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INTERBAND TRANSITIONS IN DISORDERED SYSTEMS WITH A SLOWLY VARYING RANDOM FIELD

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The specific properties of disordered systems ([1]) greatly complicate the development of a consistently microscopic theory of them (unless one speaks of purely "model" systems). In such a situation it is meaningful to take a phenomenological approach, in which the dynamical features of the system are reflected by several experimentally determined parameters. The theory must find these parameters and indicate the corresponding experiments.

In the present note a model is considered of independent quasiparticles moving in a static slowly varying random field. By definition, the latter is characterized by a smooth function of spatial correlation, varying slowly on the characteristic "electronic" length. The system is assumed to be macroscopically homogeneous in the sense of ([2]). Problems of this type arise in the theory of substances with large Maxwell relaxation times, in surface physics, in studies of the interaction of charge carriers with low-frequency disordered acoustic oscillations ("noise"), and also in the theory of strongly alloyed semiconductors*. Apparently, the model also has a certain meaning in application to amorphous and liquid semiconductors or to glasses.

The density of states in such a system has been calculated by a number of authors (see, for example, ([2–9])). In particular, the works ([2–4,9]) were based on a quasiclassical approximation consisting of a certain expansion in powers of the spatial derivatives of the random potential V. In the present work the same approach is used to study interband optical transitions**. This formulation of the problem is meaningful if the mean fluctuation $\langle (V - \langle V \rangle)^2 \rangle$ is small in comparison with the width of the forbidden band Δ. The same problem was considered earlier in the works ([10,11]). The first of them, however, was based on an approximation opposite to that adopted here; on the other hand, in ([11]) a purely classical approximation was used (all spatial derivatives of the random potential were discarded)***. As was noted in ([12]), this is sometimes justified in

calculating the density of states (but not in kinetics, since momentum scattering is then completely excluded). We shall take into account the first nonvanishing quantum correction.

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* In the latter case additional complications arise, connected with the divergence of the Coulomb field at small distances. They require special consideration and do not fundamentally change the results set forth below.

** Expressions of the type "band edge," etc., refer to an auxiliary system with excluded fluctuations of the force field, i.e., to an ideal crystal with a "renormalized" Hamiltonian containing the term $\langle V\rangle$; brackets here and below denote averaging over the random field.

*** For this reason the comparison of the results of ([10,11]) carried out in ([11]) appears to be of little content: the calculations were performed under mutually exclusive assumptions.

The problem consists in calculating the absorption coefficient a. In a cubic crystal (or in an isotropic substance), as is known,

$$a = \frac{4\pi e^2\Gamma}{c\hbar\omega\sqrt{\varepsilon}} \int dx \lim_{\substack{x'\to x\\ y'\to y}} \langle \operatorname{Im} K(x,x';y,y';\omega)\rangle. \tag{1}$$

Here c is the speed of light in vacuum; ε is the real part of the dielectric permittivity; ω is the frequency of light (for simplicity it is assumed to be much greater than the plasma frequency of the free carriers); $K = \langle\langle \bar{a}(x)a(x') \mid \bar{a}(y)a(y')\rangle\rangle^r$ is the corresponding two-particle Green' s function; $\bar{a}$ and a are creation and annihilation operators; $\Gamma = \frac{1}{3}\left|\int U_c^*\left(-\frac{i\hbar}{m_0}\nabla\right)U_v\,dx\right|^2$, where m_0 is the mass of a free electron; U_v and U_c are the periodic parts of the Bloch function corresponding to the band edges (provided that $\Gamma \neq 0$). In the adopted model the function K (before averaging) factorizes exactly into one-particle functions. In this case the following term in the integrand in (1) corresponds to interband transitions:

$$2\lim_{\substack{x\to x'\\ y\to y'}} \int_{-\infty}^{+\infty} d\omega' \{n_F(\omega'-\omega,\mu_v) - n_F(\omega',\mu_c)\}\times$$

$$\times \langle \operatorname{Im} G_r^+(y',x;c;\omega') \operatorname{Im} G_r^+(x',y;v;\omega'-\omega)\rangle. \tag{2}$$

Here G_r^+ is the one-particle Green' s function; the indices c and v correspond to the conduction and valence bands; n_F is the Fermi function; μ_v and μ_c are the Fermi levels in the corresponding bands (under equilibrium conditions with respect to concentration $\mu_v = |\mu_c|$). In the quasiclassical approximation we have (putting $\hbar = 2m_0 = 1$ [2])

$$G_r^+(x_1, x_2; l, E) =$$

$$= \frac{i}{(2\pi)^4} \int_0^\infty ds \int dk \, \exp\{-\varepsilon s + is(E - W_{kl}) + i(k, x_1 - x_2) + \varphi_l\}, \quad (3)$$

where $l = c, v$, $\varepsilon \to +0$, and W_{kl} is the dispersion law for the l-th band.

We shall consider the simplest case, where $W_c = \beta_c k^2$, $W_v = -\Delta - \beta_v k^2$, $\beta_l = m_0/m_l$; then

$$\varphi_c = -isU(R) + \frac{s^2}{4}\beta_c \nabla^2 U - \frac{is^3}{12}\beta_c (\nabla U)^2 -$$

$$- \left[\frac{is^3}{6}\beta_c^2 k_\alpha k_\beta - \frac{is^2}{4}\beta_c r_\alpha k_\beta + \frac{is}{8} r_\alpha r_\beta\right] \frac{\partial^2 U}{\partial R_\alpha \partial R_\beta}, \quad (4)$$

here $U = V - \langle V \rangle$, $R = (x_1 + x_2)/2$, and α, β are vector indices. The function φ_v is given by formula (4) with β_c replaced by $-\beta_v$. The most "model-dependent" part of the calculation consists in averaging, for the functional $P[U]$, which determines the probability of realization of a given function $U(R)$, must be specified *a priori*. For small fluctuations it is natural to use a Gaussian form P*. In this case the result is naturally expressed in terms of the correlation function $\langle U(R)U(R')\rangle$; in the case under consideration it depends only on $|R - R'|$, and the answer is expressed in terms of two parameters (with the dimensions, respectively, of the square and cube of energy):

$$\psi_1 = \langle U^2 \rangle, \qquad \psi_2 = \frac{1}{2}\langle (\nabla U)^2 \rangle. \quad (5)$$

These (along with m_c, m_v, and Δ) are the parameters mentioned at the beginning of the article; ψ_2 describes the first quantum correction (in Gaussian units this parameter would contain an additional factor $\hbar^2/2m_0$).

* The case of randomly distributed impurity centers requires special consideration.

Combining formulas (1)–(4) and carrying out the averaging, we find the general expression for $\alpha(\omega)$. It turns out to be rather cumbersome; therefore here we shall give only some results for the tail ($\omega < \Delta$). In the spirit of the adopted approximation we shall assume that $\psi_2^{1/3} \ll T$, $\psi_2 \ll \psi_1^{3/2}$, $\psi_1^{1/2} \ll \Delta - \omega$, where T is the temperature in energy units. However, even in this case the result depends strongly on the relations between the various quantities (μ_c, μ_v, etc.). For simplicity we shall assume that $m_v \gg m_c$, now using m_c as the unit of mass, and consider separately the cases of high and low temperatures. The latter are defined, respectively, by the conditions $\pi T \gg \psi_1^{1/2}$ and $\pi T \ll \psi_1^{1/2}$.

At high temperatures we obtain

$$\alpha = \frac{e^2\Gamma\psi_2}{T\pi c\omega\sqrt{\varepsilon}\,2^{5/4}(\Delta-\omega)^{3/2}}\,\mathrm{sh}\left(\frac{\omega+\mu_v-\mu_c}{2T}\right)\times$$

$$\times\exp\left\{-\frac{\Delta-\omega}{2T}-\frac{\Delta+\mu_c+\mu_v}{2T}-\frac{T(\Delta-\omega)^2}{6\psi_2}\right\}. \tag{6}$$

At low temperatures we distinguish two cases:

a) $\Delta+\mu_c-\omega>0, \quad \Delta+\mu_v>0$:

$$\alpha = \frac{e^2\Gamma\psi_2^{3/2}}{(2\pi)^2 c\omega\sqrt{2\varepsilon}\,(\Delta-\omega)^{5/2}}\left\{\frac{1}{(\Delta+\mu_c-\omega)^{3/2}}-\frac{1}{(\Delta+\mu_c)^{3/2}}\right\}; \tag{7a}$$

b) $\Delta+\mu_c-\omega<0, \quad \Delta+\mu_v>0$:

$$\alpha = \frac{e^2\Gamma\psi_2^{1/2}}{32\pi c\omega\sqrt{\varepsilon}}(\Delta-\omega)^{-1/2}(\omega-\Delta-\mu_c)^{-1/2}. \tag{7b}$$

Let us note that the quantity ψ_1 does not enter explicitly into the limiting formulas (6), (7a, b), but determines the limits of their applicability. Evidently, the latter circumstance constitutes one of the differences between our approach and that adopted in ([13]). It is also seen that in the tail region $\alpha = 0$, if ψ_2 is neglected: a purely classical approximation loses the entire effect.

The conditions of applicability of the quasiclassical approach have been discussed repeatedly (see, for example, ([2,11])). In the problem under consideration the main role is played by the inequality $r_F \gg \hbar(2m\psi_1^{1/2})^{-1/3}$, where r_F is the length over which the field changes appreciably. Depending on the nature of the system, this may be the screening radius or the length of the "central" sound wave in a packet, or the ratio $D/|\sigma|$, where D and σ are, respectively, the diffusion coefficient and the differential conductivity of the charge carriers.

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Note: Figure translations are in progress. See original paper for figures.