Green's functions are used to study interband transitions in a quasiclassical (i.e., slowly varying in space) irregular field. It is assumed that the irregular field is random, i.e., the mean square of the fluctuation of the potential energy of an electron in such a field is much less than the width of the forbidden band. Explicit expressions are obtained for the coefficient of interband optical absorption for the case of an anisotropic irregular field and for the case when the irregular fields that act on electrons in the conduction and the valence band are different. As examples, we consider a fluctuation random field in ferroelectrics and a random field produced by long-wave acoustic lattice vibrations. The behavior of the tail of the optical absorption coefficient in ferroelectrics in the region of a phase transition is discussed.

1. Introduction

Interest in problems connected with the behavior of electrons in irregular structures has increased considerably in recent times. This is due not only to practical requirements but also to the general progress in the development of theoretical methods of physics, in particular, solid-state physics. In its most general form, the problem of the behavior of electrons in irregular fields is associated with exceptional mathematical difficulties. In theoretical studies of the problem it has been necessary to apply crude and not always well justified assumptions. In this connection, considerable methodological interest attaches to the solution of problems in which the characteristics of such unordered systems can be calculated under assumptions that are known to be reasonable. In particular, Bonch-Bruevich [1, 2] has considered a problem in which one can carry out the calculations to the end and obtain explicit expressions for characteristics such as the density of states and the complex electrical conductivity, which have a precise meaning in unordered systems. This can be done under the assumption that the random field \( U(r) \) in which an electron moves is quasiclassical. The quasiclassical condition means that the probabilities are appreciably different from zero only for comparatively smooth functions \( U(r) \). As is shown in [1], this condition can be satisfied, in practice, for a large class of actual problems. The parameter \( \eta \) that determines the slowness of the variation of the random field in space is clearly the ratio of the characteristic field length \( r_U \) to the characteristic electron length \( r_e \). In the adopted approximation

\[
\eta = \frac{r_U}{r_e} \gg 1.
\]

The aim of the present paper is to generalize the results of [1, 2] in two directions: a) to the case of an anisotropic irregular field, when the correlation function \( \psi(r' - r'') = \langle U(r') U(r'') \rangle \), where the angular brackets denote averaging over the random field, depends not only on the magnitude but also the direction of the vector \( r = r' - r'' \); b) to the case when the irregular fields that act on the electrons in the conduction and the valence bands, \( U_C \) and \( U_V \), are different: \( U_C \neq U_V \). As an example for the first part of the paper we consider a fluctuation random field in ferroelectrics. We discuss the behavior of the tail of the optical absorption coefficient of such materials in the region of the phase transition. As an example for the second part of the paper we consider the random field produced by low-frequency lattice vibrations.
2. Anisotropic Random Field

We consider an anisotropic crystal that in the absence of the random field has forbidden band width $\Delta$ and dispersion laws $\omega(\mathbf{k})$, where $\mathbf{k} = (k_x, k_y, k_z)$ is the quasiwave vector:

\[ \omega_x = \beta_{cx} k_x^2 + \beta_{cy} k_y^2 + \beta_{cz} k_z^2 \quad \text{for the conduction band;} \]
\[ \omega_v = -\Delta - \beta_{cx} k_x^2 - \beta_{cy} k_y^2 - \beta_{cz} k_z^2 \quad \text{for the valence band.} \]

Here, the energy origin is taken to be the lower edge of the conduction band in the absence of the random field, and $\beta_{i\ell} = 1/(2m_i)$ are the components of the tensors of the reciprocal effective masses in coordinate axes coinciding with the principal symmetry axes of the crystal. Here and in what follows, $\hbar = 1$.

If a random field $U(\mathbf{r})$ is applied to the crystal, the edges of the energy bands are "smeared" and concepts such as the forbidden band width and the dispersion law become meaningless in general. However, if the random field is such that

\[ \left< U^2 \right> \ll \Delta \]

(and it is such fields that we shall consider in this paper), the above concepts can be preserved by regarding them as unrenormalized characteristics. We shall be interested in the coefficient of optical absorption $\alpha(\omega)$ associated with transitions of electrons from the valence to the conduction band at frequencies $\omega$ satisfying

\[ |\Delta - \omega| \ll \Delta. \]

In this section we shall consider the case when the irregular fields in the two bands are identical: $U_c = U_v = U$. Because in this case the forbidden band width $\Delta(\mathbf{r})$ is a constant as a function of the coordinates, $\Delta(\mathbf{r}) = \text{const}$, we can only obtain a nonvanishing tail of the absorption coefficient at frequencies $\omega < \Delta$ if we take into account the quantum effect of delocalization of an electron and the associated possibility of "oblique" (in the spatial sense) transitions. Below, we shall show that in this case the tail of the absorption coefficient is determined not by $\Psi$ itself but by its second derivative:

\[ \Psi_{\alpha 3} = -\frac{\partial^2 \Psi}{\partial r_3 \partial r_3} \bigg|_{r_0} = \left< \frac{\partial U}{\partial r_3} \frac{\partial U}{\partial r_3} \right>_r, \]

which for an anisotropic random field is a second-rank tensor.

For simplicity, we shall consider the case when the principal axes of the real permittivity and electrical conductivity tensor coincide. Then in coordinate axes that coincide with the principal symmetry axes of the crystal, the absorption coefficient is given by the well-known formula

\[ \alpha_i(\omega) = \frac{4\pi}{cn_i} \Re \sigma_{ii}(\omega), \]

where $\sigma_{ii}(\omega)$ are the diagonal components of the complex electrical conductivity tensor, $n_i$ are the principal refractive indices of the crystal (at the frequency $\omega$), and $c$ is the velocity of light in vacuum.

Following [1], we write down an expression for the real electrical conductivity in the form

\[ \Re \sigma_i(\omega) = \frac{4\pi e^2}{m_0} \int dx \lim_{y \to y'} < \imath K(x, x'; y, y'; t) >; \]

where $e$ is the electron charge, and

\[ \Gamma_i = \int u_{x_i}^* \ov v_i u_{y'} r |^2, \]

where $u_{x_i}$ and $u_{y'}$ are Bloch wave functions of an electron corresponding to the edges of the respective bands; $\ov v_i = -i/(m_0) \partial / \partial k_i$ are the components of the velocity operator; $m_0$ is the mass of a free electron; $K(\omega)$ is the Fourier transform of the two-particle retarded Green's function:

\[ K(x, x'; y, y'; t - t') = \langle \ov a(x, t) a(x', t) | \ov a(y, t') a(y', t') \rangle, \]

where $\ov a$ and $a$ are Fermi operators of creation and annihilation in the Heisenberg representation; $x$ and $y$ are spatial coordinates; and $t$ is the time.