Boundary conditions for the electron distribution function on an imperfect surface

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A boundary condition is obtained for the spin-dependent distribution function. This condition describes the scattering by the fluctuations of a short-range surface potential. For electrons that are not spin-polarized, the angular dependences of the coefficient of diffusivity are obtained. The specularity of the scattering of normally incident electrons is increased by processes with spin flip.

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1. The theoretical analysis of surface scattering of conduction electrons is based on the boundary conditions (BC) for the distribution function. The published derivation of these conditions (see the latest review[1]) is incomplete, since the interaction of the electrons with the surface is described within the framework of simple models that are equally applicable to metals and semiconductors. We consider here one more model, viz., scattering by fluctuations of a short-range surface potential of a semiconductor or semimetal, with account taken of processes with spin flip, which are important for materials with large spin-orbit splitting of the spectrum.

The interaction between a conduction electron described in a volume by the Hamiltonian $p^2/2m$ of the effective-mass approximation, and a short-range surface potential, is specified by the BC for the wave function ψ_{xz} on the surface $z=0$:

$$\{p_z+i\chi\sigma[\mathbf{e}_z\times\mathbf{p}]+ip_0(1+u_x)\}\psi_{xz}|_{z=0}=0. \tag{1}$$

This formula follows directly from the BC obtained by us earlier[2] for long-wave (compared with λ) fluctuations of the potential. In the case of short-wave fluctuations it is possible to derive Eq. (1) because of the presence of the small parameter a/λ (a is the thickness of the near-surface region and λ is the characteristic de Broglie wavelength of the electron). In the foregoing, m is the isotropic effective mass, $\mathbf{p}=-i\hbar\nabla$, σ is a Pauli matrix, the coefficient χ determines the magnitude of the spin-dependent interaction with the surface potential, and the three-dimensional coordinate is written in the form $(\mathbf{x}, z)$. The characteristic momentum p_0 describes the surface without allowance for the scattering, and the random increment u_x determines the degree of imprefection of the surface. In the limiting case when $p_0\gg\hbar/\lambda$ and $\chi=0$, the BC written above corresponds to the model of scattering by a potential wall whose height is determined by the random function u_x. We emphasize that the quantity p_0^2/m is not connected with the work function of the electron [Eq. (1) is replaced at large p_0 by the BC $\psi=0$ and the scattering mechanism discussed above is ineffective], since we consider slow electrons localized in energy at the extrema of the bands. In the general case, even the sign of p_0 is arbitrary; at $p_0<0$, "shallow" Tamm states[3] are present on a perfect surface (the assumption that p_0^2/m is of the order of the work function contradicts also the possibility of the existence of such states). The parameter χ is small in the case of weak spin-orbit interaction, but in a number of materials[2] (InSb, InAs, lead chalcogenides, bismuth) the spin-dependent interaction with the surface is not small, and this leads to singularities in the spectra of the two-dimensional electrons, and of the here-discussed rapid surface relaxation of the spin.

The quantum-mechanical problem of the scattering of an electron by an imperfect surface described by the BC (1) is solved below in the Born approximation. The obtained wave functions determine the connection between the distribution functions of the incident and reflected electrons, i.e., yield the BC for the spin-dependent distribution function. This BC describes a new surface-scattering mechanism that contributes to various kinetic effects governed by the near-surface electrons. We discuss here the angle (as well as energy) dependence of the diffusivity of the scattering of electrons that are not spin-polarized, and compare the results with the experimental data.[4,5]

2. It is convenient to consider the problem of scattering by a surface described by the condition (1) by changing over to the momentum representation in the two-dimensional coordinate x, i.e., by introducing the spinor

$$\psi(\mathbf{p}_\parallel z)=\int d\mathbf{x}\exp\left(-\frac{i}{\hbar}\mathbf{p}_\parallel\mathbf{x}\right)\psi_{xz}. \tag{2}$$

In this representation, the eigenvalues E are determined by the Schrödinger equation (in differential form with respect to the variable z), supplemented on the surface by an integral BC whose kernel is the Fourier transform of the random function u_x:

$$\frac{p_z^2}{2m}\psi(\mathbf{p}_\parallel z)=\left(E-\frac{p_\parallel^2}{2m}\right)\psi(\mathbf{p}_\parallel z),\quad z\geqslant 0,$$

$$\{p_z+i\chi\sigma[\mathbf{e}_z\times\mathbf{p}_\parallel]+ip_0\}\psi(\mathbf{p}_\parallel z)|_{z=0}+\frac{ip_0}{(2\pi\hbar)^2}\int d\mathbf{p}'\,u(\mathbf{p}_\parallel-\mathbf{p}')\psi(\mathbf{p}'0)=0. \tag{3}$$

We seek the wave function of the problem (3) on a half-space $z\geqslant 0$ in the form

$$\psi(\mathbf{p}_\parallel z)=\psi^{(-)}(\mathbf{p}_\parallel,\bar{p})\exp(-i\bar{p}z/\hbar)+\psi^{(+)}(\mathbf{p}_\parallel,\bar{p})\exp(i\bar{p}z/\hbar), \tag{4}$$

which satisfies the Schrödinger equation. Introducing a real, continuous and positive parameter $\bar{p}=(2mE$

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$-p_\parallel^2)^{1/2}$, we neglect the Tamm states (their spectrum for a perfect spectrum was obtained in Refs. 2 and 3) and the size quantization of the electrons in the z direction (the specimen is assumed to be thick enough). The spinors $\psi^{(\pm)}(\mathbf{p}_\parallel, \bar{p})$ determine the amplitudes of the reflected (+) and incident (−) waves and are connected by virtue of the BC (3) by the integral relation $[\bar{p}' = (2mE - p'^2)^{1/2}]$

$$\left\{1+\frac{\chi}{p_0}\sigma[\mathbf{e}_z\times\mathbf{p}_\parallel]-i\frac{\bar{p}}{p_0}\right\}\psi^{(+)}(\mathbf{p}_\parallel,\bar{p})=-\left\{1+\frac{\chi}{p_0}\sigma[\mathbf{e}_z\times\mathbf{p}_\parallel]+i\frac{\bar{p}}{p_0}\right\}\psi^{(-)}(\mathbf{p}_\parallel,\bar{p}) - \frac{1}{(2\pi\hbar)^2}\int d\mathbf{p}'\,u(\mathbf{p}_\parallel-\mathbf{p}')\,[\psi^{(+)}(\mathbf{p}',\bar{p}')+\psi^{(-)}(\mathbf{p}',\bar{p}')]. \tag{5}$$

We write down the solution of the scattering problem, following Fal'kovskiĭ,[6] in the second Born approximation, iterating with respect to the integral term in (5) and expressing the amplitude $\psi^{(+)}(\mathbf{p}_\parallel, \bar{p})$ of the reflected wave in terms of the amplitude $\psi^{(-)}(\mathbf{p}_\parallel, \bar{p})$ of the incident one. It is convenient to carry out these transformations by diagonalizing (5) with respect to spin with the aid of the unitary operator

$$2^{-1/2}(1+i\sigma_x\cos\varphi+i\sigma_y\sin\varphi), \tag{6}$$

where the angle φ determines the orientation of the two-dimensional vector $\mathbf{p}_\parallel = \{p_\parallel\cos\varphi, p_\parallel\sin\varphi\}$. The result of the calculation is given by the formulas (we use a nondiagonal representation)

$$\begin{aligned}
&\psi^{(+)}(\mathbf{p}_\parallel,\bar{p})\approx -i(1+v(\mathbf{p}_\parallel,\bar{p}))\psi^{(-)}(\mathbf{p}_\parallel,\bar{p})+\psi^{(1)}(\mathbf{p}_\parallel,\bar{p})+\psi^{(2)}(\mathbf{p}_\parallel,\bar{p}),\\
&\psi^{(1)}(\mathbf{p}_\parallel,\bar{p})=-\frac{i}{2(2\pi\hbar)^2}\frac{p_0}{\bar{p}}v(\mathbf{p}_\parallel,\bar{p})\int d\mathbf{p}'\,u(\mathbf{p}_\parallel-\mathbf{p}')v(\mathbf{p}',\bar{p}')\psi^{(-)}(\mathbf{p}',\bar{p}'),\\
&\psi^{(2)}(\mathbf{p}_\parallel,\bar{p})=\frac{1}{4(2\pi\hbar)^4}\frac{p_0}{\bar{p}}v(\mathbf{p}_\parallel,\bar{p})\int d\mathbf{p}'\int d\mathbf{p}''\,u(\mathbf{p}_\parallel-\mathbf{p}')\\
&\times u(\mathbf{p}'-\mathbf{p}'')\frac{p_0}{\bar{p}'}v(\mathbf{p}',\bar{p}')v(\mathbf{p}'',\bar{p}'')\psi^{(-)}(\mathbf{p}'',\bar{p}''),
\end{aligned} \tag{7}$$

in which we have introduced the operator

$$v(\mathbf{p}_\parallel,\bar{p})=2i\frac{\bar{p}}{p_0}\left\{1-i\frac{\bar{p}}{p_0}-\chi\sigma\left[\mathbf{e}_z\times\frac{\mathbf{p}_\parallel}{p_0}\right]\right\}\Big/\left\{\left(1-i\frac{\bar{p}}{p_0}\right)^2-\left(\chi\frac{p_\parallel}{p_0}\right)^2\right\}. \tag{8}$$

The macroscopic quantities calculated with the aid of the wave function (7) should be averaged over the random surface. We present here formulas for this averaging (designated hereafter by $\langle\ldots\rangle$) in the case of two surface-scattering mechanisms: by smooth (compared with a) fluctuations of the surface potential, and by point defects of the surface. For the first mechanism in the case of an isotropic and homogeneous random surface, we obtain the correlator $\langle u_{\mathbf{x}} u_{\mathbf{x}'}\rangle$, which is writtten for the Fourier transforms in the form

$$\langle u(\mathbf{p}_1)u(\mathbf{p}_2)\rangle=(2\pi\hbar)^2\delta(\mathbf{p}_1+\mathbf{p}_2)\sigma^2W(p_1). \tag{9}$$

Here σ^2 is the mean squared fluctuation of the random function $u_{\mathbf{x}}$, and $W(p_1)$ is an isotropic correlation function, usually assumed to be Gaussian. In scattering by randomly disposed point defects with low concentration, the statistical-averaging operation is determined, in analogy with the three-dimensional case,[7] by integrating with respect to the coordinates of the impurities. The resultant correlator differs from (9) only in that it contains in place of $\sigma^2W(p_1)$ a constant proportional to the surface concentration of the impurity. The integrals with respect to p_1 should be cut off at momenta of the order of $\hbar/a$ (if the impurity is localized on a surface with area a^2).

3. The one-electron statistical operator of the electrons incident on the surface and reflected from it is defined in terms of the amplitude $\psi^{(\pm)}(\mathbf{p}_\parallel, \mathbf{p}_z)$ by the formula

$$\rho^{(\pm)}(\mathbf{p}_\parallel', p_z'|\mathbf{p}_\parallel, p_z)=\frac{p_z p_z'}{m^2}\sum_{\lambda\lambda'}\delta\left(E_{\lambda'}-\frac{p_\parallel'^2+p_z'^2}{2m}\right) \times\delta\left(E_\lambda-\frac{p_\parallel^2+p_z^2}{2m}\right)\psi_{\lambda'}^{(\pm)}(\mathbf{p}_\parallel', p_z')\rho_{\lambda'\lambda}\psi_\lambda^{(\pm)}(\mathbf{p}_\parallel, p_z)^+, \tag{10}$$

in which $\rho_{\lambda'\lambda}$ satisfies the quantum-kinetic equation

$$\frac{\partial\rho_{\lambda'\lambda}}{\partial t}+\frac{i}{\hbar}(E_{\lambda'}-E_\lambda)\rho_{\lambda'\lambda}=J_{\lambda'\lambda}, \tag{11}$$

written in the representation of the eigenfunctions of the problem (2) (the subscripts λ' and λ number these states). The collision integral $J_{\lambda'\lambda}$ describes the interaction with the volume scatterers, and the character of the volume scattering can change in the near-surface region. We note that $\rho^{(\pm)}(\mathbf{p}_\parallel', p_z'|\mathbf{p}_\parallel, p_z)$ is a 2×2 matrix (whereas $\rho_{\lambda'\lambda}$ contains the spin in the set of quantum numbers λ) and the independent variables are here $\mathbf{p}_\parallel$ and p_z rather than $\mathbf{p}_\parallel$ and E as in Sec. 2.

The distribution functions $F(\mathbf{p}_\parallel, \pm p_z)$ of the incident and reflected electrons on the surface $z=0$ are expressed[1)] in terms of the diagonal elements of (10), averaged over the random surface. Writing down explicit expressions for $\langle\rho^{(+)}(\mathbf{p}_\parallel, p_z|\mathbf{p}_\parallel, p_z)\rangle$ with the aid of (7) and (9), and changing from two-dimensional integrals in (7) to integration over the half-space of the incident momenta

$$\int\limits_{p_z'>0} d^3p'\ldots$$

[the elasticity of the scattering gives rise here to the delta function $\delta(E-E')$], we arrive at the BC ($v_z=p_z/m$)

$$\begin{aligned}
F(\mathbf{p}_\parallel,p_z)&=(1+v(\mathbf{p}_\parallel,p_z))F(\mathbf{p}_\parallel,-p_z)(1+v(\mathbf{p}_\parallel,p_z)^+)\\
&+\left(\frac{\sigma p_0}{4\pi m\hbar}\right)^2\frac{1}{v_z}\int\limits_{p_z'>0}d^3p'\delta(E-E')W(|\mathbf{p}_\parallel-\mathbf{p}'|)\{v(\mathbf{p}_\parallel,p_z)v(\mathbf{p}',p_z')F(\mathbf{p}',-p_z')\\
&\times v(\mathbf{p}',p_z')^+v(\mathbf{p}_\parallel,p_z)^+-(1+v(\mathbf{p}_\parallel,p_z))F(\mathbf{p}_\parallel,-p_z)v(\mathbf{p}_\parallel,p_z)^+v(\mathbf{p}',p_z')^+v(\mathbf{p}_\parallel,p_z)^+\\
&-v(\mathbf{p}_\parallel,p_z)v(\mathbf{p}',p_z')v(\mathbf{p}_\parallel,p_z)F(\mathbf{p}_\parallel,-p_z)(1+v(\mathbf{p}_\parallel,p_z)^+)\}.
\end{aligned} \tag{12}$$

This matrix BC can be simplified by introducing the scalar and spin distribution functions $f(\mathbf{p}_\parallel, p_z)$ and $\sigma(\mathbf{p}_\parallel, p_z)$ respectively, using the relations

$$\begin{aligned}
f(\mathbf{p}_\parallel,p_z)&=\mathrm{Sp}\,F(\mathbf{p}_\parallel,p_z),\quad \sigma(\mathbf{p}_\parallel,p_z)=\mathrm{Sp}\,\sigma F(\mathbf{p}_\parallel,p_z),\\
F(\mathbf{p}_\parallel,p_z)&={}^1/_2\{f(\mathbf{p}_\parallel,p_z)+\sigma\sigma(\mathbf{p}_\parallel,p_z)\},
\end{aligned} \tag{13}$$

in which the trace is taken over the spin variable. We write the BC for these functions by acting on (12) with the operators Sp... and Spσ... and using the definitions (13). As a result, the scalar and spin components of the distribution function on the surface are connected by the relations ($i=x,y,z$)

$$\begin{aligned}
f(\mathbf{p}_\parallel,p_z)&=f(\mathbf{p}_\parallel,-p_z)+\left(\frac{\sigma p_0}{4\pi m\hbar}\right)^2\frac{1}{v_z}\int\limits_{p_z'>0}d^3p'\,\delta(E-E')W(|\mathbf{p}_\parallel-\mathbf{p}'|)\\
&\times\Big\{A(\mathbf{p}_\parallel,p_z|\mathbf{p}',p_z')[f(\mathbf{p}',-p_z')-f(\mathbf{p}_\parallel,-p_z)]\\
&+\sum_i[\sigma_i(\mathbf{p}',-p_z')C_i(\mathbf{p}_\parallel,p_z|\mathbf{p}',p_z')-\sigma_i(\mathbf{p}_\parallel,-p_z)C_i(\mathbf{p}',p_z'|\mathbf{p}_\parallel,p_z)]\Big\},
\end{aligned} \tag{14}$$

$$\sigma_i(\mathbf{p}_\parallel, p_z) = \sum_j B_{ij}(\mathbf{p}_\parallel, p_z)\sigma_j(\mathbf{p}_\parallel, -p_z) + \left(\frac{\sigma p_0}{4\pi m\hbar}\right)^2 \frac{1}{v_z} \int\limits_{p_z'>0} d^3p'\,\delta(E-E')$$
$$\times W(|\mathbf{p}_\parallel - \mathbf{p}'|)\Big\{ D_i(\mathbf{p}_\parallel p_z|\mathbf{p}', p_z')[f(\mathbf{p}', -p_z') - f(\mathbf{p}_\parallel, -p_z)]$$
$$+ \sum_j [F_{ij}(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z')\sigma_j(\mathbf{p}', -p_z') - G_{ij}(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z')\sigma_j(\mathbf{p}_\parallel, -p_z)]\Big\}, \tag{15}$$

with the tensor coefficients of these BC given by

$$A(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = {}^1/_2 \operatorname{Sp} v(\mathbf{p}_\parallel, p_z)v(\mathbf{p}', p_z')v(\mathbf{p}', p_z')^+v(\mathbf{p}_\parallel, p_z)^+,$$
$$B_{ij}(\mathbf{p}_\parallel, p_z) = {}^1/_2 \operatorname{Sp} \sigma_i(1+v(\mathbf{p}_\parallel, p_z))\sigma_j(1+v(\mathbf{p}_\parallel, p_z)^+),$$
$$C_i(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = {}^1/_2 \operatorname{Sp} v(\mathbf{p}_\parallel, p_z)v(\mathbf{p}', p_z')\sigma_i v(\mathbf{p}', p_z')^+v(\mathbf{p}_\parallel, p_z)^+,$$
$$D_i(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = {}^1/_2 \operatorname{Sp} v(\mathbf{p}', p_z')^+v(\mathbf{p}_\parallel, p_z)^+\sigma_i v(\mathbf{p}_\parallel, p_z)v(\mathbf{p}', p_z'), \tag{16}$$
$$F_{ij}(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = {}^1/_2 \operatorname{Sp} \sigma_i v(\mathbf{p}_\parallel, p_z)v(\mathbf{p}', p_z')\sigma_j v(\mathbf{p}', p_z')^+v(\mathbf{p}_\parallel, p_z)^+,$$
$$G_{ij}(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = {}^1/_2 \operatorname{Sp} \sigma_i\{(1+v(\mathbf{p}_\parallel, p_z))\sigma_j v(\mathbf{p}_\parallel, p_z)^+v(\mathbf{p}', p_z')^+v(\mathbf{p}_\parallel, p_z)^+$$
$$+v(\mathbf{p}_\parallel, p_z)v(\mathbf{p}', p_z')v(\mathbf{p}_\parallel, p_z)\sigma_j(1+v(\mathbf{p}_\parallel, p_z)^+)\}.$$

Boundary conditions similar to (14) and (15) were obtained also for other scattering models.[1] The mechanism considered here differs in that the tensor coefficients (16) are given in explicit form, and at $|\chi| \sim 1$ the probability of scattering with spin flip is not small. Tne functions $f(\mathbf{p}_\parallel, p_z)$ and $\sigma(\mathbf{p}_\parallel, p_z)$ are separated only in the case of spin-independent surface scattering (at $\chi = 0$), when $C_i = D_i = 0$ and all the tensor coefficients are proportional to δ_{ij}.

Upon substitution of the equilibrium distribution $f_{eq}(E)$, $\sigma_{eq} = 0$, these BC turn into identities because the surface scattering is elastic. Let us verify that (14) and (15) correspond to a zero particle flux through the surface. Defining the fluxes of the incident (J_-) and reflected (J_+) electrons as

$$J_- = \int\limits_{p_z>0} d^3p\, p_z f(\mathbf{p}_\parallel, p_z), \quad J_+ = \int\limits_{p_z>0} d^3p\, p_z f(\mathbf{p}_\parallel, -p_z), \tag{17}$$

we apply the operator

$$\int\limits_{p_z>0} d^3p \ldots$$

to the BC (14). The integral term then vanishes (we use the symmetry condition $A(\mathbf{p}_\parallel, p_z|\mathbf{p}'p_z') = A(\mathbf{p}', p_z'|\mathbf{p}_\parallel, p_z)$ and we obtain the equality $J_- = J_+$, meaning no particle flux through the surface.

4. The diffusivity $P(E, \theta)$ of the scattering of the electrons that are not spin-polarized, is defined as the integral probability from a given state into all other states.[2)] The quantity $P(E, \theta)$ enters in the BC (14) alongside the function $f(\mathbf{p}_\parallel, -p_z)$ [the factor $1 - P(E, \theta)$ determines the degree of specularity of the scattering] and is expressed in terms of the coefficient

$$A(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = 16\frac{p_z^2 p_z'^2}{p_0^4} a(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z').$$

Using the explicit expression

$$a(\mathbf{p}_\parallel, p_z|\mathbf{p}', p_z') = \left\{\left[1 + \left(\frac{p_z}{p_0}\right)^2 + \left(\chi\frac{p_\parallel}{p_0}\right)^2\right]\left[1 + \left(\frac{p_z'}{p_0}\right)^2 + \left(\chi\frac{p'}{p_0}\right)^2\right]\right.$$
$$\left. + (2\chi)^2\frac{\mathbf{p}_\parallel\mathbf{p}'}{p_0^2}\right\}\left\{\left[1 - \left(\frac{p_z}{p_0}\right)^2 - \left(\chi\frac{p_\parallel}{p_0}\right)^2\right]^2\right.$$
$$\left. + \left(2\frac{p_z}{p_0}\right)^2\right\}^{-1}\left\{\left[1 - \left(\frac{p_z'}{p_0}\right)^2 - \left(\chi\frac{p'}{p_0}\right)^2\right]^2 + \left(2\frac{p_z'}{p_0}\right)^2\right\}^{-1} \tag{18}$$

and changing to integration with respect to the two-dimensional momentum for the diffusivity, we obtain the equation

$$P(E, \theta) = \left(\frac{\sigma}{\pi\hbar}\right)^2 \int d\mathbf{p}' W(|\mathbf{p}_\parallel - \mathbf{p}'|)\frac{p_z\bar{p}_z}{p_0^2} a(\mathbf{p}_\parallel, p_z|\mathbf{p}', \bar{p}_z),$$
$$p_\parallel = (2mE)^{1/2}\cos\theta, \quad p_z = (2mE)^{1/2}\sin\theta, \quad \bar{p}_z = (2mE - p'^2)^{1/2}, \tag{19}$$

in which θ is the electron incidence angle.

The integration with respect to the momentum transfer $\mathbf{q} = \mathbf{p}_\parallel - \mathbf{p}'$ is carried out in (19) for the limiting cases of long-wave and short-wave surface inhomogeneities [the correlation function $W(q)$ cuts off the integral at $q > q_{max}$]. In the case of long-wave correlations [$\hbar/q_{max} \gg \hbar/(2mE)^{1/2}$] we obtain a formula

$$P(E, \theta) \approx P_0\frac{E}{E_0}\sin^2\theta\left\{\left[1 + \frac{E}{E_0}(\sin^2\theta + \chi^2\cos^2\theta)\right]^2\right.$$
$$\left. + 4\chi^2\frac{E}{E_0}\cos^2\theta\right\}\left\{\left[1 - \frac{E}{E_0}(\sin^2\theta + \chi^2\cos^2\theta)\right]^2 + 4\frac{E}{E_0}\sin^2\theta\right\}^{-2}, \tag{20}$$
$$P_0 = (\sigma/\pi\hbar)^2\int d\mathbf{q}\, W(q), \quad E_0 = p_0^2/2m,$$

that is not suitable in the case of normal incidence of the electron [$(2mE)^{1/2}\cos\theta \sim q_{max}$]. For normal incidence we obtain a different asymptotic form, but at $\theta = \pi/2$ the formulas coincide and therefore (20) describes approximately the angular dependence in the entire range of variation of the angle θ.

If the inverse inequality $\hbar/q_{max} \ll \hbar/(2mE)^{1/2}$ holds (short-wave inhomogeneity), we obtain an angular dependence of the form

$$P(E, \theta) \approx P_1\left(\frac{E}{E_0}\right)^{1/2}\sin\theta\left\{1 + \frac{E}{E_0}(\sin^2\theta + \chi^2\cos^2\theta)\right\}$$
$$\times\left\{\left[1 - \frac{E}{E_0}(\sin^2\theta + \chi^2\cos^2\theta)\right]^2 + 4\frac{E}{E_0}\sin^2\theta\right\}^{-1}, \tag{21}$$
$$P_1 = \left(\frac{\sigma}{\pi\hbar}\right)^2\int d\mathbf{q}\, W(q)\frac{q}{p_0}\frac{1 + (1+\chi^2)(q/p_0)^2}{[1 - (1+\chi^2)(q/p_0)^2]^2 + 4(q/p_0)^2}$$

The last formula describes also scattering by point defects, and $\sigma^2 W(q)$ must be replaced by a constant. The coefficient P_1 diverges at large momentum transfers, and the integral should be cut off at $q_{max} \sim \hbar/a$, i.e., only an order-of-magnitude estimate of the amplitude of the diffusivity is obtained for this scattering mechanism.

The angular dependences (20) and (21) are shown in the figure for different values of E/E_0 and χ. The grazing electrons are specularly reflected on account of the factors $\sin^2\theta$ and $\sin\theta$. This angular dependence is preserved over the entire range of variation of θ for extremely slow particles $E/E_0 \to 0$ (or in the case of a high potential wall). With increasing E/E_0 the diffusivity increases more slowly with θ, and at finite values of χ (which take into account the scattering with spin flip) a situation is possible wherein the function $P(E, \theta)$ becomes nonmonotonic. The maximum of this function approaches the point $\theta = 0$ as $E/E_0 \to 1$ and $|\chi| \to 1$, and when the parameters E/E_0 and $|\chi|$ are equal to unity the diffusivity diverges like $(\sin\theta)^{-2}$ and $(\sin\theta)^{-1}$ for the cases (20) and (21), respectively. At these values of the parameters, the scattering of the grazing electrons turns out to be strong, and we cannot make for them the assumptions made in the derivation of the BC. With increasing E/E_0, the functions (20) and (21) fall off respectively as $(E/E_0)^{-1}$ and $(E/E_0)^{-1/2}$,

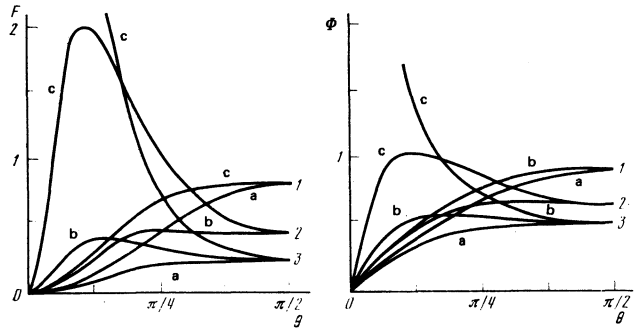

FIG. 1. Angular and energy dependences of the scattering diffusivity. The functions $F = [P(E, \theta)/P_0]E_0/E$ and $\Phi = [P(E, \theta)/P_1](E_0/E)^{1/2}$, defined by Eqs. (20) and (21), were calculated here for the values $E/E_0 = 0.1$ (1), $E/E_0 = 0.5$ (2), $E/E_0 = 1$ (3) and $\chi = 0$ (a), $|\chi| = 0.5$ (b), $|\chi| = 1$ (c).

and the form of the angular dependences does not vary with energy.

An experimental investigation of the angular dependences of $P(E, \theta)$ was made for bismuth[4,5] (a number of results were obtained also for other semimetals and metals). The model considered here does not describe in detail the structure of bismuth (no account is taken of the anisotropic and multivalley character of the spectrum, nor of its strong nonparabolicity), but does reflect certain characteristic features of the experiment. Thus, the almost-specular reflection of the normally incident electrons, which was observed already in the first studies (see Ref. 4), is obtained here at $\chi = 1$ (corresponding to the case of bismuth) in a wide range of E/E_0. Another distinguishing feature is the very large difference between the values and angular dependences of $P(E, \theta)$ on surfaces oriented along different crystallographic planes; this fact can be attributed to the different values of the parameter p_0 in the BC(1) on these surfaces.

5. The formulas given above can be used directly to describe surface kinetic effects in III-V semiconductors at $E/\varepsilon_g \ll 1$ (ε_g is the forbidden-band width). The structure of the BC(14) and (15) obtained here is standard, so that it is possible to treat various kinetic effects in the usual manner.[1] For example, the condition (15) is transformed (see Ref. 8) into the BC for the magnetization, which leads at $|\chi| \sim 1$ to a rapid surface relaxation of the spin. Using (14), we can describe galvanomagnetic size effects. The scattering mechanism introduced here should then be treated as supplementing (assuming the scattering to be weak) the mechanism already discussed in the literature[1,9] and is effective in the case of a surface enriched with electrons. A weak scattering can be ensured both by small fluctuations of the surface parameters ($P_{0,1} \ll 1$) and by a "nonresonant" character of the scattering (at $E/E_0 \gg 1$ or $E/E_0 \ll 1$).

The analysis of almost-specular reflection (the only one carried out theoretically) is vital also for the solution of the inverse scattering problem on a diffuse surface,[5,10] since it makes it possible to set the energy and angular dependences of the scattering probability in such a way that only several parameters of this dependence are determined in experiment.

[1)] Such a connection is obtained if (10) is used to express the Wigner distribution function on a half-space and the quasiclassical limit is taken. Then (11) is transformed into the usual kinetic equation.

[2)] Another definition of the diffusivity is necessary in a number of problems.[1]

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