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ELECTRON SCATTERING AND THE CONDUCTIVITY OF A FILM WITH SURFACE DEFECTS

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The decay of electron states and the conductivity of a quantum or classical film with surface defects (impurities, surface roughness) are investigated. Scattering by widely-spaced roughnesses reduces to scattering by potential centers randomly distributed over the surface. The amplitude of scattering from a surface center in the film is determined in the approximation in which the transverse center dimension is small compared with the film thickness. Boundary conditions for the electron distribution function are found for a classical film. The dependence of the film conductivity on the film thickness is discussed.

THERE are many papers devoted to a theoretical description of the influence of scattering from the surface on the kinetics of electrons in a film. These papers can be divided into two groups. One group[1-4] considers classical films, in which the film thickness a is large compared with the characteristic wavelength of the electron. For such films, it is possible to use a classical distribution function $n(\mathbf{r}, \mathbf{p})$ satisfying the kinetic equation inside the film and a certain boundary condition on its averaged surface. The simplest boundary condition of this type is the condition that the total particle flux through the surface S vanish:[3]

$$\int \mathbf{p}\mathbf{n}n(\mathbf{r} \in S, \mathbf{p})\, d^3p = 0, \tag{1}$$

where $\mathbf{n}$ is the normal to the surface. However, being an integral condition, it does not yield complete information for the determination of the conductivity and other kinetic coefficients. It is therefore necessary to use model assumptions concerning the isotropic distribution of the scattered particles (total or partial "diffuseness"),[3,4] or to connect the boundary condition on the distribution function with the microscopic scattering mechanism:[1,2]

$$n(\mathbf{r}, \mathbf{p}) = \int n(\mathbf{r}, \mathbf{p}')\, \alpha(\mathbf{p}', \mathbf{p})\, \delta(E(p) - E(p'))\, d^3p',$$
$$\mathbf{p}\mathbf{n} > 0, \quad \mathbf{p}'\mathbf{n} < 0, \quad \mathbf{r} \in S. \tag{2}$$

The function $\alpha(\mathbf{p}', \mathbf{p})$ describes scattering by the surface, which is assumed to be elastic; $\alpha(\mathbf{p}', \mathbf{p})$ should conserve the number of particles and make Eq. (2) an identity when the equilibrium distribution function is substituted. This imposes on $\rho(\mathbf{p}', \mathbf{p})$ the limitations:

$$\mathbf{p}'\mathbf{n} = -\int \mathbf{p}\mathbf{n}\alpha(\mathbf{p}', \mathbf{p})\, \delta(E(p) - E(p'))\, d^3p, \tag{3}$$

$$\int \alpha(\mathbf{p}', \mathbf{p})\, \delta(E(p) - E(p'))\, d^3p' = 1. \tag{4}$$

However, the form of the scattering function and its connection with the transition probability have been determined so far quasiclassically,[1,5,6] or else from semi-intuitive consideration.[2]

Another group of papers[7-9] considers a quantum film with a slightly-roughened surface. The applicability of the results of these papers is limited to the condition that the height of the roughnesses be small compared with the transverse wavelength of the electron, a condition apparently rather rarely satisfied.

In this paper we consider the relaxation of the electron states and the conductivity of a quantum film with isotropic dispersion in the presence of surface defects. The boundary condition on the carrier distribution function is obtained in the classical limit. The scattering of the electrons by volume defects is neglected (the film thickness a is much smaller than the volume mean free path). If the normal component of the electron momentum is much smaller than the reciprocal interatomic distance, then the boundary condition for the wave function on the surface has the form $\psi(\mathbf{r} \in S) = 0$. The problem of scattering by a rough surface is then equivalent to the problem of scattering on potential centers distributed along the surface, with a potential that is infinite in a limited spatial region, outside of which the potential vanishes. Indeed, when the potential tends to infinity the wave function will tend to zero on the boundary of this region.

1. RELAXATION TIME OF THE ELECTRON STATES

We consider a quantum film occupying the region $0 \le z \le a$; on the surface $z = 0$ there are potential centers with potential

$$V(\rho, z) = \sum_i u(\rho - \rho_i, z).$$

The coordinates of the centers $\rho_i = (x_i, y_i, 0)$ are distributed randomly and independently, and have a density c. The second surface, for simplicity, is assumed to be specular.

As is well known, the relaxation of the electron states and the conductivity are determined by the mean values of the Green's function and its derivatives averaged over the positions of the centers.[10] In the representation of the eigenfunctions of the unperturbed problem, the equation for the Green's function is

$$G_{nn'}(\mathbf{p}, \mathbf{p}') = \delta_{nn'}\delta(\mathbf{p} - \mathbf{p}')\, G_n{}^0(p)$$
$$+ (2\pi)^{-2} G_n{}^0(p) \sum_{i,n_1} \int u_{nn_1}(\mathbf{p} - \mathbf{p}_1)\, G_{n_1n'}(\mathbf{p}_1, \mathbf{p}') \exp\{i(\mathbf{p} - \mathbf{p}_1)\rho_i\}\, d^2p_1. \tag{5}$$

Here **p** and **p**′ are the longitudinal momenta, n and n′ the transverse quantum numbers

$$G_n^0(p) = [E - E_n(p) + i\delta]^{-1}, \quad E_n(p) = {}^1/_2 p^2 + {}^1/_2 \pi^2 n^2 a^{-2},$$

and $u_{nn'}(\mathbf{p})$ is the matrix element of the potential of one center.

The usual diagram technique is obtained for the average Green's function.[9] Summation of diagrams with unclosed dotted lines corresponds to the potential produced by the centers (bending of the bands), and therefore leads to an immaterial renormalization of the energy eigenvalues $E_n(p)$ and of the matrix elements $u_{nn'}(\mathbf{p})$. In the approximation when the self-energy part $\Sigma_{nn'}(\mathbf{p})$ satisfies the inequalities

$$\Sigma_{nn'}(p) \ll E_{n+1}(p) - E_n(p) = \Delta E, \quad \Sigma_{nn}(p) \ll E_n(p), \tag{6}$$

the Green's function contains only diagonal elements in the essential energy region $E - E_n(p) \sim \operatorname{Im} \Sigma_{nn}(p)$:

$$G_{nn'}(p, p') = \delta(p - p')\{(2\pi)^2 \delta_{nn'}[E - E_n(p) - \Sigma_{nn}(p) + i\delta]^{-1} + o(\Sigma_{nn'}/\Delta E)\}. \tag{7}$$

For the relaxation time of the electron state we obtain

$$\tau^{-1} = \operatorname{Im} \Sigma_{nn}(p). \tag{8}$$

Let us find τ for scattering by screened Coulomb centers. When the screening radius q_0^{-1} is smaller than the film thickness, the screening occurs as in an unbounded sample:

$$u(r) = \frac{e^2}{\varepsilon r} \exp(-q_0 r). \tag{9}$$

In the Born approximation we have

$$u \ll [kq_0, \; q_0^4/k^2], \qquad k = \sqrt{2E}, \tag{10}$$

$$\Sigma_{nn_1}(p) = c(2\pi)^{-2} \sum_{n'} \int d^2p' G_{n'}^0(p') u_{nn'}(\mathbf{p} - \mathbf{p}') u_{n'n_1}(\mathbf{p}' - \mathbf{p}). \tag{11}$$

If only one subband of transverse quantization is filled, then the electron energy lies in the range $2\pi^2/a^2 > E > \pi^2/2a^2$, only one term with $n' = n + 1$ remains of the sum (11), and

$$\tau^{-1} = 2\pi^2 e^4 c / \varepsilon^2 a^6 q_0^8. \tag{12}$$

In the opposite classical case $(E \gg 2\pi^2/a^2)$ it is possible to go over in (11) to integration with respect to $p_z = n\pi/a$, and

$$\tau^{-1} = \frac{(2\pi)^2 e^4 kc}{\varepsilon^2 a} \left\{ \frac{2}{q_0^2(q_0^2 + 4k^2)} - \frac{1}{k^2 \cos\theta} \frac{1}{\sqrt{A}} \times \ln \frac{2A + B + 2(q_0^2 + k^2\cos\theta)\sqrt{A}}{2A - B + 2(q_0^2 - k^2\cos\theta)\sqrt{A}} \right\}, \tag{13}$$

where

$$\mathbf{k} = (\mathbf{p}, \mathbf{p}_z), \; \cos\theta = p_z/k, \; A = q_0^4 - k^4 \sin^2\theta, \; B = 2q_0^2 k^2 \cos\theta.$$

In the limit as $q_0 \gg k$, we obtain

$$\tau^{-1} = 2^7 \pi^3 e^4 p_z^2 k^3 c / 3a\varepsilon^2 q_0^8. \tag{14}$$

In semiconductors usually $q_0 \ll k$. The time of relaxation of the electron state depends in this case strongly on the angle between the surface and **k**:

$$\tau^{-1} = 2\pi^3 e^4 c / a\varepsilon^2 k q_0^2 \tag{15}$$

At not too slow a decrease $(p_z \gg q_0)$, and

$$\tau^{-1} = (2\pi)^3 e^4 p_z^2 c / 3a\varepsilon^2 q_0^4 k \tag{16}$$

when $p_z \ll q_0$.

The Born approximation is not applicable to scattering by roughnesses, since the perturbation potential becomes infinite. It is therefore necessary to sum diagrams containing more than two dashed lines per center (see [10]). The self-energy part is expressed in terms of the vertex part $\Gamma_{nn'}(\mathbf{p}, \mathbf{p}', E)$:

$$\Sigma_{nn'}(\mathbf{p}) = c\Gamma_{nn'}(\mathbf{p}, \mathbf{p}, E),$$

which satisfies the equation

$$\Gamma_{nn'}(\mathbf{p}, \mathbf{p}', E) = u_{nn'}(\mathbf{p} - \mathbf{p}') - \sum_{n_1} \int \frac{d^2 p_1}{(2\pi)^2} \times \frac{u_{nn_1}(\mathbf{p} - \mathbf{p}_1)\Gamma_{n_1 n'}(\mathbf{p}_1, \mathbf{p}', E)}{E - E_{n_1}(p_1) + i\delta} \tag{17}$$

Comparing (17) with (A.3), we see that when $E - E_n(p) \ll E_n(p)$, the quantity $2a\pi^{-1}\Gamma_{nn'}(\mathbf{p}, \mathbf{p}', E)$ coincides with the amplitude $F_{nn'}(\mathbf{p}, \mathbf{p}')$ for scattering by a surface center.

We confine ourselves to the case of a centrally-symmetrical potential of a center. The corresponding surface roughnesses have the form of hemispherical craters of different radii. The final result is averaged over the dimension of the crater. Using the known formulas for the amplitude of scattering by a solid sphere, we obtain for the relaxation time the following results (we confine ourselves to the case of a classical film):

1. Radius of crater r much smaller than the wavelength k^{-1} $(rk \ll 1)$,

$$\tau^{-1} \approx \frac{3\pi^2}{2^3 a} p_z^2 k^3 \langle r^6 \rangle c; \tag{18}$$

2. $rk \gg 1$,

$$\tau^{-1} \approx \begin{cases} \pi/a \, \langle r^2 \rangle \, kc, & \text{if} \quad p_z r \gg 1, \\ \pi/8a \, \langle r^4 \rangle \, p_z^2 kc, & \text{if} \quad p_z r \ll 1. \end{cases} \tag{19}$$

2. CONDUCTIVITY

The conductivity is expressed in terms of the electron Green's function with the aid of the Greenwood–Peierls formula in the same manner as in [9]:

$$\sigma = -4\pi e^2 \sum_{n,m} \int \mathbf{q}\mathbf{p} \langle \tilde{G}_{nm}(\mathbf{p}, \mathbf{q}) \tilde{G}_{mn}(\mathbf{q}, \mathbf{p}) \rangle \frac{\partial f_0}{\partial E} \frac{d^2 p \, d^2 q}{(2\pi)^4} dE, \tag{20}$$

where $\bar{G} = G_R - G_A$ is the difference between the retarded and advanced Green's function, obtained in the first part of the paper; $f_0(E)$ is the Fermi distribution function per unit volume.

Without stopping to discuss the intermediate calculations, we present the final formulas obtained in the approximation (6):

$$\sigma = -4\pi e^2 \sum_n \int \frac{M_n(p)}{\operatorname{Im} \Sigma_{nn}(p)} \frac{\partial f_0}{\partial E} \delta(E - E_n(p)) \, d^2 p \, dE; \tag{21}$$

$M_n(p)$ is defined by the equation

$$M_n(p) = p^2 + c \sum_l \int |F_{nl}(\mathbf{p}, \mathbf{p}_1)|^2 \frac{\mathbf{p}\mathbf{p}_1}{p_1^2} d\varphi \frac{M_l(p_1)}{\operatorname{Im} \Sigma_{ll}(\mathbf{p}_1)},$$
$$p_1^2 + \frac{\pi^2 l^2}{a^2} = p^2 + \frac{\pi^2 n^2}{a^2}, \quad \cos\varphi = \frac{\mathbf{p}\mathbf{p}_1}{pp_1}. \tag{22}$$

In the limit of a thick film, the sums in (21) and (22) go over into integrals, $\sum \rightarrow a\pi^{-1}\int dp_z$. The approximation (6) remains in force, since the condition $\Sigma_{nn_1} \gg \Delta E$ does not depend on the film thickness. Indeed, according to (A.4), in the classical limit

$$\operatorname{Im}\Sigma_{nn'}(p)=c\frac{\pi}{2a}\operatorname{Im}\left[f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right]$$
$$\equiv c\frac{\pi}{2a}\cdot\frac{k}{4\pi}\int d\Omega'\left|f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right|^2,$$

while $\Delta E \sim p_z/a$ and (6) reduces to the inequality

$$c\frac{\mathbf{k}}{p_z}\int d\Omega'\left|f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right|^2\ll 1,\quad \tilde{f}\equiv f\left(\frac{\mathbf{k}\tilde{\mathbf{k}}'}{k^2}\right). \qquad (23)$$

This condition requires that the scattering cross sections of individual centers, projected on the surface of the film, must not overlap. From (14), (16), (18), and (19) we see that (23) is satisfied also at small values of p_z (glancing incidence).

On the other hand, the problem of determining the conductivity of a classical film reduces to a solution of the kinetic equation for the distribution function $n(\mathbf{r}, \mathbf{p})$ with boundary condition (2). In this case we obtain for the conductivity

$$\sigma=ae^2\int\frac{\partial f_0}{\partial E}\left(2D(k)-\frac{p^2}{p_z}\right)d^3k, \qquad (24)$$
$$\mathbf{k}=(\mathbf{p},\ p_z),\quad E=k^2/2,$$

where the functions $D(\mathbf{k})$ are defined by

$$D(k)=\frac{p^2}{p_z}+2\int\alpha(\mathbf{k}',\mathbf{k})\delta(k'^2-k^2)\frac{\mathbf{pp}'}{p'^2}D(k')d^3\mathbf{k}', \qquad (25)$$

and $\alpha(\mathbf{k}', \mathbf{k})$ is taken from the boundary condition (2)

We separate explicitly in the scattering function $\alpha(\mathbf{k}', \mathbf{k})$ the specular part $1-\bar{\alpha}(\mathbf{k})$:

$$2\delta(k'^2-k^2)\alpha(\mathbf{k}',\mathbf{k})=(1-\bar{\alpha}(k))\delta(\mathbf{k}'-\mathbf{k})+2\alpha_1(\mathbf{k}',\mathbf{k})\delta(k'^2-k^2). \qquad (26)$$

Substituting (26) in (25) and comparing with the corresponding quantum formulas (with allowance for (A.4)), we find that $\alpha(\mathbf{k}', \mathbf{k})$ is expressed in terms of the amplitude for scattering by surface centers

$$\bar{\alpha}(\mathbf{k})=\frac{4\pi}{p_z}c\operatorname{Im}\left[f(1)-f\left(\frac{\mathbf{k}\tilde{\mathbf{k}}}{k^2}\right)\right],$$
$$\alpha_1(\mathbf{k}',\mathbf{k})=\frac{c}{p_z}\left|f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right|^2. \qquad (27)$$

This form of the scattering function satisfies the conditions (3) and (4).

It is easy to understand the physical meaning of the results. In one unit of time, $p_z n(k)$ particles are emitted from a unit surface area in the direction of $\mathbf{k}$; from among these particles,

$$c\int k\left|f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right|^2 n(k')\,d\Omega'$$

are scattered and

$$p_z n(\tilde{k})-cn(\tilde{k})\int k\left|f\left(\frac{\mathbf{kk}'}{k^2}\right)-\tilde{f}\right|^2 d\Omega'$$

are reflected specularly. Comparing with (26) and using the optical theorem, we get formulas (27).

3. DISCUSSION

The results of this paper are valid in the "gas" approximation (6). We note that in this approximation it is easy to take into account also the potential centers that are distributed in the volume of the film. Indeed, the amplitude for scattering in the film, given in Appendix 1, is applicable also to the description of scattering by centers inside the film. The final result must only be averaged over the transverse coordinate of the scattering centers. The entire diagram technique remains the same as before, Σ consists of two independent parts, Σ_S and Σ_V, which are connected respectively with the surface and volume scattering, and the reciprocal relaxation times are additive.

It is interesting to trace the transition to a nonquantum film in the formulas for the relaxation time and the conductivity. As expected, when averaging over the transverse coordinates of the impurities, the nondiagonal matrix elements in Σ_V vanish, and condition (6) assumes the usual form $\Sigma_V(\mathbf{p}) \ll E$.

Thus, the approach of the present paper makes it possible in principle to determine various kinetic coefficients in the film. However, for classical films it is more convenient to solve the kinetic equation with the corresponding boundary conditions. The obtained boundary condition (27) and (2) is linear in the distribution function, in accordance with the Greenwood–Peierls formula. The linearity of the boundary condition corresponds to linearity of the collision term in the kinetic equation in the case of elastic scattering. Green's nonlinear boundary condition[2] is apparently the consequence of an incorrect allowance for the Pauli principle.

The boundary condition (2) and (27) simplifies greatly if the amplitude for scattering by a surface center is isotropic in the plane of the film (the case of a center whose dimension is small compared with the wavelength), and the nonequilibrium part of the distribution function of the electrons incident on the surface of the film is proportional to the electron-momentum component parallel to the surface. This is satisfied, for example, in the problem of the conductivity of the film with impurities. We obtain a boundary condition of the type given by Fuchs,[4]

$$n(\mathbf{r},\ \mathbf{k})=(1-\bar{\alpha}(\mathbf{k}))n(\mathbf{r},\ \tilde{\mathbf{k}}),\quad \mathbf{kn}>0.$$

As seen from (14), (16), (18), (19), and (27), the diffuseness coefficient $\bar{\alpha}(\mathbf{k})$ depends strongly on p_z, vanishing like $\bar{\alpha}(\mathbf{k}) \sim p_z$.

This result has apparently a general character. Indeed, the model of [9] can be employed for values of p_z small compared with the reciprocal height of the surface roughness. The relaxation time obtained in [9] determines the diffuseness coefficient in accordance with the formula

$$\bar{\alpha}(\mathbf{k})=T/\tau, \qquad (28)$$

where $T = 2a/p_z$ is the period of the transverse motion of the particle. Using the results of [9], we see that $\bar{\alpha} \sim p_z$ at small p_z. Physically this is attributed to the well known phenomenon that a rough surface is specular with respect to waves incident on it at a small angle.

If we investigate the conductivity of a film with a transverse bending of the bands,

$$T=\oint dz/\sqrt{2E-p^2-2\varphi(z)}$$

($\varphi(z)$ is the potential energy of the electron in the transverse electric field), $\bar{\alpha}$ as a function of the momentum of the particle near the wall remains the same as before if the characteristic of the center is smaller than the region of the transverse motion. Then (28) yields the dependence of the relaxation time on the magnitude of the bending of the bands.

If the scattering from the surface is isotropic in the plane of the film, then the mobility μ_f in a classical film is expressed in terms of the relaxation time in the usual manner

$$\mu_f = -\frac{e^2}{2}\int \frac{\partial f_0}{\partial E} p^2 \tau_S(k)\, d^3k\, (2\pi)^{-3}. \tag{29}$$

Here $\tau_S(k)$ is the previously-obtained relaxation time in scattering by surface centers (see formulas (14), (16), (18), and (19)). At small p_z, the integral in (29) diverges like p_z^{-1}. The divergence is connected with neglect of quantization and with volume scattering mechanisms. As shown above, when volume scattering is taken into account, the relaxation time is determined by the formula

$$\tau^{-1} = \tau_S^{-1} + \tau_V^{-1}$$

(τ_V is the volume relaxation time). If $\tau_V \ll \tau_{0S}$, where τ_{0S} is the minimum value of τ_S as a function of p_z, then the conductivity of the sample is determined only by the value of scattering.

Let us consider the case $\tau_V \gg \tau_{0S}$. If $\tau_V \gg \tau_{0S}\pi^2 \times \pi^{-2} \min(1/b^2, k^2)$, where $b = r, q_0^{-1}$, then the lower limit of integration in (29) is determined by quantization of the transverse motion, and $\mu_f/\mu_V \sim \tau_{0S}/\tau_V$. If $\tau_V \ll \tau_{0S} a^2 \pi^{-2} \min[1/b^2, k^2]$, then the integration limit is determined by the volume scattering and $\mu_f/\mu_V \sim \sqrt{\tau_{0S}/\tau_V}$. As seen from these formulas, the well known result

$$\frac{\mu_f}{\mu_V} \sim \frac{\tau_{0S}}{\tau_V} \ln \frac{\tau_V}{\tau_{0S}},$$

which has been derived for the case of fully diffuse scattering,[1] does not hold in this approximation in any region of the parameters.

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APPENDIX 1

SCATTERING BY A SURFACE CENTER IN A FILM

In analogy with the amplitude of scattering in an infinite volume, we introduce the amplitude of scattering in a film. At infinity, the wave function has the asymptotic form

$$\psi_{n'}(\rho) = \delta_{nn'} e^{i\mathbf{Q}\mathbf{p}} + \sqrt{\frac{\pi i}{2}}\, F_{nn'}(\mathbf{p}, \mathbf{p}') \frac{\exp(ip'\rho)}{a\sqrt{p'\rho}}, \tag{A.1}$$

where

$$\psi_{n'}(\rho) = \sqrt{\frac{2}{a}} \int \psi(\rho, z) \sin\frac{\pi n'}{a} z\, dz. \tag{A.2}$$

The quantity $F_{nn'}(\mathbf{p}, \mathbf{p}')$ plays the role of the scattering amplitude. It is similar to the scattering amplitude in the inelastic process,[11] if n′ denotes the decay channel and n the initial channel. Therefore relations analogous to the optical theorem, etc., should be satisfied for F. It is easy to derive the equation satisfied by $F_{nn'}(\mathbf{p}, \mathbf{p}')$:

$$F_{nn'}(\mathbf{p}, \mathbf{p}') = \frac{2a}{\pi} u_{nn'}(\mathbf{p} - \mathbf{p}') - \sum_{n_1} \int \frac{d^2p_1}{(2\pi)^2} \frac{u_{nn_1}(\mathbf{p} - \mathbf{p}_1') E_{n_1 n'}(\mathbf{p}_1, \mathbf{p}')}{[E_n(p) - E_{n_1}(p_1) + i\delta]} \tag{A.3}$$

The problem of finding the amplitude of scattering in a film entails certain difficulties. However, in the case of interest to us, that of a film which is thick compared with the characteristic dimension of the center (the screening radius, the transverse dimension of the roughnesses), the amplitude of scattering in a film can be expressed in terms of the volume-scattering amplitude:

$$F_{nn'}(\mathbf{p}, \mathbf{p}') = f\left(\frac{\mathbf{k}\mathbf{k}'}{kk'}\right) - f\left(\frac{\mathbf{k}\tilde{\mathbf{k}}'}{kk'}\right),$$

$$\mathbf{k} = (\mathbf{p}, p_z), \quad \tilde{\mathbf{k}} = (\mathbf{p}, -p_z), \quad p_z = \pi n / a. \tag{A.4}$$

APPENDIX 2

BOUNDARY CONDITION FOR THE CLASSICAL DISTRIBUTION FUNCTION

As is well known, in the absence of collisions the classical distribution function $n(\mathbf{r}, \mathbf{q})$ can be expressed in terms of the single-particle density matrix $\rho(\mathbf{r}_1, \mathbf{r}_2)$:

$$n(\mathbf{r}, \mathbf{q}) = \int \exp(2i\mathbf{q}\boldsymbol{\xi})\, \rho(\mathbf{r} + \boldsymbol{\xi}, \mathbf{r} - \boldsymbol{\xi})\, d\boldsymbol{\xi}. \tag{A.5}$$

Let us examine the density matrix of the pure state corresponding to particles incident on the surface of a semi-infinite sample with momentum **k**. In this case

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \psi_k^*(\mathbf{r}_1)\, \psi_k(\mathbf{r}_2). \tag{A.6}$$

In scattering on widely-spaced (in a sense of condition (6)) surface centers, the wave function of such a state is given at large distances from the surface by

$$\psi_k(\mathbf{r}) = \sin p_z z\, e^{i\mathbf{p}\boldsymbol{\rho}} + \frac{1}{2i} \sum_n \frac{\exp(ik|\mathbf{r} - \boldsymbol{\rho}_n|)}{|\mathbf{r} - \boldsymbol{\rho}_n|} e^{i\rho_n p} \left[f\left(\frac{\mathbf{k}, (\mathbf{r} - \boldsymbol{\rho}_n)}{k|\mathbf{r} - \boldsymbol{\rho}_n|}\right) - \tilde{f} \right], \tag{A.7}$$

where $\mathbf{r} = (\rho, z)$, and $\rho_n = (\rho_n, 0)$ is the coordinate of the surface center.

The boundary condition for the distribution function is imposed in that region near the surface, where z is much larger than the electron wavelength k^{-1}, but is at the same time small compared with the characteristic dimension of variation of the distribution function (the mean free path in the volume or the thickness of the film). Using this, we obtain the distribution function near the surface:

$$\begin{aligned} n(\mathbf{r}, \mathbf{q}) = \delta(\boldsymbol{\eta} - \mathbf{p}) \Big\{ & \delta(q_z - p_z) + \delta(q_z + p_z) \\ & \times \left[1 - c\frac{4\pi}{p_z} \operatorname{Im}\left(f(1) - f\left(\frac{\mathbf{k}\tilde{\mathbf{k}}}{k^2}\right)\right)\right] + \frac{2c}{q_z} \delta(q^2 - k^2) \left| f\left(\frac{\mathbf{k}\mathbf{q}}{kq}\right) - \tilde{f} \right|^2, \end{aligned} \tag{A.8}$$

$$\mathbf{q} = (\boldsymbol{\eta}, q_z).$$

The term proportional to $\delta(q_z - p_z)$ describes the distribution function of the incident particles, and the term with $\delta(q_z + p_z)$ describes the distribution function of the particles that are specularly reflected. The third term in (A.8) gives the contribution of the scattered particles. Separating the contributions of the incoming and outgoing particles, we get (27).

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53