CONTRIBUTION TO THE THEORY OF ABSORPTION OF LOW-FREQUENCY ELECTROMAGNETIC WAVES IN DISORDERED SEMICONDUCTORS

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The Dyson statistical theory of energy levels is used to calculate the frequency dependence of the real part of the electric conductivity, connected with the electronic transitions between discrete local levels in a disordered system. The region considered is that of "extremely low" frequencies, satisfying the condition $\hbar\omega \ll \bar{E}$, where $\bar{E}$ ($\sim 10^{-2}$ eV) is the characteristic energy in which the density of state changes noticeably. In particular, the static electric conductivity of such a system is calculated and is found to differ from zero only when account is taken of the lattice deformation occurring during the electronic transition.

1. INTRODUCTION

BY now it has apparently been established[1-6] [1)] that the "forbidden band" [2)] of a disordered semiconductor is actually completely filled with "tails" of the density of states produced by a random field caused by one factor or another. Near the boundaries of the allowed bands, the states on the tail of the density of states belong to the continuous spectrum, and the electrons (holes) occupying these states take part in the transport of the direct current. Somewhere deep in the forbidden band, however, these states apparently give way to localized ones. Each of the latter, of course, should belong to a discrete spectrum; in their aggregate, however, these levels (connected with sufficiently deep potential wells of random origin) form an almost continuous sequence. The question of the contribution of these states to the transport of the direct current is still not fully clear (see the discussion in[5]).

In this paper we investigate the real part of the electric conductivity at low frequencies ω, corresponding to transitions between closely-lying discrete levels. The exact meaning of this expression is determined by the inequality

$$\hbar\omega \ll \bar{E}, \tag{1}$$

where $\bar{E}$ is the characteristic energy over which the density of state changes noticeably. Obviously, such a formulation of the problem is meaningful precisely for an aggregate of closely-lying discrete levels, the average distance D between them (in the energy region under consideration) satisfies an inequality of the type (1): $D \ll \bar{E}$.[3)] By virtue of the random character of the forced field in the system in question and the relative moments of D, the true distances between the levels, of course, fluctuate strongly and they can be regarded as perfectly random numbers. In other words, we are under conditions of applicability of the statistical theory of Dyson and Mehta[8,9], the results of which we shall use from now on[4)].

In the analysis of the behavior of electrons and holes in the systems (and problems) of interest to us, it suffices to use the single-particle approximation, with collective effects taken into account (if necessary) only via a screened potential. Accordingly, we can introduce a representation in which the single-particle Green's function (not yet averaged over the random field) is diagonal:

$$G_r(\lambda, \lambda'; E) = -\frac{1}{2\pi}\delta_{\lambda\lambda'}\frac{1}{E - W_\lambda + i\varepsilon}. \tag{2}$$

Here G_r is the retarded anticommutator Green's function, E is the real energy variable, and $\epsilon \to +0$, λ and λ' are sets of quantum numbers characterizing the states with energies W_λ and $W_{\lambda'}$. Inasmuch as in a random field there is hardly any probability of finding spatial symmetry, λ contains, generally speaking, only the energy itself and also the triplet of coordinates R, indicating the position of the given potential well. In a macroscopically homogeneous system, W does not depend on R[5)].

It is convenient to calculate first the density of states $\rho(E)$, defined by the standard formula

$$\rho(E) = \frac{2}{\Omega}\langle \mathrm{Sp}\,\mathrm{Im}\,G_r(E)\rangle. \tag{3}$$

Here Ω is the volume of the system, and the angle brackets denote averaging over the random field. We denote by $P_W(R)$ the density of the probability that near R there is formed a potential well containing a level W. Noting that in a macroscopically homogeneous system P_W it is practically independent of R, we have, using (2) and (3):

[1)] The author is grateful to Professor I. Stuke for his preprint.

[2)] The concepts of allowed and forbidden bands in such a system can be correctly determined without resorting to any model representation [7].

[3)] We note, however, that by the very definition of the concept "discrete level" the quantity D cannot be arbitrarily small: it should exceed at least the sum of the proper widths of two neighboring levels.

[4)] The results of [8,9] were used also in [10] in a similar problem (but having a different formulation) in solid-state theory.

[5)] The spin variables in our problem need not be indicated explicitly: in the case of a sufficiently strong spin-orbit interaction, different values of the spin variables correspond to different values of the energy, and in the absence of the aforementioned interaction the electrons can be regarded simply as having no spin.

$$\rho(E)=\sum_{w}P_{w}\delta(E-W)\approx\int dW\frac{P(W)}{D}\delta(E-W)\equiv\frac{P(E)}{D}. \quad (4)$$

Here D is the average distance between two successive levels in the given energy region; the transition from summation to integration in (4) is meaningful if the function P(E) (and by the same token $\rho(E)$) changes only slowly over the "distance" D.

As seen from (4) the density of states, strictly speaking, is a "palisade" of δ functions; under the conditions indicated above, however, it is approximated by continuous "envelope" P(E).

2. LOW-FREQUENCY ELECTRIC CONDUCTIVITY IN A "RIGID" MATERIAL

In the study of the electronic transitions between discrete levels, allowance for the possible deformations of the lattice, and particularly multi-phonon transitions, may turn out to be very important. It is convenient methodologically, however, to consider first the simple problem of the electric conductivity of a "rigid" material, in which the positions of equilibrium and the oscillation frequencies of the heavy particles do not change during the course of the electronic transition. Within the framework of the model employed above, we have (omitting the constant factors which are immaterial in what follows)

$$\operatorname{Re}\sigma(\omega)\sim\frac{1}{\omega}\sum_{W',W''}\int d\mathbf{R}'\,d\mathbf{R}''P(\mathbf{R}',\mathbf{R}'')\,|\,(W',\mathbf{R}'|j|W'',\mathbf{R}'')\,|^{2}\times\{n_{F}(W')-n_{F}(W'')\}\,\delta(W'-W''+\hbar\omega). \quad (5)$$

Here n_F is the Fermi function, $(W', \mathbf{R}'|j|W'', \mathbf{R}'')$ is the matrix element of the current density, and $P(\mathbf{R}', \mathbf{R}'')$ is the density of the probability that potential wells containing the levels W′ and W″ respectively will appear near the points $\mathbf{R}'$ and $\mathbf{R}''$. In a macroscopically homogeneous and isotropic medium, obviously,

$$P(\mathbf{R}',\mathbf{R}'')=\Omega^{-1}\Phi(\mathbf{R}),$$

where $\mathbf{R}'-\mathbf{R}''=\mathbf{R}$, and the function Φ describes the spatial correlation in the positions of the wells; neglecting the latter, we have $\Phi = 1/\Omega$.

Averaging the expressions (5) over the distribution of the levels reduces to a replacement of the sum over W′ and W″ by the integral

$$\int dW'\,dW''\,\rho(W')\rho(W'')\Omega^{2}[1-Y_{2}(W'-W'')]\;(\ldots), \quad (6)$$

where the dots stand for the expression under the summation sign in (5), and $Y_W(W'-W'')$ is the correlation function calculated in[8,9].

To calculate the current-density matrix element, we use the asymptotic form of the wave functions of the discrete spectrum

$$\psi_{W,\mathbf{R}}\sim\gamma^{3/2}(W)\,\exp\{-\gamma(W)\,|\mathbf{r}-\mathbf{R}|\}, \quad (7)$$

where $\gamma=\hbar^{-1}\sqrt{2m^{*}I}$, I is the ionization energy of the given level (I = const − W), and m* is a quantity with the dimension of mass (generally speaking, it does not coincide with either the effective mass as usually defined or the free-electron mass; the exact value of m* does not matter in this case)[6].

[6] We do not use the effective-mass method. It is easy to verify that formula (7) remains valid also in the case when the random potential wells occur against a background of a periodic field.

Using formulas (7), we obtain (again omitting inessential factors):

$$|(W',\mathbf{R}'|j|W'',\mathbf{R}'')|^{2}\sim(W'-W'')^{2}\gamma^{6}(W')R^{8}\cdot\times\frac{e^{-2a}}{a^{2}}\left(\frac{2\operatorname{sh}b}{b^{2}}-\frac{6\operatorname{ch}b}{b^{3}}+\frac{6\operatorname{sh}b}{b^{4}}\right)^{2}, \quad (8)$$

where

$$a=\gamma(W')R,\quad b=\frac{W'-W''}{4I}\gamma(W')R.$$

In the derivation of (8) we used the inequalities[7]

$$\hbar\omega\ll I,\quad a\gg 1.$$

When $b \ll 1$ (the case of greatest interest) Eq. (8) takes the form

$$|(W',\mathbf{R}'|j|W'',\mathbf{R}'')|^{2}\sim(W'-W'')^{4}R^{8}\gamma^{6}(W')\exp\{-2R\gamma(W')\}. \quad (9)$$

We note that the vanishing of the right side of (8) (or (9)) at W″ = W′ is not connected with the choice of the wave functions in the form (7). Indeed, the factor $(W'-W'')^2$ in (8) comes from the relation between the matrix elements of the current density and the coordinate (the second factor in (8)). The latter should also vanish in the system under consideration when W″ = W′, by virtue of the obvious symmetry considerations and by virtue of the absence of any quantum numbers other than the energy itself and the coordinates of the center of the well. Moreover, even if some additional accidental symmetry does occur (or if the model is made complicated in any other manner), the matrix element of the coordinate will be inevitably bounded at W′ = W″, so long as it is calculated with the aid of the wave functions of the discrete spectrum. Accordingly, when W″ → W′ the square of the matrix element of the current density vanishes not slower than $(W'-W')^2$.

Substituting (9) and (5) and using inequality (1), we obtain, taking (6) into account:

$$\operatorname{Re}\sigma\sim\omega^{4}[1-Y_{2}(\hbar\omega)]A, \quad (10)$$

where

$$A=\int dW'\,\rho^{2}(W')\frac{1}{\omega}[n_{F}(W')-n_{F}(W'+\hbar\omega)]\gamma^{6}(W')\times\int_{0}^{\infty}dR\,R^{10}\Phi(R)\exp[-2R\gamma(W')]. \quad (11)$$

In accordance with the previously adopted formulation of the problem, we confine ourselves to the case when

$$\hbar\omega\ll\mu\ \text{ or }\ \hbar\omega\ll kT \quad (12)$$

(μ is the Fermi level; the first inequality is for a degenerate system and the second for a nondegenerate one). Then the integral A ceases to depend on ω, and its value at T = 0 is determined, as expected, only by the situation at W′ = μ, and the entire frequency dependence of Re σ is given by an expression which is explicitly written out in (10). The first factor (ω^4) is due here to the matrix element of the current density and is connected with the inequality $(\hbar\omega/4I)R\gamma(W') \ll 1$ (see also the remark made in front of formula (10)). The second factor describes the statistical

[7] Actually it will be shown below that an important role is played by the values $a \sim 5$; allowance for terms of order 1/a, however, would be an exaggeration of the accuracy, so long as the function (7) is employed.

correlation between the levels. As is well known[8,9] it has a different form for the orthogonal, symplectic, and unitary ensembles, namely:

$$Y_2^{\text{ortho}} = \left(\frac{\sin t}{t}\right)^2 + \int_1^\infty \frac{\sin ty}{y}\,dy\,\frac{d}{dt}\left(\frac{\sin t}{t}\right), \tag{13a}$$

$$Y_2^{\text{sympl}} = \left(\frac{\sin t}{t}\right)^2 + \int_0^1 \frac{\sin ty}{y}\,dy\,\frac{d}{dt}\left(\frac{\sin t}{t}\right)^2, \tag{13b}$$

$$Y_2^{\text{unit}} = \left(\frac{\sin t}{t}\right)^2. \tag{13c}$$

Here (in our notation) $t = \pi\hbar\omega/D$.

An orthogonal ensemble is realized in the absence of a magnetic field if the system as a whole is invariant against the spatial rotations (for example, the material in question is not ferroelectric) or has an integer spin. The symplectic ensemble is realized (also in the absence of a magnetic field) if there is no invariance against the spatial rotation, and the total spin is half-integer. Finally, the unitary ensemble corresponds to the case of the system in a magnetic field whose intensity satisfies the inequality $\beta H \gg D$ (β is the Bohr magneton). As seen from formulas (10) and (13a)–(13c), inclusion of such a magnetic field should noticeably alter the frequency dependence of the absorption coefficient of the low-frequency electromagnetic waves. We note also the difference in the frequency dependence of the absorption coefficient for systems with integer and half-integer spin at sufficiently large spin-orbit coupling or in the case of ferroelectrics (transition from the orthogonal to the symplectic ensemble).

When $\hbar\omega \ll D$ we have

$$1 - Y_2^{\text{ortho}} = \pi^2\hbar\omega/D, \tag{14a}$$

$$1 - Y_2^{\text{sympl}} = {}^1/_3(\pi\hbar\omega/D)^2, \tag{14b}$$

$$1 - Y_2^{\text{unit}} = {}^2/_3(\pi\hbar\omega/D)^2. \tag{14c}$$

From this, taking (10) into account, we see that under the conditions in question (for any ensemble)

$$\operatorname{Re}\sigma(\omega) \to 0 \text{ as } \omega \to 0. \tag{15}$$

The form of the matrix element influences here only the law according to which Re σ tends to zero as $\omega \to 0$; the very fact of the vanishing of the static electric conductivity is already imposed by formulas (14a) and (14b), i.e., the effect of "level repulsion"[8]. We note, however, that this result is essentially connected with the approximation of the "rigid" material; when account is taken of the interaction with the phonons, the situation is different (Sec. 3).

At first glance it might appear that the result (15) contradicts the general theorem[7,11] concerning the finite value of Re $\sigma(0)$ at $T = 0$, so long as the density of states $\rho(E)$ is finite and continuous at $E = \mu$. Actually, however, there is no such contradiction, for in proving the theorem we used explicitly the assumption that the spectrum is continuous (in the exact mathematical sense of the word); on the other hand, in the case considered now the density of states only seems to be continuous (see the discussion following formula (4)).

[8]In fact, these considerations do not differ from those discussed in [2b]; the quantitative results, however, are somewhat different.

3. CASE OF DEFORMABLE MATERIAL

The possible role of phonons in the system under consideration is obvious: because of their emission or absorption, electronic transitions become possible, for example, between the unequal-energy levels, and this, as we shall show, leads in particular to a finite value of $\sigma(0)$.

For our purposes, the Condon approximation is sufficient and the frequency effect can be neglected. We can then readily obtain for the electric conductivity σ_{ph}, calculated with allowance for the deformation of the material in the electronic transitions, the expression (see[12])

$$\sigma_{ph}(\omega) = \int_{-\infty}^{+\infty} d\nu\, K(\nu)\,\sigma(\omega - \nu), \tag{16}$$

where σ is the electric conductivity calculated for a non-deformable material (see the preceding section) and $K(\nu)$ is a function defined by the well known formulas of the theory of multiphonon transitions (see, for example,[13]):

$$K(\nu) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt \exp\{i\nu t - \varphi(t)\}, \tag{17}$$

$$\varphi = \varphi_\infty + \psi(t), \tag{18}$$

$$\varphi_\infty = -\sum_k \frac{2N_k + 1}{2\hbar^2\omega_k^2}|B(k)|^2, \tag{19}$$

$$\psi(t) = \sum_k \frac{|B(k)|^2}{\hbar^2\omega_k^2}\{e^{i\omega_k t} + 2N_k\cos\omega_k t\}. \tag{20}$$

Here k are the quantum numbers determining the state of the phonon, ω_k are the corresponding frequency, N_k is the Planck function, B(k) the mean value of the energy of interaction of the electron with the phonons in the state (W", R"). The explicit form of B(k) cannot yet be readily established with complete assurance, if for no other reason than that the very form of the electron-phonon interaction energy operator calls for a special investigation for the systems under consideration. For our purposes, however, it suffices to remark that the functions $\psi_{W'',R''}$ correspond to a sufficiently deep (and therefore strongly localized) state. For this reason, we can assume for most phonons that $B(k)^2$ is practically independent of the form of $\psi_{W'',R''}$.

Noting that $\psi(t) \to 0$ as $t \to \infty$ and $\psi(-t) = \psi^*(t)$, we can rewrite formula (16) in the form

$$\operatorname{Re}\sigma_{ph}(\omega) = \operatorname{Re}\sigma(\omega)e^{\psi_\infty} + e^{\psi_\infty}\int_0^\infty d\nu\, F(\nu)\,[\operatorname{Re}\sigma(\nu - \omega) + \operatorname{Re}\sigma(\nu + \omega)]. \tag{21}$$

Here

$$F(\nu) = \frac{1}{\pi}\int_0^\infty dt\{e^{\psi_1}\cos(\nu t + \psi_2) - \cos\nu t\}, \tag{22}$$

and ψ_1 and ψ_2 are the real and imaginary parts of the function ψ.

The first term in (21) describes the "phononless line," and the second describes transitions with phonons taking part. As expected, the statistical electric conductivity is now different from zero even at zero temperature.

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