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 in a crystal is due to the appearance of transverse forces that cannot be expressed in terms of the scattering amplitude. The specific correlations 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 dislocations. It was found that the transport cross section is determined mainly by the angular 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 problem that is specific to dislocations.

Analogous effects arise in the interaction of excitations with vortices in superfluid He\(_2\), where, as one of the present authors has shown,\(^3\) the long-range field of a vortex gives rise to the Born scattering to an anomalous transverse force that cannot be expressed directly in terms of the transport cross section. It was later shown that this force is directly analogous to the Aharanov-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.\(^5\) It was shown in Ref. 6 that the Aharanov-Bohm effect was also present 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 excitations with dislocations, 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.\(^6\) We perform a crystallographic transformation matching the deformed unit cell with the undeformed cell:

\[
x_{\text{def}} = x_{\text{def}}^0 + \delta x,
\]

where \(x_{\text{def}}^0\) is the position of the deformed unit cell and \(\delta x\) is the displacement of the cell.

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

\[\epsilon(x) = \epsilon(0) + \sum_{\mathbf{A}_i} (\mathbf{A}_i \cdot \nabla)^2 \epsilon_{i\mathbf{A}_i}(x),\]

where \(\mathbf{A}_i\) are the components along \(\mathbf{A}_i\), satisfies the condition of the perpendicular plane, and

\[
\mathbf{A}_i = \mathbf{V}_i \times \mathbf{x}_{\text{def}}^0.\]

If the minimum of \(\epsilon\) is found at the point \(k = 0\), then

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\[
\begin{align*}
\frac{\partial \psi}{\partial t} + \left( \frac{\partial \psi}{\partial x} \right)_x + \left( \frac{\partial \psi}{\partial y} \right)_y + \left( \frac{\partial \psi}{\partial z} \right)_z &= 0, \\
\frac{\partial \psi}{\partial x} &= \left( \frac{1}{m_1} \nabla_x \cdot \mathbf{p}_x \right) + \left( \frac{1}{m_2} \nabla_x \cdot \mathbf{p}_y \right) + \left( \frac{1}{m_3} \nabla_x \cdot \mathbf{p}_z \right), \\
\frac{\partial \psi}{\partial y} &= \left( \frac{1}{m_2} \nabla_y \cdot \mathbf{p}_y \right) + \left( \frac{1}{m_3} \nabla_y \cdot \mathbf{p}_z \right), \\
\frac{\partial \psi}{\partial z} &= \left( \frac{1}{m_3} \nabla_z \cdot \mathbf{p}_z \right).
\end{align*}
\]

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

\[
f = \psi(x, z) + t \frac{\partial \psi}{\partial t}.
\]

whereupon the equation is easily integrated to give

\[
f(x, z) = \frac{1}{4 \pi} \int \frac{\mathbf{v} \cdot \mathbf{n}}{\mathbf{p} - \mathbf{p}_0} \psi(x, z) \, dx \, dz,
\]

where \( \mathbf{v} = \mathbf{v} + \mathbf{n} \) is the velocity of the transverse wave perpendicular to the excitation. We note that \( \partial \mathbf{v} / \partial \mathbf{p} \) is a vector of intensity per area. It is directed out of the medium in the direction of the velocity of the incident excitations. The scattering of excitations by the incident excitations is a second-order process. We therefore multiply both sides by \( \mathbf{p}_0 \) and integrate over all \( \mathbf{p} \) to obtain the final result of the form

\[
f = \int \frac{\mathbf{v} \cdot \mathbf{n}}{\mathbf{p} - \mathbf{p}_0} \psi(x, z) \, dx \, dz.
\]

Equations (1.7)–(1.9) give the solution in all regions. We note that if the incident excitations are directed along \( \mathbf{v} = \mathbf{n} \), the equation for the transverse wave is the same as the equation for the incident excitation. The only difference is the additional term \( \mathbf{n} \cdot \mathbf{v} \) on the right-hand side of the equation.

Importantly, the solution we have constructed is not in the form of a sum of two separate solutions, each for a different process. The solution we have constructed is a single solution that includes both processes. The equation for the transverse wave is the same as the equation for the incident excitation, but the equation for the transverse wave includes an additional term \( \mathbf{n} \cdot \mathbf{v} \) on the right-hand side of the equation.

\[
\mathbf{v} = \mathbf{v}_0 + \mathbf{n} \mathbf{v}_1.
\]

The change in momentum along the direction of the velocity \( \mathbf{v} = \mathbf{v}_0 + \mathbf{n} \mathbf{v}_1 \) is

\[
\int \Delta \mathbf{v} \cdot \mathbf{n} \, dx \, dz = \int \frac{\mathbf{n} \cdot \mathbf{v} \cdot \mathbf{n}}{\mathbf{p} - \mathbf{p}_0} \psi(x, z) \, dx \, dz.
\]

We are interested in small angles and large distances to the diffraction near the axis \( x = z = 0 \) and below the axis along the unperturbed trajectory. The particle is given by the expression

\[
\psi = \frac{1}{2 \pi} \int \frac{\mathbf{v} \cdot \mathbf{n}}{\mathbf{p} - \mathbf{p}_0} \psi(x, z) \, dx \, dz.
\]

where the contour integral (Fig. 1) is taken over a horizontal narrow rectangle surrounding the axis and enclosing the term \( \mathcal{F} \). This is the area bounded by the contour \( \mathcal{F} \), 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 excitations. We therefore multiply both sides by \( \mathbf{n} \cdot \mathbf{v} \) and below the axis along the unperturbed trajectory.

\[
\mathbf{v} \cdot \mathbf{n} = \frac{1}{2} \left( \frac{\partial \mathbf{v}}{\partial x} \right)_x + \frac{1}{2} \left( \frac{\partial \mathbf{v}}{\partial y} \right)_y + \frac{1}{2} \left( \frac{\partial \mathbf{v}}{\partial z} \right)_z.
\]

where the last term \( \mathcal{F} \) is the area bounded by the contour \( \mathcal{F} \), 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 excitations. The solution permits evaluation of the momentum carried off by the excitations in the small-angle region (where we can drop \( \mathcal{F} \)).

FIG. 1. Contour along which the integration is performed in the plane perpendicular to the direction of the excitations (the x axis is directed along the direction of the group velocity of the incident excitations on the plane perpendicular to the excitations). The region inside the contour \( \mathcal{F} \) is the area bounded by the contour \( \mathcal{F} \), 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 excitations.
2 at the boundary). The diffusion equations for carriers from different valleys are
\[ \frac{\partial n_{i}}{\partial t} - \frac{\partial n_{i}}{\partial x_{i}} = \frac{n_{i} n_{j}}{\tau_{ij}} - \frac{n_{i} n_{j}}{\tau_{i}} \]
where \( \tau_{ij} \) is the time for transfer from one valley to the other and \( \tau_{i} \) is the lifetime within the valley. In the appropriate approximation, we find
\[ \frac{\partial n_{i}}{\partial t} = \frac{n_{i} n_{j}}{\tau_{ij}} - \frac{n_{i} n_{j}}{\tau_{i}} \]
\( \tau_{ij} \) is the characteristic time for a transition from valley \( i \) to valley \( j \), and the angle brackets denote an averaging over the impurity distribution. The first term in square brackets in (3.1) gives the valley ignorance correction arising on account of the symmetry of the Hamiltonian with respect to change in the valley. The second term gives a contribution due to the time-reversal symmetry of the Hamiltonian (we shall call this the valley correction). Let us first consider the valley correction. The equation
\[ C_{i}^{\nu \nu'}(x_{i}) = \frac{1}{2} \sum_{\alpha} \int \frac{d\alpha}{2\pi} \frac{d\beta}{2\pi} \int \frac{d\gamma}{2\pi} \int \frac{d\delta}{2\pi} \frac{d\epsilon}{2\pi} C_{i}^{\nu \nu'}(x_{i}) \]
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 of a 1D line (mean free path) is of the form
\[ C_{i}^{\nu \nu'} = C_{i}^{\nu \nu'}(x_{i}) + \frac{1}{2} \sum_{\alpha} \int \frac{d\alpha}{2\pi} \frac{d\beta}{2\pi} \int \frac{d\gamma}{2\pi} \int \frac{d\delta}{2\pi} \frac{d\epsilon}{2\pi} C_{i}^{\nu \nu'}(x_{i}) \]
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\[ C_{i}^{\nu \nu'}(x_{i}) = \frac{1}{2} \sum_{\alpha} \int \frac{d\alpha}{2\pi} \frac{d\beta}{2\pi} \int \frac{d\gamma}{2\pi} \int \frac{d\delta}{2\pi} \frac{d\epsilon}{2\pi} C_{i}^{\nu \nu'}(x_{i}) \]
and \( \tau_{ij} \) is the time for disruption of the phase on account of distortion of the band.

Substituting (3.2) and (3.3) into the definition of \( C_{i}^{\nu \nu'}(x_{i}) \) and invoking the condition that there be no change in the sign of the group velocity within a valley, the condition of valley ignorance arises due to the interference between trajectories from one valley but traversed in opposite directions. In a brief communication, the current authors have shown that the presence of dislocations breaks this symmetry and strongly influences the corrections to the conductivity. In the present section, we consider the question in more detail.

The quantum correction to the conductivity in the many-valley case can be written in the form
\[ \gamma_{i}^{\nu \nu'}(x_{i}) = \frac{1}{2} \sum_{\alpha} \int \frac{d\alpha}{2\pi} \int \frac{d\beta}{2\pi} \int \frac{d\gamma}{2\pi} \int \frac{d\delta}{2\pi} \frac{d\epsilon}{2\pi} C_{i}^{\nu \nu'}(x_{i}) \]
(3.1)
where \( C_{i}^{\nu \nu'}(x_{i}) \) are coorponders containing the valley indices, the retarded and advanced Green functions are of the form
\[ C_{i}^{\nu \nu'}(x_{i}) = \frac{1}{2} \sum_{\alpha} \int \frac{d\alpha}{2\pi} \int \frac{d\beta}{2\pi} \int \frac{d\gamma}{2\pi} \int \frac{d\delta}{2\pi} \frac{d\epsilon}{2\pi} C_{i}^{\nu \nu'}(x_{i}) \]

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(3.1)
we note that the dislocations reaching the surface have not yet completed their movement to the surface. If there is such a component, each dislocation is associated with a step on the surface, and the scattering by this step will lead to a decrease in the conductivity that is much larger than the expected effect. A proper system in which to observe this effect is the (111) surface. Since all the valleys are situated identically with respect to the surface, the stair-rod valley geometry is preserved on this surface (see Ref. 17). In addition, the typical 60-degree dislocations for the diamond-type 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 excitons with dislocations to be essentially different from the interaction with point impurities or linear imperfections. The difference is manifested most strongly in the scatter 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 quantum corrections to the conductivity is of a specific form and can be measured experimentally.

In closing, we wish to thank D. E. Khmel’nikskii and I. Rashba for helpful discussions.