

Interaction of excitations with dislocations in a crystal

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A study is made of how the topology change due to the presence of dislocations in a crystal influences the motion of excitations. It is shown that the scattering of excitations involves anomalous transverse forces that cannot be expressed in terms of the scattering amplitude. The specific corrections to the conductivity due to the disturbance of the phase in the presence of a finite dislocation density are investigated for many-valley semiconductors.

INTRODUCTION

The interaction of excitations with dislocations is important for understanding a number of kinetic phenomena in solids.¹ The majority of papers on this subject have either used the effective-mass method or directly employed the Born approximation for scattering by the deformation potential created by the elastic fields around the dislocation. It was found that the transport cross section is determined mainly by large scattering angles, i.e., by the poorly understood region near the core of the dislocation (see, e.g., Ref. 2). The goal of this paper is to study the effects associated with large distances from the core and to investigate the scattering anomalies that are specific to dislocations.

Analogous effects arise in the interaction of excitations with vortices in superfluid He₄, where, as one of the present authors has shown,³ the long-range field of a vortex gives rise in the phonon scattering to an anomalous transverse force that cannot be expressed directly in terms of the transport scattering cross section. It was later shown that this force is directly due to a feature analogous to the Aharonov-Bohm effect in the scattering of electrons by a narrow solenoid.⁴ A similar effect has been detected in the scattering of excitations by screw dislocations, for which the deformation potential is absent in the isotropic approximation and terms of a purely geometric nature must be included in the Hamiltonian.^{5–7} It was shown in Ref. 8 that the Aharonov-Bohm effect arises in this case.

In the present paper we consider the general case of the interaction of excitations with an arbitrary dislocation and study both the scattering anomalies and certain other effects due to a topological interaction.

1. INTERACTION AND ANOMALIES IN SCATTERING BY DISLOCATIONS

In considering the interaction of dislocations with excitations, we will be interested in large distances, where the deformations are small and slowly varying, so that the effective mass method can be used.

The general approach for obtaining the effective Hamiltonian is presented in the monograph of Bir and Pikus.⁹ We perform a coordinate transformation matching the deformed unit cell with the undeformed cell:

$$x_i^0 = x_i^0(x_i), \quad x_i = x_i^0 + u_i(x_i^0). \quad (1.1)$$

To a linear approximation in the deformations, the energy of the excitations after transformation should be of the form

$$\varepsilon = \varepsilon^0(\delta p_i) + \Gamma_{ijk} \delta p_i u_{jk} + \Xi_{jk} u_{jk}, \quad (1.2)$$

where $u_{jk} = \frac{1}{2}(\partial u_j / \partial x_k + \partial u_k / \partial x_j)$ is the deformation tensor, δp_j is the (assumed small) deviation of the quasimomentum from its value at the minimum $\varepsilon^0(\mathbf{p})$, Ξ_{jk} is the tensor of the deformation-potential constants, Γ_{ijk} is the tensor which specifies the displacement of the minimum of $\varepsilon(\mathbf{p})$ in the reciprocal cell (both these quantities depend on the interaction of the excitations with the lattice and cannot be evaluated in general form). In order to write the Hamiltonian for the interaction with dislocations, we must express $\delta p_j = (i\partial / \partial x_j^0 - k_j)$ in terms of the deformed coordinates x_j :

$$\delta p_j \approx \left(i \frac{\partial}{\partial x_j} + i \frac{\partial}{\partial x_n} \frac{\partial u_n}{\partial x_j} - k_j \right)$$

and assume that $\varepsilon(\delta \mathbf{p}, \mathbf{x})$ gives the local energy density. Here the multivaluedness of transformation (1.1) is unimportant, since the distortion tensor $w_{jk} = \partial u_j / \partial x_k$ is single-valued.

We shall assume the simplest case of cubic symmetry and suppose that the vectors \mathbf{k} corresponding to the position of the minima in the cell of the reciprocal lattice have a two-fold symmetry axis, so that the most important tensor here, Γ_{ijn} , is of the form

$$\Gamma_{ijn} = \tilde{\gamma}_1 k_i \delta_{jn} + \tilde{\gamma}_2 k_i (k_j k_n / k^2) + \tilde{\gamma}_3 (\delta_{ij} k_n + \delta_{in} k_j),$$

where $\tilde{\gamma}_i$ is generally of the order of $1/m$ when k is of the order of the unit cell dimension. If \mathbf{k} occupies a position of special symmetry (the Brillouin zone center, reciprocal lattice sites), then Γ vanishes, there are no terms linear in $\delta \mathbf{p}$, and the deformation corrections to the effective-mass tensor must be taken into account. We will be interested in the corrections to the "kinetic" part of the energy; we therefore collect all the remaining terms into an effective potential $U(r)$ created by the dislocations, so that

$$\mathcal{H} = \frac{1}{2m_{\parallel}} \sum_{\mathbf{k}} (\hat{p}_{\parallel} - A_{\parallel} - k)^2 + \frac{1}{2m_{\perp}} \sum_{\mathbf{k}} (\hat{p}_{\perp} - \mathbf{A}_{\perp})^2 + U(r), \quad (1.3)$$

where A_{\parallel} is the component along \mathbf{k} , \mathbf{A}_{\perp} consists of the components in the perpendicular plane, and

$$A_j = -k_j w_{ij} + \gamma_1 k_j u_{ii} + \gamma_2 k_j (k_i k_n / k^2) u_{in} + \gamma_3 k_i u_{ji}. \quad (1.4)$$

If the minimum of ε is found at the point $\mathbf{k} = 0$, then

$$A_j = -p_i w_{ij} + \gamma_1 p_j u_{ii} + \gamma_2 p_i u_{ji}. \quad (1.4')$$

In considering the interaction of charge carriers with the dislocation, we shall assume that the semiconductors are

highly enough doped that there is a finite density of charge carriers, no large Read cylinders of ionized donors form around the dislocations, and the situation is close to metallic. We note in this regard that the deformation potential at large distances is decreased substantially by screening, whereas the effective vector potential A_j does not alter the charge density and is therefore not screened.

We will be interested in systematic effects which do not vanish on averaging over the distribution of the dislocations, which are assumed to be rectilinear and parallel.

At large distances the transfer of excitations from one valley to another by the dislocation field is extremely rare, and so the excitations in each valley can actually be treated independently.

Let us consider the case in which k is directed along the dislocation, which we assume is parallel to the z axis, so that

$$A_j = -(1 - \gamma_3/2)kw_{zj} + \gamma_1 k u_{ii} \delta_{zj}. \quad (1.5)$$

The first term here is of the form of the vector potential of the magnetic field, which is concentrated at the core of the dislocation. The second term gives rise to a magnetic field in the plane perpendicular to the dislocation. Let us consider the influence of the second term on the motion of the excitations. The corresponding classical equations of motion are of the form

$$m \frac{dv_x}{dt} = \frac{\partial A_z}{\partial x} v_z, \quad m \frac{dv_y}{dt} = \frac{\partial A_z}{\partial y} v_z, \\ m \frac{dv_z}{dt} = -\frac{\partial A_z}{\partial y} v_y - \frac{\partial A_z}{\partial x} v_x,$$

from which we get for the change in the velocity along the unperturbed trajectory

$$m\delta v_z(r) = \gamma_1 k (u_{ii}(r) - u_{ii}(0)) = \delta A_z.$$

Because u_{ii} changes sign along the trajectory because of the random distribution of the dislocations, we see that there is no systematic change in v_z to first order in A_z . In an analogous way it can be shown that there are no systematic contributions of second order in v_x and v_y .

If we consider the phase acquired along some excitation trajectory owing to the presence of A_j , then because of the random distribution of the dislocations it too will lack a systematic nature for a trajectory with a general position.

The case in which k_j lies in the plane perpendicular to the dislocation is more complicated, since all the terms in (1.4) are nonzero and A_j itself also lies in this plane, so that there is an effective magnetic field parallel to the dislocations. The value of A_j depends on the entire set of forces applied to the body and not only on the density of dislocations and the deformations they cause.

The features in the small-angle scattering are due to the singular component of A_j , which gives the main contribution to the circulation integral

$$\varphi = \int_C A_j dx_j,$$

where the center C is a rectangle enclosing the dislocations, with a side of length L along the projection of the velocity of the incident excitations onto the plane perpendicular to the dislocation and with a short side $(L\lambda)^{1/2}$, where λ is the

wavelength of the incident excitations, and $l, n_d^{-2} \gg L \gg \lambda$, where l is the mean free path of the incident excitations and n is the dislocation density per unit area. The main contribution to the circulation, $\sim \mathbf{b} \cdot \mathbf{k}$, where \mathbf{b} is the Burgers vector of the dislocation, is from the singular terms in A_j due to the presence of dislocations and to anomalies of the distortion tensor.

The contribution to the circulation from the regular elastic deformations, which vary over distances of order \mathcal{L} (where \mathcal{L} is the dimension of the object), is smaller by a factor of $\sim n_d L^2 (\lambda/L)^{1/2}$. For this reason we shall henceforth consider only effects due to the first term in (1.4); this gives an exact treatment of screw dislocations with $\mathbf{k} \parallel \mathbf{b}$ in the isotropic approximation of the theory of elasticity ($u_{ii} = 0$) if one allows for an additional coefficient $(1 - \gamma_3/2)$ in A_j . Our approximation corresponds to allowance for only the "topological" interactions;⁷ here one gets comparatively simple physical answers. Because $A_j = -k_i \partial u_i / \partial x_j$, the corresponding magnetic field is parallel to the dislocation and concentrated in the core, with dimensions of an atomic scale; we have the same situation as in the Aharonov-Bohm effect: The vector potential can be eliminated locally by a gradient transformation, but it is impossible to do this over all space.

There is an extensive literature on the Aharonov-Bohm effect, which was reviewed in detail in Ref. 10. Let us briefly show how calculations can be done in the case of an arbitrary dispersion relation.

The wave function of the excitations at large distances from the dislocation core consists of a distorted incident wave and a scattered wave. We assume that the latter is known from the solution of the problem of scattering by a given entity (which takes into account the influence of the dislocation core) everywhere except in the region of small scattering angles, where we must find the specific form of the wave function. This singular diffraction region should clearly be directed along the group velocity of the excitations in the region of the dislocation core.

To construct the solution we use the local solution of the Schrodinger equation with Hamiltonian (1.3) (for a single valley), whereby the vector potential is eliminated by the gradient transformation

$$\psi = e^{i\mathbf{k}\mathbf{r}} e^{i\delta\mathbf{p}\mathbf{r}} + \exp \left[i \int_{-\infty}^{\infty} A_j dx_j \right], \quad (1.6)$$

where $-\infty$ corresponds to the direction along which the incident particles arrive. Function (1.6) is not single-valued, since $\varphi = \oint A_j dx_j \neq 0$, and we should make a cut along the singular diffraction region, where function (1.6) has a discontinuity; in the exact solution this discontinuity is replaced by a relatively narrow transition zone. In this zone the derivatives of ψ in the perpendicular direction are large compared to the derivatives in the parallel direction (at large distances all the derivatives remain small after the exponentials $e^{i\mathbf{k}\mathbf{r}} e^{i\delta\mathbf{p}\mathbf{r}}$ have been factored out). In addition, we can neglect the small vector potential inside the transition zone, since the Schrodinger equation for $\psi = e^{i\mathbf{k}\mathbf{r}} e^{i\delta\mathbf{p}\mathbf{r}} f(x,y)$ with Hamiltonian (1.3) is of the form

$$\begin{aligned} \frac{\partial \varepsilon}{\partial p_x} \left(i\hbar \frac{\partial f}{\partial x} \right) - \frac{1}{2} \frac{\partial^2 \varepsilon}{\partial p_y^2} \frac{\partial^2 f}{\partial y^2} &= 0, \\ \frac{\partial \varepsilon}{\partial p_x} &= \left(\frac{1}{m_{\parallel}} - \frac{1}{m_{\perp}} \right) \frac{k_x}{k} (\delta \mathbf{p} \mathbf{k}) + \frac{\partial p_x}{m_{\perp}}, \\ \frac{\partial^2 \varepsilon}{\partial p_y^2} &= \left(\frac{1}{m_{\parallel}} - \frac{1}{m_{\perp}} \right) \frac{k_y^2}{k^2} + \frac{1}{m_{\perp}}. \end{aligned} \quad (1.7)$$

The x axis is directed along the group velocity $\partial \varepsilon / \partial \mathbf{p}$ of the incident excitations. Equations (1.7) is the familiar parabolic equation introduced by Leontovich in the theory of diffraction. We require a solution of the form

$$f = f(\zeta), \quad \zeta = \frac{y}{x^{1/2}} \left(\frac{\partial \varepsilon}{\partial p_x} / \hbar \frac{\partial^2 \varepsilon}{\partial p_y^2} \right)^{1/2}, \quad (1.8)$$

whereupon the equation is easily integrated to give

$$\begin{aligned} f(\zeta) &= \left[e^{i\varphi_+} \int_{-\infty}^{\zeta} e^{i\eta^{3/2}} d\eta + e^{i\varphi_-} \int_{\zeta}^{+\infty} e^{i\eta^{3/2}} d\eta \right] \left[\int_{-\infty}^{+\infty} e^{i\eta^{3/2}} d\eta \right]^{-1}, \\ \varphi_+ &= \int_{-\infty}^{+\infty} A(x, y) dx, \quad y \rightarrow +0; \\ \varphi_- &= \int_{-\infty}^{+\infty} A(x, y) dx, \quad y \rightarrow -0. \end{aligned} \quad (1.9)$$

Equations (1.7)–(1.9) give the solution in all regions. We note that if the singular region is not directed along $\partial \varepsilon / \partial \mathbf{p}$, there will be no solution that admits joining, since the first derivatives with respect to y remain in the equation.

Importantly, the solution we have constructed is not in the form of a sum of the incident wave and a diverging cylindrical wave. In a formal calculation by expansion in angular harmonics, we obtain both a divergence in the total cross section σ and a logarithmic divergence in the “transverse” transport cross section $\sigma_{\perp} = \int \sin \varphi d\sigma(\varphi)$, while the ordinary “longitudinal” transport cross section $\sigma_{\parallel} = \int (1 - \cos \varphi) d\sigma(\varphi)$ converges (φ is the angle to the direction of the incident excitations). The divergence in the transverse force is fictitious; this force can be evaluated directly by using the solution just obtained. Using the Schrodinger equation with Hamiltonian (1.3), we easily obtain an identity which expresses the law of momentum conservation:

$$\begin{aligned} \oint_{\mathcal{L}} \left[-\frac{1}{2m_k} \left(i\hbar \frac{\partial \psi^*}{\partial x_k} - A_k \psi^* \right) \left(-i\hbar \frac{\partial \psi}{\partial x_j} - A_j \psi \right) \right. \\ \left. + \text{c.c.} + \frac{\hbar^2}{4m_k} \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_j} (\psi \psi^*) \right] n_k dl + \int_{S(\mathcal{L})} \psi^* \hat{P}_j \psi d^2x = 0, \end{aligned}$$

where the last term [$S(\mathcal{L})$ is the area bounded by the contour \mathcal{L}], which does not have the form of a divergence, gives the average value of the force acting on the excitations, and the first term gives the momentum carried off by the scattered excitations (n_k is the vector normal to the contour \mathcal{L}). Our solution permits evaluation of the momentum carried off by the excitations in the small-angle region (where we can drop A):

$$\langle F_y \rangle = \hbar n v \sin \varphi, \quad \varphi = \oint A_j dx_j = \mathbf{k} \mathbf{b}, \quad (1.10)$$

where \mathbf{b} is the Burgers vector of the dislocation, n is the density of incident excitations, and $v = (\partial \varepsilon / \partial \mathbf{p})_{\perp}$ is the projection of the velocity of the incident excitations onto the plane perpendicular to the dislocation. We note that Burgers vector is a lattice vector, and so this force vanishes if $\mathbf{k} = m \mathbf{k}_0 / 2$, where \mathbf{k}_0 is a reciprocal lattice vector and m is an integer.

$$\text{If we consider only the topological interaction, then} \quad \varphi_0 = (\mathbf{k} + \delta \mathbf{p}) \mathbf{b}; \quad (1.10')$$

if we allow for corrections to \mathbf{A} of the type written in (1.4'), Eq. (1.10') remains valid for $\mathbf{k} = 0$.

The flow of excitations to a dislocation thus gives rise to a transverse force perpendicular to the flow. This force is of a specific, diffractive origin and cannot be expressed in terms of the scattering cross section. If there is a large number of dislocations (with a density n_d) with the same orientation and the same Burgers vector, there will be an average force density $F_y n_d$ acting on the excitations. In the equilibrium situation, when the \mathbf{k} and $-\mathbf{k}$ valleys are identically occupied, there is no net force because the contributions of the different valleys cancel. Any breakdown of equilibrium between the \mathbf{k} and $-\mathbf{k}$ valleys will give rise to a Hall current (for example).

In concluding this section we note that the scattering features we have found are general for the scattering of excitations by topological defects. Suppose that the excitations in the field of linear defects are described by a certain Hamiltonian $\mathcal{H}(\mathbf{p}, \mathbf{r})$ that can be represented at large distances as $\mathcal{H} = \mathcal{H}_0(\mathbf{p}) + \delta \mathcal{H}(\mathbf{p}, \mathbf{r})$, where $\delta \mathcal{H}$ is a small correction. The change in momentum along the direction of the group velocity $\mathbf{v} = \partial \mathcal{H}_0 / \partial \mathbf{p}$ is

$$\delta p_x = \int_{-\infty}^{\zeta} \frac{\partial \delta \mathcal{H}}{\partial \mathbf{r}} \frac{\mathbf{v}}{v} dt = \frac{1}{v} [\delta \mathcal{H}(\mathbf{r}) - \delta \mathcal{H}(-\infty)].$$

We are interested in small angles and large distances; then the diffraction in the phase acquired above the x axis (along \mathbf{v}) and below the x axis along the unperturbed trajectory of the particle is given by the expression

$$\varphi = \oint_c \frac{\delta \mathcal{H}}{v} dl,$$

where the contour integral (Fig. 1) is taken over a long and narrow rectangle surrounding the x axis and enclosing the

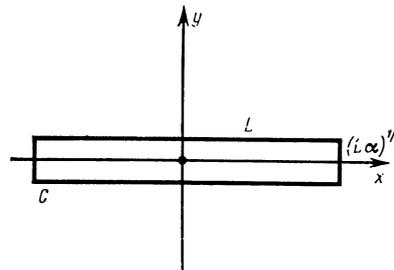


FIG. 1. Contour along which the integration is performed in the plane perpendicular to the dislocation (the x axis is directed along the projection of the group velocity of the incident excitations onto this plane).

defect. If $\varphi \neq 0$, we have the Aharonov-Bohm situation described above, which leads, in particular, to an anomalous transverse force. The anomalies in the scattering of different excitations by topological defects in He_4 and He_3 can be described in the same way (in particular, for phonons scattering off vortices in He_4 we get the familiar result³ for the transverse force). We note that the phase difference φ determines the additional transverse force perpendicular to the group velocity. We also note that all the scattering anomalies for dislocations are due to the lack of a center of inversion for dislocations, but unlike scattering by point defects, where the leading role for excitations with small momenta is played by isotropic s scattering, they incorporate no specific small quantity whatever.

2. SOME NONEQUILIBRIUM EFFECTS IN THE PRESENCE OF A FINITE DENSITY OF IDENTICAL DISLOCATIONS

The anomalies in the scattering of excitations by dislocations are very specific and have a number of macroscopic consequences. Unlike scattering by impurities and in general by scatterers which act through some potential $U(\mathbf{r})$ for which the average $\langle U(\mathbf{r}) \rangle$ reduces in the homogeneous case to a trivial shift of the chemical potential, here we have an essentially inhomogeneous situation, since the transverse force evaluated in the previous section is the same for all dislocations with identical Burgers vectors and so does not vanish on averaging over the dislocation distribution for a finite dislocation density. In writing the kinetic equation for the excitations one must include this force (as an external macroscopic force or a certain average vector potential $\langle \mathbf{A} \rangle$) in addition to the collision integral of the excitations with the dislocations. Accordingly, the Hamiltonian of the excitations is of the form

$$\mathcal{H} = \varepsilon(p_j - \langle A_j \rangle), \quad \langle A_j \rangle = \frac{1}{2} \hbar n_d \sin \varphi [\boldsymbol{\tau} \mathbf{r}]_j, \quad (2.1)$$

where $\boldsymbol{\tau}$ is a unit vector along the dislocation and n_d is the dislocation density. The gauge of $\langle A_j \rangle$ is unimportant, since the kinetic equation contains only the field strengths. The form of the average vector potential is adjusted so that the average force which arises agrees with (1.10). We take only the leading term in δp into account, so that $\varphi = \mathbf{k} \cdot \mathbf{b}$. The kinetic equation is of the form

$$\frac{\partial f}{\partial t} + \left(\frac{\partial \mathcal{H}}{\partial \mathbf{p}} \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial \mathcal{H}}{\partial \mathbf{r}} \frac{\partial f}{\partial \mathbf{p}} \right) = J(f). \quad (2.2)$$

Because of the lack of a center of symmetry, the collision integral including collisions with dislocations gives different scattering probabilities for the processes $\mathbf{p} \rightarrow \mathbf{p}'$ and $\mathbf{p}' \rightarrow \mathbf{p}$. However, this happens only in the second Born approximation, and the corresponding effects differ little from scattering by asymmetric impurities.¹¹ These effects will not be considered here, as we discuss only the τ approximation for the collision integral.

Let us take as an example the "photothermal" effect: the appearance of an electronic heat flux under illumination by a circularly polarized electromagnetic wave in the presence of parallel screw dislocations with an area density n_d . We shall consider the single-valley case, when $\varphi = \mathbf{p} \cdot \mathbf{b}$,

where \mathbf{p} is referred to the center of the Brillouin zone. Assuming that $\mathbf{p} \cdot \mathbf{b} \ll 1$, we have

$$\mathcal{H} = \frac{1}{2m} \left[\left(p_x - \frac{1}{2} n_d b y p_z \right)^2 + \left(p_y + \frac{1}{2} n_d b x p_z \right)^2 + p_z^2 \right]. \quad (2.3)$$

As independent variables in the kinetic equation it is convenient to take $v_x = \partial \mathcal{H} / \partial p_x, v_y = \partial \mathcal{H} / \partial p_y, p_z$. Then, in the presence of a circularly polarized alternating electric field $E_x = E \cos \omega t, E_y = E \sin \omega t$ the kinetic equation becomes

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial v_x} \left(\frac{eE}{m} \cos \omega t - \omega_z \right) + \frac{\partial f}{\partial v_y} \left(\frac{eE}{m} \sin \omega t + \omega_z \right) = -\frac{f - f_0}{\tau_0}, \quad (2.4)$$

where $\omega_z = n_d b p_z / \hbar m$, and τ_0 is the time between collisions due to the short-range impurities.

If the solution of equation (2.4) is sought in the form of a series in powers of eE , a time-independent correction to the distribution function appears in second order:

$$f_2 = \frac{(eE)^2}{m} \frac{1}{(\omega - \omega_z)^2 + 1/\tau_0^2} \frac{\partial}{\partial \varepsilon_{\perp}} \left(\varepsilon_{\perp} \frac{\partial f_0}{\partial \varepsilon_{\perp}} \right),$$

where $\varepsilon_{\perp} = mv_{\perp}^2/2$. Using this correction, we can get an expression for the heat flux:

$$\mathbf{q} = \frac{(eE)^2 n}{m} \left\langle \frac{p_z}{(\omega - \omega_z)^2 + 1/\tau_0^2} \right\rangle, \quad (2.5)$$

where n is the electron density and $\langle \dots \rangle$ denotes an average over the equilibrium distribution function $f_0(\varepsilon)$ of the electrons. At low dislocation densities we have $\omega_z \ll \omega, 1/\tau_0$, and this expression becomes

$$\mathbf{q} = \frac{4n_d b n \varepsilon \omega}{3m^2 (\omega^2 + 1/\tau_0^2)^2} (eE)^2,$$

where ε is the average value of the electron energy ($\varepsilon = \frac{3}{2} kT$ for a nondegenerate electron gas and $\varepsilon = \frac{3}{5} \varepsilon_F$ for a degenerate electron gas). For a thermally isolated sample of finite length L , the temperature difference arising at the ends is

$$\Delta T = \frac{n_d b l^2}{k^2 T} (eE)^2 \frac{\omega \tau_0}{(1 + (\omega \tau_0)^2)^2} L,$$

so that the total heat flux is zero: $\mathbf{q} + \kappa \nabla T = 0$ (nondegenerate electron gas; l is the mean free path).

For the second effect, let us consider a semiconductor having two valleys, \mathbf{k}_0 and $-\mathbf{k}_0$, with $\mathbf{k}_0 \parallel z$ —the direction of parallel dislocations with Burgers vector \mathbf{b} .

If we apply a voltage and a current j flows along the y axis, the Hall currents of carriers from opposite valleys arise:

$$j_{1,2}^x = \pm \frac{g}{2} j, \quad g = \frac{\tau n_d}{m} \sin(\mathbf{b} \mathbf{k}_0).$$

The total current along the x direction is the sum of the Hall current and the diffusion current:

$$j_{1,2} = j_{1,2}^x + j_{1,2}^D = \pm \frac{g}{2} j - D \frac{\partial n^{1,2}}{\partial x}.$$

At the boundary of the sample we have $j_{1,2} = 0$ (we assume that there is no transition of electrons from valley 1 to valley

2 at the boundary). The diffusion equations for carriers from different valleys are

$$-D \frac{\partial^2 n_1}{\partial x^2} = -\frac{n_1 - n_2}{\tau_v}, \quad -D \frac{\partial^2 n_2}{\partial x^2} = -\frac{n_2 - n_1}{\tau_v},$$

where τ_v is the time for transfer from one valley to the other in the interior of the semiconductor. Solving these equations and applying the boundary conditions, we find

$$n = n_1 + n_2 = \text{const}, \quad n_1 - n_2 = \frac{gjl_v}{2V\sqrt{2}D} \exp\left[\frac{\sqrt{2}}{l_v}\left(x - \frac{L}{2}\right)\right]$$

$$l_v = (D\tau_v)^{1/2}, \quad L \gg l_v, \quad L/2 - x \ll L,$$

i.e., an excess of electrons from one of the valleys arises on the surface.

If, under the same assumptions, we impose a static magnetic field along the z axis (the direction of the dislocations), the electrons in different valleys will feel a different effective magnetic field. Thus, many-valley semiconductors having dislocations oriented along the magnetic field should exhibit a splitting of the cyclotron resonance lines.

3. INFLUENCE OF DISLOCATIONS ON LOCALIZATION EFFECTS IN MANY-VALLEY SEMICONDUCTORS

The interference between electron trajectories returning to the same point but traversed in opposite directions leads to a singular quantum-mechanical correction to the conductivity.¹² A consequence of time-reversal symmetry is that the electron acquires the same phase on these trajectories, and so the correction depends strongly on perturbations which break this symmetry, e.g., a magnetic field.^{13,14}

In many-valley semiconductors whose valleys do not lie at the Brillouin zone edges (Si, Te, Bi₂Te₃), the situation is more complicated.^{12,15} At long intervalley relaxation times $\tau_v \gg \tau_i$ (τ_v is the momentum relaxation time within a valley) and for scattering solely by a scalar potential, the electron Hamiltonian has an approximate symmetry with respect to a change in the sign of the group velocity within a valley¹¹: $\varepsilon_k(\mathbf{p}) = \varepsilon_k(-\mathbf{p})$. As a result, an additional quantum correction arises due to the interference between trajectories from the same valley but traversed in opposite directions. In a brief communication¹⁶ the present authors have shown that the presence of dislocations breaks this symmetry and strongly influences the correction to the conductivity. In the present section we consider this question in more detail.

The quantum correction to the conductivity in the many-valley case can be written in the form^{11,13}

$$\delta\sigma_{ij}^{\text{qm}} = -\frac{2e^2}{\pi\hbar} \sum_{\mathbf{k}} \tau D_{ij}(\mathbf{k}) [C_{\mathbf{k}\mathbf{k}}^{\mathbf{k}\mathbf{k}}(\mathbf{r}, \mathbf{r}) + C_{-\mathbf{k}-\mathbf{k}}^{-\mathbf{k}\mathbf{k}}(\mathbf{r}, \mathbf{r})], \quad (3.1)$$

where

$$C_{\mathbf{k}_1\mathbf{k}_2}^{\mathbf{k}_3\mathbf{k}_4}(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi v \tau} \langle G_{\mathbf{k}_1\mathbf{k}_2}^R(\mathbf{r}, \mathbf{r}') G_{\mathbf{k}_3\mathbf{k}_4}^A(\mathbf{r}, \mathbf{r}') \rangle$$

($\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$) are cooperons containing the valley indices, the retarded and advanced Green functions are of the form

$$\langle G_{\mathbf{k}\mathbf{k}'}^{R/A}(p) \rangle = \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\varepsilon_F - \varepsilon_{\mathbf{k}}(\mathbf{p}) \pm i/2\tau},$$

v is the single-valley density of states (with allowance for the spin degeneracy), $D_{ij}(\mathbf{k})$ is the tensor describing the diffusion of electrons from the valley centered at \mathbf{k} , τ is the total momentum relaxation time,

$$\frac{1}{\tau} = \frac{1}{\tau_i} + \frac{1}{\tau_v}, \quad \frac{1}{\tau_v} = \sum_{\mathbf{k}_1} \frac{1}{\tau_{\mathbf{k}\mathbf{k}_1}},$$

$\tau_{\mathbf{k}\mathbf{k}_1}$ is the characteristic time for a transition from valley \mathbf{k} to valley \mathbf{k}_1 , and the angle brackets denote an averaging over the impurity distribution.

The first term in square brackets in (3.1) gives the single-valley interference correction arising on account of the symmetry of the Hamiltonian with respect to change in the velocity within a single valley, and the second term is the correction due to the time-reversal symmetry of the Hamiltonian (we shall call this the two-valley correction).

Let us first consider the two-valley correction. The cooperons

$$C_{-\mathbf{k}\mathbf{k}'}^{-\mathbf{k}'\mathbf{k}'}(q) = \frac{1}{V} \iint d\mathbf{r}_1, d\mathbf{r}_2 \exp(-iq(\mathbf{r}_1 - \mathbf{r}_2)) C_{-\mathbf{k}\mathbf{k}'}^{-\mathbf{k}'\mathbf{k}'}(\mathbf{r}_1, \mathbf{r}_2)$$

can be determined from the following system of equations, shown graphically in Fig. 2. For illustration, let us consider the simplest case, in which there are only two valleys and the corresponding system of equations in the case $q \ll 1/l$ (l is the mean free path) is of the form

$$C_{-\mathbf{k}\mathbf{k}}^{-\mathbf{k}\mathbf{k}} = C_{-\mathbf{k}\mathbf{k}}^0 \left(1 + \frac{\tau}{\tau_i} C_{-\mathbf{k}\mathbf{k}}^{-\mathbf{k}\mathbf{k}} + \frac{\tau}{\tau_v} C_{-\mathbf{k}\mathbf{k}}^{\mathbf{k}-\mathbf{k}} \right),$$

$$C_{-\mathbf{k}\mathbf{k}}^{\mathbf{k}-\mathbf{k}} = C_{-\mathbf{k}\mathbf{k}}^0 \left(\frac{\tau}{\tau_i} C_{-\mathbf{k}\mathbf{k}}^{-\mathbf{k}\mathbf{k}} + \frac{\tau}{\tau_v} C_{-\mathbf{k}\mathbf{k}}^{-\mathbf{k}\mathbf{k}} \right), \quad (3.2)$$

where

$$C_{-\mathbf{k}\mathbf{k}}^0 = \frac{1}{\pi v \tau} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \langle G_{-\mathbf{k}}^R(-\mathbf{p} + \frac{\mathbf{q}}{2}) \rangle \times \langle G_{\mathbf{k}}^A(\mathbf{p} + \frac{\mathbf{q}}{2}) \rangle$$

$$\approx 1 - \frac{\tau}{\tau_\varphi} - \tau D_{ij} q_i q_j, \quad (3.3)$$

and τ_φ is the time for disruption of the phase by inelastic processes. From (3.2) and (3.3) we easily find

$$C_{-\mathbf{k}\mathbf{k}}^{\mathbf{k}-\mathbf{k}} = \frac{1}{2\tau} \left(\frac{1}{1/\tau_\varphi + D_{ij} q_i q_j} - \frac{1}{1/\tau_\varphi + 2/\tau_v + D_{ij} q_i q_j} \right).$$

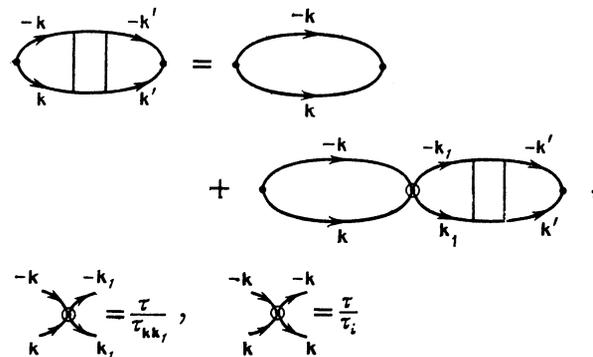


FIG. 2. Equations determining the cooperons $C_{-\mathbf{k}\mathbf{k}'}^{-\mathbf{k}'\mathbf{k}'}(\mathbf{q})$. The scattering is assumed isotropic.

Substituting this expression into (3.1), we find the corresponding correction to the conductivity:

$$\delta\sigma_{ij}^{qm} = \frac{e^2}{2\pi^2\hbar} \frac{D_{ij}}{D_{\perp}D_{\parallel}^{1/2}} \left[\frac{1}{\tau_{\varphi}^{1/2}} - \left(\frac{1}{\tau_{\varphi}} + \frac{2}{\tau_v} \right)^{1/2} \right].$$

Let us now consider the single-valley correction. We introduce the notation

$$C_{\mathbf{k}}(q) = C_{\mathbf{k}\mathbf{k}^*}(q), \quad C_{\mathbf{k}}^0(q) = \frac{1}{\pi v \tau} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \times \left\langle G_{\mathbf{k}^R} \left(\mathbf{p} + \frac{\mathbf{q}}{2} \right) \right\rangle \left\langle G_{\mathbf{k}^A} \left(-\mathbf{p} + \frac{\mathbf{q}}{2} \right) \right\rangle.$$

Summing the series of ladder diagrams, we get the following expressions for the cooperon:

$$C_{\mathbf{k}}(q) = C_{\mathbf{k}}^0(q) \left[1 - \frac{\tau}{\tau_1} C_{\mathbf{k}}^0(q) \right]^{-1}. \quad (3.4)$$

Let us evaluate $C_{\mathbf{k}}^0(q)$ for $q \ll 1/l$, taking into account the nonparabolic distortion of the band.¹⁴ To do this, we separate the energy $\varepsilon_{\mathbf{k}}(\mathbf{p})$ into parts which are symmetric and antisymmetric in \mathbf{p} :

$$\varepsilon_{\mathbf{k}}(\mathbf{p}) = \varepsilon_{\mathbf{k}}^+(\mathbf{p}) + \varepsilon_{\mathbf{k}}^-(\mathbf{p}), \quad \varepsilon_{\mathbf{k}}^+(-\mathbf{p}) = \varepsilon_{\mathbf{k}}^+(\mathbf{p}), \\ \varepsilon_{\mathbf{k}}^-(-\mathbf{p}) = -\varepsilon_{\mathbf{k}}^-(\mathbf{p}).$$

At a low occupation of the valleys we have $|\varepsilon_{\mathbf{k}}^-(\mathbf{p})| \ll \varepsilon_{\mathbf{k}}^+(\mathbf{p})$. In a crystal of cubic symmetry with valleys situated along the faces of the cube (silicon), the leading terms in the expansion is small p are

$$\varepsilon_{\mathbf{k}}^+(\mathbf{p}) = \frac{p_z^2}{2m_z} + \frac{p_{\perp}^2}{2m_{\perp}}, \quad \varepsilon_{\mathbf{k}}^-(\mathbf{p}) = \gamma p_z p_{\perp}^2. \quad (3.5)$$

Substituting $\varepsilon_{\mathbf{k}}(\mathbf{p})$ into the definition of $C_{\mathbf{k}}^0(q)$ and invoking the condition $q \ll 1/l$, we get

$$C_{\mathbf{k}}^0(q) = 1 - \tau \left(\frac{1}{\tau_{\varphi}} + \frac{1}{\tau_1} \right) - \tau D_{ij} q_i q_j. \quad (3.6)$$

Here τ_{φ} is the time for disruption of the phase on account of the distortion of the band¹⁴:

$$\frac{1}{\tau_{\varphi}} = \frac{4\tau}{\hbar^2} \langle [\varepsilon_{\mathbf{k}}^-(\mathbf{p})]^2 \rangle_{S_F},$$

where the angle brackets denote an averaging over the Fermi surface within a single valley. If $\varepsilon_{\mathbf{k}}^-$ is given by (3.5), we have

$$\frac{\tau}{\tau_{\varphi}} = \frac{256}{105} \gamma^2 \varepsilon_F m_{\perp}^2 m_z \left(\frac{\varepsilon_F \tau}{\hbar} \right)^2.$$

Substituting (3.6) into (3.4), we obtain the following expression for the single-valley cooperon:

$$C_{\mathbf{k}}(q) = \left[\tau \left(\frac{1}{\tau_{\varphi}} + D_{ij} q_i q_j \right) \right]^{-1},$$

where $1/\tau_1 = 1/\tau_{\varphi} + 1/\tau_{\gamma} + 1/\tau_v$.

According to formula (3.1), the corresponding single-valley correction to the conductivity will be of the form

$$\delta\sigma_{ij}^{qm} = \frac{e^2}{2\pi^2\hbar} \frac{1}{D_{\perp}(D_{\parallel}\tau_1)^{1/2}} \sum_{\mathbf{k}} D_{ij}(\mathbf{k}).$$

Let us now consider how dislocations affect the quantum corrections to the conductivity. It was shown in Sec. 1 that dislocations create an effective vector potential $A_j(\mathbf{k})$

for the electrons of each valley [Eq. (1.3)]. In the quasiclassical approximation the vector potential alters the Green function in the following way¹⁶:

$$\tilde{G}_{\mathbf{k}}^{R,A}(\mathbf{r}, \mathbf{r}') = \exp \left(i \int_{\mathbf{r}}^{\mathbf{r}'} A(\mathbf{k}) d\mathbf{l} \right) G_{\mathbf{k}}^{R,A}(\mathbf{r}-\mathbf{r}')$$

(the integration in the exponent is over a straight line joining the points \mathbf{r} and \mathbf{r}'). Let us consider the effect of this vector potential on the two-valley contribution. The quantity

$$C_{-\mathbf{k}\mathbf{k}}^0(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi v \tau} \langle G_{-\mathbf{k}^R}(\mathbf{r}, \mathbf{r}') \rangle \langle G_{\mathbf{k}^A}(\mathbf{r}, \mathbf{r}') \rangle$$

which determines the two-valley cooperon in the quasiclassical approximation is not affected, since $A(-\mathbf{k}) = -A(\mathbf{k})$, and the phase factors in the retarded and advanced Green functions therefore cancel. Thus, the two-valley contribution is affected by the dislocations only to the extent of a slight change in the mean free path, since this contribution is related to the time-reversal symmetry, which is not broken by dislocations. The situation is different in the case of the single-valley correction. The velocity-reversal symmetry within a single valley is broken by dislocations, and the single-valley interference will be suppressed. The quantity

$$C_{\mathbf{k}}^0(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi v \tau} \langle G_{\mathbf{k}^R}(\mathbf{r}, \mathbf{r}') \rangle \langle G_{\mathbf{k}^A}(\mathbf{r}, \mathbf{r}') \rangle$$

that determines the single-valley cooperon is altered in the presence of dislocations in the following way:

$$\tilde{C}_{\mathbf{k}}^0(\mathbf{r}_1, \mathbf{r}_2) = \exp \left[2i \int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{A}(\mathbf{k}) d\mathbf{l} \right] C_{\mathbf{k}}^0(\mathbf{r}_1, \mathbf{r}_2).$$

Using this expression, we can introduce the following equation for the single-valley cooperon¹⁶:

$$\left[\frac{1}{\tau_1} + D_{\perp} (\hat{\mathbf{p}}_{\perp} - 2\mathbf{A}_{\perp}) + D_{\parallel} (\hat{\mathbf{p}}_{\parallel} - 2\mathbf{A}_{\parallel})^2 \right] C_{\mathbf{k}}(\mathbf{r}, \mathbf{r}') = \frac{1}{\tau} \delta(\mathbf{r}-\mathbf{r}'). \quad (3.7)$$

We shall take into account only the topological interaction of the electrons with dislocations [the first term in (1.4)]. As we have pointed out, in this case a dislocation is equivalent to a narrow solenoid with a flux $\Phi = (\hbar c/e) \mathbf{k} \cdot \mathbf{b}/2\pi$. The distortion tensor appearing in A_j combines the contributions of different dislocations in an additive way. We shall assume that the dislocations are rectilinear, parallel, and distributed uniformly with a density n_d . Thus

$$A_j(\mathbf{r}) = - \sum_i k_i w_{ij}(\mathbf{r}_{\perp} - \mathbf{r}_{\perp i}).$$

Equation (3.7) can be made isotropic by the change of variables:

$$\mathbf{r}_{\perp} = \left(\frac{D_{\perp}}{D_a} \right)^{1/2} \tilde{\mathbf{r}}_{\perp}, \quad z = \left(\frac{D_{\parallel}}{D_a} \right)^{1/2} \tilde{z};$$

$$\tilde{A}_{\perp} = \left(\frac{D_{\perp}}{D_a} \right)^{1/2} A_{\perp}, \quad \tilde{A}_{\parallel} = \left(\frac{D_{\parallel}}{D_a} \right)^{1/2} A_{\parallel}, \quad \tilde{n}_d = \frac{D_c}{D_a} n_d,$$

$$D_a = (D_{\perp}^2 D_{\parallel})^{1/2}, \quad D_c^2 = D_{\perp} (D_{\perp} \cos^2 \alpha + D_{\parallel} \sin^2 \alpha);$$

here α is the angle between \mathbf{k} and the direction of the dislocations. In the new variables Eq. (3.7) becomes

$$\left[\frac{1}{\tau_1} + D_a (\tilde{\mathbf{p}} - 2\tilde{\mathbf{A}})^2 \right] C_{\mathbf{k}}(\mathbf{r}', \mathbf{r}') = \frac{1}{\tau} \delta(\mathbf{r} - \mathbf{r}'). \quad (3.8)$$

Formally, this equation is identical to the equation for the Green function of a particle of mass $1/2D_a$ moving in the field of parallel solenoids of density n_d , each of which carries a flux of $(2\hbar c/e)\mathbf{k} \cdot \mathbf{b}$.

At a low density of dislocations, when $D_c n_d \sin \varphi \ll 1/\tau_1$ ($\varphi = \mathbf{k} \cdot \mathbf{b}$), the linear (in n_d) correction to the cooperon, averaged over the dislocation distribution, is given by the expression

$$\Delta C(\tilde{\mathbf{r}}, \tilde{\mathbf{r}}) = \tilde{n}_d \int (C^1(\tilde{\mathbf{r}}, \tilde{\mathbf{r}}) - C^0(\tilde{\mathbf{r}}, \tilde{\mathbf{r}})) d\tilde{\mathbf{r}}_{\perp}. \quad (3.9)$$

Here C^0 is the free Green function, while the Green function in the field of a solenoid is

$$C^1(\tilde{\mathbf{r}}, \mathbf{r}') = \frac{1}{\tau} \sum_{m=-\infty}^{\infty} \int \frac{p_{\perp} dp_{\perp} dp_z}{(2\pi)^2} \times \frac{J_{|m+\varphi/\pi|}(p_{\perp} \tilde{r}_{\perp}) J_{|m+\varphi/\pi|}(p_{\perp} \tilde{r}'_{\perp}) \exp\{im(\theta - \theta') + ip_z(z - z')\}}{1/\tau_1 + D_a(p_{\perp}^2 + p_z^2)}$$

(here $J_{\nu}(x)$ is the Bessel function of order ν , and we have used the Aharonov-Bohm eigenfunctions¹⁰). Integral (3.9) can be evaluated exactly:

$$\Delta C(\mathbf{r}, \tilde{\mathbf{r}}) = -\frac{\Phi}{4\pi} \left(1 - \frac{\Phi}{\pi} \right) \tilde{n}_d \frac{\tau_1^{1/2}}{\tau D_a^{1/2}}.$$

Substituting this result into (3.1), we obtain the linear (in n_d) correction to the conductivity:

$$\Delta \sigma_{ij}^{\text{qm}} = \frac{n_d e^2 \tau_1^{1/2}}{2\pi D_a^{1/2}} \sum_{\mathbf{k}} D_c(\mathbf{k}) D_{ij}(\mathbf{k}) \frac{|\mathbf{k}\mathbf{b}|}{\pi} \left(1 - \frac{|\mathbf{k}\mathbf{b}|}{\pi} \right). \quad (3.10)$$

If there are several types of dislocations in the crystal, the correction is the sum of the contributions from the various dislocations.

In the case of a high dislocation density, $D_c n_d \gg 1/\tau_1$, it is extremely difficult to obtain an exact answer. For purposes of estimation, however, it is sufficient to replace τ_1 by $(D_c n_d)^{-1}$ in the formula for the quantum correction, since in this limiting case the phase disturbance is mainly due to dislocations (we assume $\sin \varphi \sim 1$); we thus obtain

$$\Delta \sigma_{ij}^{\text{qm}} \approx \frac{e^2 n_d^{1/2}}{2\pi^2 \hbar D_a^{1/2}} \sum_{\mathbf{k}} D_c^{1/2} D_{ij}. \quad (3.11)$$

We note that this effect can be substantially larger than the change in the conductivity due to the change in the mean free path. The same effects can also occur in the two-dimensional case under analogous assumptions about the many-valley spectrum of the carriers, e.g., in inversion layers at the surfaces of many-valley semiconductors. Dislocations reaching the surface lead to suppression of the single-valley interference corrections and to a decrease in the conductivity of the two-dimensional electrons. By analogy with the three-dimensional case, in the two limiting cases the change in the conductivity in the presence of dislocations is of the form

$$\Delta \sigma_{ij} = \frac{e^2}{\pi \hbar} n_d \sum_{\mathbf{k}} D_{ij}(\mathbf{k}) \frac{|\mathbf{k}\mathbf{b}|}{\pi} \left(1 - \frac{|\mathbf{k}\mathbf{b}|}{\pi} \right),$$

$$(D_{\perp} D_{\parallel})^{1/2} n_d \ll 1/\tau_1,$$

$$\Delta \sigma_{ij} \approx \frac{e^2}{2\pi^2 \hbar} \sum_{\mathbf{k}} \frac{D_{ij}(\mathbf{k})}{(D_{\perp} D_{\parallel})^{1/2}} \ln[(D_{\perp} D_{\parallel})^{1/2} n_d \tau_1],$$

$$(D_{\perp} D_{\parallel})^{1/2} n_d \gg \frac{1}{\tau_1}.$$

We note that the dislocations reaching the surface should not have a component of the Burgers vector perpendicular to the surface. If there is such a component, each dislocation is associated with a step on the surface, and the scattering of electrons by the steps will lead to a decrease in the conductivity that is much larger than the expected effect. A promising system in which to observe this effect is the (111) surface of silicon. Since all the valleys are situated identically with respect to this surface, the sixfold valley degeneracy is preserved on this surface (see Ref. 17). In addition, the most typical 60-degree dislocations for the diamond-type lattice have Burgers vectors parallel to this surface.

CONCLUSION

The change in the topology of the crystal due to the presence of dislocations causes the interaction of excitations with dislocations to be essentially different from the interaction with point impurities or linear filamentary defects. This difference is manifested most strongly in the scattering anomalies and in the appearance of an additional transverse force that cannot be expressed in terms of the scattering amplitude. For this reason the influence of dislocations on the quantum corrections to the conductivity is of a specific form and can be measured experimentally.

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¹⁾ In this section \mathbf{p} denotes the deviation of the momentum from the point of the minimum ϵ_0 .

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