\pi)^3}\Big[\theta(\mathbf{r})\sum_{\mathbf{K},j}\sigma_j(\mathbf{q},\mathbf{K}-\mathbf{q})$$

$$\times\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'+\mathbf{q}}+E_{j0})W(\mathbf{p}-\mathbf{K}+\mathbf{q},\mathbf{p}'+\mathbf{q};\mathbf{r},\mathbf{r}';t)$$

$$-\sum_{\mathbf{K},j}\sigma_j(\mathbf{K}-\mathbf{q},\mathbf{q})\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'+\mathbf{q}}-E_{j0})W(\mathbf{p},\mathbf{p}'+\mathbf{K};\mathbf{r},\mathbf{r}';t)\Big],$$

where $E_{j0}=E_j-E_0$ is the excitation energy of the electron subsystem. The summation over $\mathbf{K}$ in (2.6) is carried out over all the reciprocal-lattice vectors of the crystal, and the function $\vartheta(\mathbf{r})$ is defined by

$$\theta(\mathbf{r})=\begin{cases}1; & \mathbf{r}\in\Omega\\ 0; & \mathbf{r}\notin\Omega\end{cases} \tag{2.7}$$

and specifies the region of the space which is occupied by the scattering medium.

In kinetic equation (2.6), the terms which contain the Fourier components of the regular potential,

$$\Lambda(\mathbf{K})=N\sum_{\alpha}U_\alpha(\mathbf{K})\exp(-i\mathbf{K}\mathbf{r}_\alpha)\exp\Big(-\frac{1}{2}M_\alpha(\mathbf{K})\Big), \tag{2.8}$$

describe processes of coherent Bragg diffraction. The quantity

$$\sigma_0(\mathbf{q},\mathbf{k})=N\sum_{n}\exp(-i\mathbf{k}(\mathbf{R}_n-\mathbf{R}_m))F(\mathbf{q},\mathbf{k},\mathbf{R}_n-\mathbf{R}_m),$$

$$F(\mathbf{q},\mathbf{k},\mathbf{R}_n-\mathbf{R}_m)=\sum_{\alpha,\beta}U_\alpha(\mathbf{q})U_\beta(\mathbf{k})\exp(-i\mathbf{q}\mathbf{r}_\alpha-i\mathbf{k}\mathbf{r}_\beta) \tag{2.9}$$

$$\times\Big\{\exp\Big(-\frac{1}{2}M_\alpha(\mathbf{q})-\frac{1}{2}M_\beta(\mathbf{k})\Big)$$

$$\times[\exp(Y_{\alpha\beta}(\mathbf{q},\mathbf{k},\mathbf{R}_n-\mathbf{R}_m))-1]\Big\}$$

is the cross section for scattering by thermal fluctuations of the crystal potential. The cross section for inelastic scattering accompanied by excitation of atomic electrons is

$$\sigma_j(\mathbf{q},\mathbf{k})=N\frac{(4\pi e^2)^2}{q^2k^2}\sum_{\alpha}\exp(-i(\mathbf{k}+\mathbf{q})\mathbf{r}_\alpha)$$

$$\exp\Big(-\frac{1}{2}M_\alpha(\mathbf{q}+\mathbf{r})\Big)f_{0j}^{(\alpha)}(\mathbf{q})f_{j0}^{(\alpha)}(\mathbf{k}), \tag{2.10}$$

where

$$f_{0j}^{(\alpha)}(\mathbf{q})=\langle 0|\sum_{s}\exp(-i\mathbf{q}\boldsymbol{\rho}_{\alpha s})|j\rangle \tag{2.11}$$

and $M_\alpha(\mathbf{q})=\langle(\mathbf{q}\mathbf{u}_\alpha)^2\rangle$, so that $\exp(-\frac{1}{2}M_\alpha(\mathbf{q}))$ is the Debye-Waller factor, and N is the number of unit cells of the crystal per unit volume. The summation over α and β in (2.8)–(2.10) is carried out over the atoms of an individual cell; the indices n and m specify the positions of the centers of the different cells.

Afanas'ev and Kagan[16] have worked out a method for evaluating the cross sections in(2.8)–(2.10). Maslen and Rossouw[17] have analytically calculated the amplitudes for the atomic ionization processes in (2.11) from a hydrogenlike model.

According to (1.6) and (2.2), $W(\mathbf{p},\mathbf{p}';r,r';t)$ is continuous over $\mathbf{r}$ and $\mathbf{r}'$ at the boundaries of the scattering medium Ω, which are specified by the functions $\theta(\mathbf{r})$ and $\theta(\mathbf{r}')$. In order to specify boundary conditions on (2.6) we note that in free space $W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}';t)$ would be independent of the coordinates and would be the density matrix in the momentum representation. For a plane wave which is incident on a medium, and with $\mathbf{r},\mathbf{r}'\in\Omega$, the boundary condition on (2.6) is

$$W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}';t)=(2\pi)^3\delta(\mathbf{p}-\mathbf{\Pi})\delta(\mathbf{p}-\mathbf{p}'), \tag{2.12}$$

wher $\mathbf{\Pi}$ is the initial momentum of the electrons.

If we ignore the terms with $K\neq 0$ (this approach is equivalent to assuming a random arrangement of the atoms), Eq. (2.6) becomes the kinetic equation for an amorphous medium:

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\frac{\partial}{\partial \mathbf{r}}+\frac{\mathbf{p}'}{m}\frac{\partial}{\partial \mathbf{r}'}\right)W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}',t) \tag{2.13}$$

$$+i(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'})W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}',t)$$

$$=-i\Lambda(0)(\theta(\mathbf{r})-\theta(\mathbf{r}'))W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}';t)$$

$$+\pi\theta(\mathbf{r})\theta(\mathbf{r}')\int\frac{d^3q}{(2\pi)^3}\sum_{j}\sigma_j(-\mathbf{q},\mathbf{q})$$

$$\times[\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}-E_{j0})+\delta(\varepsilon_{\mathbf{p}'+\mathbf{q}}-\varepsilon_{\mathbf{p}}-E_{j0})]$$

$$\times W(\mathbf{p}+\mathbf{q},\mathbf{p}'+\mathbf{q};\mathbf{r},\mathbf{r}',t)$$

$$-\pi(\theta(\mathbf{r})+\theta(\mathbf{r}'))\int\frac{d^3q}{(2\pi)^3}\sum_{j}\sigma_j(-\mathbf{q},\mathbf{q})[\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}+E_{j0})$$

$$+\delta(\varepsilon_{\mathbf{p}'+\mathbf{q}}-\varepsilon_{\mathbf{p}}+E_{j0})]W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}',t).$$

In approximation (1.6), according to (1.1)–(1.2), the quantity

$$W(\mathbf{p},\mathbf{r},t)=W(\mathbf{p},\mathbf{p};\mathbf{r},\mathbf{r};t) \tag{2.14}$$

is positive definite and may be interpreted as the local semiclassical distribution of the probabilities for various values of the momentum. According to (2.13), $W(\mathbf{p},\mathbf{r},t)$ in this case satisfies the transport equation[9]

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\frac{\partial}{\partial \mathbf{r}}\right)W(\mathbf{p},\mathbf{r},t)$$

$$=\theta(\mathbf{r})\left[\int\frac{d^3q}{(2\pi)^2}\sum_j\sigma_j(-\mathbf{q},\mathbf{q})\,\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}-E_{j0})\right.$$

$$\times W(\mathbf{p}+\mathbf{q},\mathbf{r},t)$$

$$\left.-\int\frac{d^3q}{(2\pi)^2}\sum_j\sigma_j(-\mathbf{q},\mathbf{q})\,\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}+E_{j0})\,W(\mathbf{p},\mathbf{r},t)\right]. \tag{2.15}$$

The boundary condition on $W(\mathbf{p},\mathbf{r},t)$ corresponding to (2.12) is

$$W(\mathbf{p},\ \mathbf{r},\ t)=\delta(\mathbf{p}-\mathbf{\Pi});\qquad \mathbf{r}\in\Omega. \tag{2.16}$$

3. MUTUAL COHERENCE FUNCTION FOR SCATTERING IN AN AMORPHOUS MEDIUM

To analyze the mutual coherence of the wave field in a medium with a sharp boundary we consider the problem of the passage of fast electrons through a plate of thickness $L\lesssim l_{tr}$ of an amorphous medium, with the particles incident on the plate nearly along the normal to the surface. According to boundary condition (2.12), $W(\mathbf{p},\mathbf{p}';\mathbf{r},\mathbf{r}';t)$ does not depend on the time and can be written in the form

$$W(\mathbf{p},\ \mathbf{p}';\ \mathbf{r},\ \mathbf{r}';\ t)=(2\pi)^3\delta(\mathbf{p}-\mathbf{p}')f(\mathbf{p},\ z,\ z'), \tag{3.1}$$

where the z axis runs along the inward normal ($\mathbf{n}$) to the surface on which the particles are incident.

The function $f(\mathbf{p},z,z')$ satisfies the equation

$$\frac{(\mathbf{pn})}{m}\left(\frac{\partial}{\partial z}+\frac{\partial}{\partial z'}\right)f(\mathbf{p},z,z')$$

$$=-i\Lambda(0)\,(\theta(z)-\theta(z'))f(\mathbf{p},z,z')$$

$$+\theta(z)\theta(z')\int\frac{d^3q}{(2\pi)^2}$$

$$\times\sum_j\sigma_j(\mathbf{q},-\mathbf{q})\,\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}-E_{j0})f(\mathbf{p}+\mathbf{q},z,z')$$

$$-\frac{\theta(z)+\theta(z')}{2}\int\frac{d^3q}{(2\pi)^2}$$

$$\times\sum_j\sigma_j(\mathbf{q},-\mathbf{q})\,\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}+E_{j0})f(\mathbf{p},z,z') \tag{3.2}$$

with the boundary condition

$$f(\mathbf{p},\ z,\ z')=\delta(\mathbf{p}-\mathbf{\Pi})\qquad z,\ z'<0. \tag{3.3}$$

The function $\theta(z)$ in (3.2) is equal to 1 for $0<z<L$ and equal to 0 outside the plate.

Since the plate thickness satisfies $L\lesssim l_{tr}$, and the electron scattering cross section has a sharp maximum in the "forward" direction, we may ignore the reflection of particles from the medium in solving (3.2), (3.3).

Denoting by $A(\mathbf{p},\mathbf{\Pi},z)$ the solution corresponding to (3.2) of transport equation (2.15), with boundary condition (2.16), we can find $f(\mathbf{p},z,z')$ by the method of characteristics:

$$f(\mathbf{p},z,z')=\exp\left(-i(z-z')\,\frac{m\Lambda(0)}{(\mathbf{\Pi n})}-|z-z'|\,\frac{m\Gamma}{2(\mathbf{\Pi n})}\right)$$

$$\times A(\mathbf{p},\mathbf{\Pi},\min(z,z')), \tag{3.4}$$

$$0<z,z'<L;$$

$$f(\mathbf{p},z,z')=\exp(-i(z-z')\,m\Lambda(0)\left(\frac{1}{(\mathbf{\Pi n})}-\frac{1}{(\mathbf{pn})}\right)$$

$$\times\exp\left(-|z-z'|\frac{m\Gamma}{2}\left(\frac{1}{(\mathbf{\Pi n})}+\frac{1}{(\mathbf{pn})}\right)\right)$$

$$\times A(\mathbf{p},\mathbf{\Pi},L-|z-z'|)\quad z,z'>L,$$

$$|z-z'|<L; \tag{3.5}$$

where

$$\Gamma=\int\frac{d^3q}{(2\pi)^2}\sum_j\sigma_j(\mathbf{q},-\mathbf{q})\,\delta(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}+E_{j0})$$

is the total scattering cross section.

According to (1.4), we can express the mutual coherence function in terms of $f(\mathbf{p},z,z')$ from (3.1)–(3.3):

$$\rho(\mathbf{r},\mathbf{r}')=\int\frac{d^3p}{(2\pi)^3}\exp(i\mathbf{p}(\mathbf{r}-\mathbf{r}'))f(\mathbf{p},z,z'). \tag{3.6}$$

It can be seen from (3.4)–(3.5) that when the vacuum-medium interface is abrupt (in comparison with the mean free path v/Γ) the function $f(\mathbf{p},z,z')$ does not reduce to a function of the single variable $R=(r+r')/2$, as was assumed in Refs. 7 and 8. Furthermore, $f(\mathbf{p},z,z')$ is not a solution of the transport equation, and even in the small-angle approximation $(\mathbf{pn})\approx(\mathbf{\Pi n})$ it differs from $A(\mathbf{p},\mathbf{\Pi},z)$ in that it contains a factor which decays exponentially rapidly in the longitudinal direction:

$$\rho(z,z')\sim f(\mathbf{p},z,z')\sim\exp\left(-|z-z'|\,\frac{m\Gamma}{(\mathbf{\Pi n})}\right). \tag{3.7}$$

The reason for the onset of this behavior is the loss of the mutual coherence of the electron wave functions at a distance exceeding the mean free path $l_{\text{mf}}=v/\Gamma$.

The results in (3.4)–(3.6) may be pertinent to experiments carried out to measure quantum correlation effects.[18,19]

4. REFLECTION OF FAST ELECTRONS FROM A SINGLE CRYSTAL IN THE CASE OF INCOHERENT MULTIPLE SCATTERING

At glancing angles $\vartheta>5°$ of the incident beam we may ignore the diffraction of the electrons by crystallographic planes running parallel to the surface. The reflection of the particles in this case occurs through incoherent multiple scattering, for which the primary mechanism is the quasielastic scattering by thermal fluctuations of the crystal potential.[20] Because of the pronounced anisotropy of the cross section for incoherent electron scattering, the numerous theories based on the model of single collisions yield only qualitative results (these studies are reviewed by Humphreys[15]). Spencer and Humphreys[21] have constructed a phenomenological description of multiple-scattering processes with the help of an inhomogeneous transport equation. However, that description ignores the coherence of the wave field of the incident electrons, so that incorrect expressions are derived for the sources [expression (6) in Ref. 21]. That study also ignores the energy loss, which significantly reduces the total reflection coefficient. Furthermore, none of these theo-

retical papers has succeeded in calculating those orientational effects in the angular distribution of reflected electrons which result from the diffraction of the incoherent wave field by the crystallographic planes.[23,24]

To calculate the distribution of electrons reflected from a single crystal in the case of incoherent multiple scattering, we use Eq. (2.6) with boundary condition (2.12). The wave field of the electrons in a crystal can be resolved into an incoherent component—the field of the particles which have undergone inelastic scattering—and a coherent component—the field which is phase-matched with the plane wave incident on the crystal. The coherent field consists of both the transmitted wave and the waves reflected through diffraction by the regular array of atoms, and it is described by the set of functions

$$\{W_{lh}(\mathbf{r},\mathbf{r}')\}=\{W(\Pi+\mathbf{G}_l;\ \Pi+\mathbf{G}_h;\ \mathbf{r},\ \mathbf{r}')\}, \tag{4.1}$$

where $\{\mathbf{G}_l\}$ is the set of reciprocal-lattice vectors of the crystal. Since inelastic processes lead to only an escape of particles from the states of the coherent field, a system of equations for W_{lh} can be found from (2.6):

$$\left(\frac{\Pi+\mathbf{G}_l}{m}\frac{\partial}{\partial\mathbf{r}}+\frac{\Pi+\mathbf{G}_h}{m}\frac{\partial}{\partial\mathbf{r}'}\right)W_{lh}+i(\varepsilon_l-\varepsilon_h)W_{lh}$$
$$=-i\theta(\mathbf{r})\sum_s\left(\Lambda_{ls}-\frac{i}{2}\gamma_{ls}{}^h\right)W_{sh}+i\theta(\mathbf{r}')$$
$$\times\sum_s W_{ls}\left(\Lambda_{sh}+\frac{i}{2}\gamma_{sh}{}^l\right) \tag{4.2}$$

with boundary condition (2.12),

$$W_{sl}(r,\ r')=\delta_{s0}\delta_{l0};\quad r,\ r'\notin\Omega, \tag{4.3}$$

where

$$\Lambda_{ls}=\Lambda(\mathbf{G}_l-\mathbf{G}_s);\quad \varepsilon_l=(\Pi+\mathbf{G}_l)^2/2m,$$
$$\gamma_{ls}{}^h=\int\frac{d^3p}{(2\pi)^2}\sum_j\sigma_j(\Pi+\mathbf{G}_l-\mathbf{p},\ \mathbf{p}-\Pi-\mathbf{G}_s)\,\delta(\varepsilon_p-\varepsilon_l+E_{j0}).$$

It can be seen from (4.2) that the inelastic scattering gives rise to imaginary increments in the Fourier components of the regular crystal potential, (2.8), in the equations for the coherent field.[25,26]

The diffraction of incoherently scattered electrons gives rise to narrow Kikuchi bands with an angular width

$$\vartheta_K\sim G/\Pi\ll\varkappa/\Pi\sim\vartheta_{\text{sngl. sc}} \tag{4.4}$$

against the diffuse multiple-scattering background.[23] By virtue of (4.4), we can ignore the diffraction of the incoherent field in a first approximation. An equation for the distribution function of the inelastically scattered electrons, $C(\mathbf{p},\mathbf{r})=W_{\text{in}}(\mathbf{p},\mathbf{p};\mathbf{r},\mathbf{r})$, can then be found from (2.6) with (4.2):

$$\frac{\mathbf{p}}{m}\frac{\partial}{\partial r}C(\mathbf{p},\mathbf{r})$$
$$=\int\frac{d^3q}{(2\pi)^2}\sum_j\sigma_j(\mathbf{q},-\mathbf{q})\,(C(\mathbf{p}+\mathbf{q},\mathbf{r})\,\delta(\varepsilon_{p+q}-\varepsilon_p-E_{j0})$$
$$-C(\mathbf{p},\mathbf{r})\,\delta(\varepsilon_{p+q}-\varepsilon_p+E_{j0}))$$
$$+\frac{1}{(2\pi)^2}\sum_{h,l}\sum_j\sigma_j(\Pi+\mathbf{G}_l-\mathbf{p},\ \mathbf{p}-\Pi-\mathbf{G}_h)\,W_{hl}(\mathbf{r},\mathbf{r}) \tag{4.5}$$
$$\times\frac{1}{2}\{\delta(\varepsilon_p+E_{j0}-\varepsilon_h)+\delta(\varepsilon_p+E_{j0}-\varepsilon_l)\}.$$

By solving this inhomogeneous kinetic equation with the boundary condition[22]

$$C(\mathbf{p},\mathbf{r})=\begin{cases}0; & (\mathbf{pn})>0\\ S(\mathbf{p}); & (\mathbf{pn})<0\end{cases}$$

for $\mathbf{r}$ at the boundary of Ω, we can find the total reflection coefficient for the electrons as a function of the orientation of the initial particle beam with respect to the atomic planes of the crystal (this function is called the "channeling pattern"[21,23]). Here the orientational effects are determined by the matrix elements of the coherent field, (4.1). Integrating (4.5), and summing with the diagonal elements in (4.2), we find the semiclassical flux conservation law

$$\operatorname{div}\left(\int\frac{\mathbf{p}}{m}C(\mathbf{p},\mathbf{r})\,d^3p+\sum_h\frac{\Pi+\mathbf{G}_h}{m}W_{hh}(\mathbf{r},\mathbf{r})\right)=0. \tag{4.6}$$

Equation (4.6) shows that the escape of particles from the states of the coherent field serves as sources in transport equation (4.5). Accordingly, with an increase in the depth to which the electrons of the coherent field penetrate into the crystal under anomalous-transmission conditions,[5,26] for example, there will be a decrease in the total particle reflection coefficient.

5. DIFFRACTION EFFECTS IN THE DISTRIBUTION OF BACK-SCATTERED ELECTRONS

The diffraction of the incoherently scattered electrons leads to the formation of a fine structure in the distribution of reflected particles near the Bragg directions corresponding to close-packed crystallographic planes. This effect, known as "back-scattering patterns" or "Kikuchi patterns,"[23,24] is exploited for precise orientation of bulk single-crystal samples.

Let us consider electrons which are moving out of the interior of a single crystal toward a surface nearly along a Bragg direction corresponding to reflection through a reciprocal-lattice vector $\mathbf{G}$. Under the "weak-coupling condition"[27]

$$G^2/2m|\Lambda(G)|\gg 1 \tag{5.1}$$

the local change which occurs in the reflected background can be derived analytically in the two-wave approximation of the theory of diffraction.[5] Here the off-diagonal elements of $W(\mathbf{p}+\mathbf{G},\mathbf{p},\mathbf{r},\mathbf{r}')$ $W(\mathbf{p},\mathbf{p}+\mathbf{G};\mathbf{r},\mathbf{r}')$ must be taken into account in (2.6). Denoting the deformation of the background near the $\mathbf{p}$ and $\mathbf{p}+\mathbf{G}$ directions by

$$\varphi(\mathbf{p},\ z)=W(\mathbf{p},\ \mathbf{p};\ z,\ z)-C(\mathbf{p},\ z),$$
$$\chi(\mathbf{p}+\mathbf{G},\ z)=W(\mathbf{p}+\mathbf{G},\ \mathbf{p}+\mathbf{G};\ z,\ z)-C(\mathbf{p}+\mathbf{G},\ z), \tag{5.2}$$

respectively, and using (4.4), we find the following system of equations in the small-angle approximation:

$$w\frac{\partial}{\partial z}\varphi=-\Gamma\varphi+i\Lambda(\beta-\alpha)-\frac{\gamma}{2}(\alpha+\beta),$$
$$w\frac{\partial}{\partial z}\chi=-\Gamma\chi+i\Lambda(\alpha-\beta)-\frac{\gamma}{2}(\alpha+\beta), \tag{5.3}$$
$$w\frac{\partial}{\partial z}\alpha+iE\alpha=-\Gamma\alpha+i\Lambda(\varphi-\chi)-\frac{\gamma}{2}(\varphi+\chi)+w\frac{\partial}{\partial z}C(\mathbf{p},z),$$

$$w\frac{\partial}{\partial z}\beta - iE\beta = -\Gamma\beta + i\Lambda(\chi-\varphi) - \frac{\gamma}{2}(\varphi+\chi) + w\frac{\partial}{\partial z}C(\mathbf{p},z),$$

where

$$\varphi(\infty)=\chi(\infty)=\alpha(\infty)=\beta(\infty)=0,$$
$$w=\frac{(\mathbf{pn})}{m}\approx\frac{(\mathbf{p}+\mathbf{G},\mathbf{n})}{m}=v\mu<0,\quad E=\varepsilon_{\mathbf{p}+\mathbf{G}}-\varepsilon_{\mathbf{p}},$$
$$\Lambda=\Lambda(\mathbf{G})=\Lambda_{10}=\Lambda_{01};\quad \gamma=\gamma_{10}=\gamma_{01},$$

and the z axis runs along the inward normal ($\mathbf{n}$) to the surface of the crystal.

Equations (5.3) can be solved at $z = 0$ by Laplace transforms:

$$\varphi(\mathbf{p},0)=-\int_0^\infty dxw\frac{\partial C}{\partial z}\Big|_{x|w|}e^{-\Gamma x}\left\{\frac{1}{(1+y^2)^{1/2}}\operatorname{sh}\left(\frac{\gamma x}{(1+y^2)^{1/2}}\right)\right.$$
$$\left.+\frac{y}{1+y^2}\left[\operatorname{ch}\left(\frac{\gamma x}{(1+y^2)^{1/2}}\right)-\cos(2\Lambda(1+y^2)^{1/2}x)\right]\right\}, \tag{5.4}$$

where $y = (\varepsilon_{\mathbf{p}+\mathbf{G}} - \varepsilon_{\mathbf{p}})/2\Lambda$. The expression for $\chi(\mathbf{p}+\mathbf{G}, 0)$ differs from (5.4) in the sign of y.

Since the scale length for a change in $C(\mathbf{p}, z)$ is the transport length $l_{tr} \gg l_{mf} = v/\Gamma$, we can calculate a specific result in (5.4):

$$\varphi(\mathbf{p},0)\approx\mu\frac{v}{\Gamma}\frac{\partial}{\partial z}C(\mathbf{p},z)|_{z=+0}I(y), \tag{5.5}$$

where the universal function $I(y)$ is

$$I(y)=\frac{y}{1+y^2}\frac{1}{1+(2\Lambda/\Gamma)^2(1+y^2)}-\frac{y+\gamma/\Gamma}{1+y^2-\gamma^2/\Gamma^2}. \tag{5.6}$$

To determine the contrast of a Kikuchi band which arises on a photographic plate near a Bragg direction, we must integrate (5.5) over the absolute value of p at a fixed observation direction. Since the energy spectrum of the reflected electrons has a sharp maximum near the initial energy,[22,23] we find

$$\mathcal{K}(y)=\mu\frac{v}{\Gamma}\frac{\partial}{\partial z}\ln C|_{z=+0}I(y). \tag{5.7}$$

The angular distribution of reflected electrons near the copper (220) Bragg direction calculated from (5.7) is shown in Fig. 1. To calculate the logarithmic derivative of the average field at the surface of the crystal, we used the results of Ref. 22, estimating the scattering cross sections for a screened Coulomb potential in Einstein's thermal-motion model.[5,20]

The shape of the Kikuchi band in Fig. 1 agrees qualitatively with the observations of Refs. 23 and 24. Unfortunately, there has been no detailed experimental analysis of the electron back-scattering patterns, so that we cannot make a quantitative comparison with (5.7).

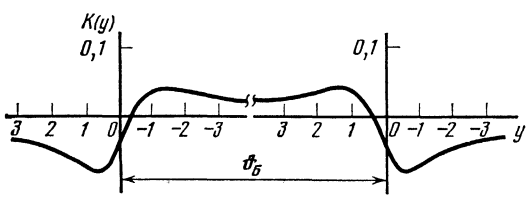

FIG. 1. Contrast of a (220) Kikuchi band in the reflection of 20-keV electrons from a copper single crystal. The reflection parameters Γ, γ, and Λ correspond to the experimental values in Ref. 28.

6. CONCLUSION

A stationary quantum kinetic equation for an inhomogeneous scattering medium (a crystal or an amorphous medium) has been derived in the "locally eikonal" approximation, (1.4), which is also introduced in this paper. The resulting kinetic equation, Eq. (2.6), incorporates the coherent diffraction by the regular array of atoms, on the one hand, and the incoherent scattering by thermal fluctuations and the ionizational energy loss, on the other. An expression has been derived for the mutual coherence function, (3.4)–(3.6), for the problem of the passage of particles through a thin plate of an amorphous medium with a sharp boundary. The longitudinal coherence is shown to be determined by the mean free path of the particles in the medium. A system of equations has been derived for determining the orientational dependence of the coefficient for the back scattering of electrons with an energy on the order of a few tens of keV from a single crystal [Eqs. (4.2)–(4.5)]. The angular distribution of reflected particles near Bragg directions has been derived in the two-wave approximation of a dynamic theory [Eqs. (5.5)–(5.7)].

It has thus been shown that the locally eikonal approximation in a quantum kinetic equation makes it a comparatively simple matter to solve several stationary scattering problems in inhomogeneous media which present difficulties in attempts to find solutions by other methods.[2–8]

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