CALCULATION OF THE CONDUCTIVITY OF A DISORDERED SEMICONDUCTOR IN A STRONG FIELD MIXED WITH A RANDOM FIELD

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A study is made of the importance of the random field when the conductivity of a disordered semiconductor is determined by the delocalization of some of the bound carriers. The random field weakens the voltage dependence of the current.

1. INTRODUCTION

It has repeatedly been pointed out that it is virtually impossible to produce ordinary heating of the free-carrier gas in a disordered semiconducto because of the short mean-free path. There are then the three possible mechanisms responsible for the deviation from Ohm's law in such a material:

1. Delocalization of some of the carriers, which lie in not very deep discrete levels in the absence of the voltage. (By delocalization here and subsequently is meant the passage of a carrier to a state lying above the bottom of the conduction band, which does not necessarily coincide with the classical one).

2. Direct action of electric field on the jump probability.

3. Electron redistribution over the local levels in response to the field (this is sometimes called heating of the localized carriers).

Here we consider the first of these mechanisms, although the general arguments on the random field apply also to the second.

It is usual to calculate the delocalization probability in interpreting the data, as this is responsible for the change in shape of the fluctuation potential well in a homogeneous field, when the field strength is then equated with

$$\mathbf{E} = \frac{V}{L}\boldsymbol{\nu}, \tag{1}$$

where V is the potential difference across the specimen, L is the length in the current direction, and $\boldsymbol{\nu}$ is the unit vector in that direction.

Such a procedure is justified in application to a sufficiently large specimen without a random field, since the possible inhomogeneity of the field in such a specimen is related only to boundary effects. However, random band curvature may occur if there is random field in the material, i.e., the specimen may be internally inhomogeneous [5]. The spatial scale of this inhomogeneity is large by comparison with the characteristic localization radius (which justifies the technique used in solving the quantum-mechanical part of the problem), but it is

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small by comparison with the dimensions of the specimen (the specimen is macroscopically homogeneous). Also, the random field of itself does not of course produce the resultant current (whose density is proportional to the electric potential gradient ∇F), but all the same it appears in the Hamiltonian, which means that the delocalization probability must be calculated on the effective field:

$$\mathbf{E} = \frac{1}{e} \nabla U - \nabla \delta\varphi. \tag{2}$$

Here e is the absolute electronic charge, which in future is taken as 1, $U(\mathbf{x})$ is the potential energy of an electron in the random field (normalized in such a way that the mean is zero), and $\delta\varphi(\mathbf{x})$ is the change in potential associated with the voltage V. The function $U(\mathbf{x})$ may also have a nonelectrostatic part $U_1(\mathbf{x})$ due for example to the deformation interaction between the carriers and the random density variations (in what follows it is assumed that U_1 is independent of V; in principle, we could incorporate this dependence within the framework of the approach, but it only results in some complication in the symbols):

$$U(\mathbf{x}) = -\varphi_0(\mathbf{x}) + U_1(\mathbf{x}). \tag{3}$$

Here $\varphi_0(\mathbf{x})$ is the random electrical potential in the specimen for V = 0, and the total potential is

$$\varphi = \varphi_0 + \delta\varphi. \tag{4}$$

When we use (2) we must bear in mind two circumstances.

Firstly, by $U(\mathbf{x})$ is meant only the smooth part of the random field (in the above sense), which does not produce fluctuation levels of the relevant type.

Secondly, the smooth fluctuations in the random field cannot of themselves cause carrier delocalization in the absence of the external field. We incorporate this via the corresponding normalization factor N in the expression for the observed current density. We have in mind experiments in which direct measurements are made of the potential difference across the specimen and the current, and the current density can be written as

$$\mathbf{j} = N\langle \sigma(F + \delta\varphi - U, \quad \nabla\delta\varphi - \nabla U)\nabla F\rangle. \tag{5}$$

Here the <> denote averaging with respect to the random field, while σ is the local conductivity; the mean value of σ would determine the observed conductivity in the absence of the random part ∇F. The dependence of σ on the first and second arguments is related to the corresponding statistical and dynamic factors. The explicit form of N may be given subsequently.

2. BASIC EQUATIONS: APPARENT-NEUTRALITY APPROXIMATION

We write standard equations to determine the forms of $\varphi(\mathbf{x})$ and $F(\mathbf{x})$:

$$\operatorname{div} \mathbf{j} = 0; \tag{6}$$

$$\nabla^2 \varphi_0 = \frac{4\pi}{\varepsilon} [n_0 - n(F_0 + \varphi_0 - U_1)]; \tag{7}$$

$$\nabla^2 \varphi = \frac{4\pi}{\varepsilon}[n_0 - n(F + \varphi - U_1)]. \tag{8}$$

Here ε is the dielectric constant of the specimen, while F_0 is the electrochemical potential (constant in space) for V = 0, and $n_0 = \langle n(F_0 + \varphi_0 - U_1)\rangle$; n_0 is independent of the coordinates by virtue of the macroscopic homogeneity. The boundary conditions to (6)-(8) are standard and are therefore not written out here. We combine (7) and (8) and use (4) to get

$$\nabla^2 \delta\varphi = \frac{4\pi}{\varepsilon}[n_0(F_0 + \varphi_0 - U_1) - n(F + \varphi - U_1)]. \tag{9}$$

Equations (6)-(9) simplify considerably for a homogeneous specimen ($\varphi_0 = 0$), whose dimensions are large by comparison with the screening length. Then the condition for local neutrality $n = n_0$ is met in nearly all of the specimen and (1) follows from this. The author is indebted to M. I. Kaganov for discussion of this point). In the materials considered here, local neutrality does not apply (even for V = 0). However, we can assume that here also there will be no substantial charge redistribution in the bulk of the specimen on applying the field. This is termed the apparent-neutrality approximation. In fact (9) has a solution that satisfies the necessary boundary conditions:

$$\delta\varphi = -\delta F = \frac{V}{L} x \tag{10}$$

(the x axis is taken in the current direction).

Equation (6) is also satisfied, because $\langle\sigma\rangle = \text{const}$ in a macroscopically homogeneous specimen; however, it is not in general guaranteed that the more general equality of (6) is obeyed, which contains an unaveraged expression for the current density at each point in the specimen. For this reason we speak of an approximation, not of an exact solution.

Under the conditions of (10) we have from (2) for e = 1 that

$$\mathbf{E} = -\frac{V}{L}\mathbf{x} + \nabla U. \tag{11}$$

It is not necessary to calculate the last term on the right in (11), because the above formulation implies that this is a random function, whose statistical characteristics are assumed to be known.

3. CURRENT DENSITY EXPRESSION

We consider the first of the mechanisms stated in Section 1 and assume that only free carriers are involved in the current transport that arise by delocalization (the F_0 level lies sufficiently far from the edge of the gap for mobility). Then the expression for the local conductivity in (5) should be put as

$$\sigma = n_{fr}\ \mu_0 = \mu_0 n(F_0 - U) W(|E|). \tag{12}$$

Here n_{fr} and μ_0 are the concentration and mobility of the free carriers, n is the concentration of the localized carriers and W is the delocaliation probabil-

ity. (One can represent the local conductivity of a polycrystalline semiconductor in analogous form, where the current flowing is limited for example by random barriers at the boundaries between the crystallites. Then the function W will determine the probability of passage through the barriers.) For definiteness we assume as follows (the relationship is due to the form of W):

$$\sigma \sim \exp\left\{\frac{|E|}{E_0}\right\}, \tag{13}$$

where E_0 is a constant. A relationship of this type has been used in various studies [1], and in [2] it is said to be obtained from the quantum mechanical scattering for an electron in a Debeye potential well in a certain field range. Here $E_0 = \frac{3}{2} T r_0^{-1}$, where T is the temperature in energy units and r_0 is the screening radius. However, for what follows it is unimportant what are the reasons for the origin of (13), and this is considered as illustrative. The quantity E_0 is strictly speaking also random. However, in order not to complicate the problem by introducing additional arbitrary elements we consider it simply as a parameter. Further, the system of localized carriers is degenerate under the above conditions and therefore the dependence of n on $F_0 - U$ is not exponential. Therefore, we obtain with exponential accuracy as follows by combining (5) and (11)-(13):

$$j \sim \left\langle \exp\left\{\frac{\sqrt{V^2/L^2 - 2V/L\frac{\partial U}{\partial x} + (\nabla U)^2}}{E_0}\right\}\right\rangle \cdot \left\langle \exp\frac{|\nabla U|}{E_0}\right\rangle^{-1}. \tag{14}$$

The last cofactor on the right in (14) is simply the normalization factor N written for this particular case. For brevity we will not write this out and understand its presence.

4. RANDOM-FIELD AVERAGING

It is convenient to perform a Laplace transformation in order to carry out the averaging on the right of (14) on the basis

$$V^2/L^2 - 2V/L\frac{\partial U}{\partial x} + (\nabla U)^2 = t; \tag{15}$$

$$f(p) = \int_0^\infty e^{-pt + t^{1/2}/E_0}\, dt, \tag{16}$$

where $\mathrm{Re}\, p > 0$; then

$$j \sim \frac{1}{2\pi i}\int_{\sigma - i\infty}^{\sigma + i\infty} f(p)\exp(pV^2/L^2)\, B(p)\, dp, \tag{17}$$

where

$$B(p) = \left\langle \exp\left\{-2\frac{V}{L}p\frac{\partial U}{\partial x} + p(\nabla U)^2\right\}\right\rangle. \tag{18}$$

The mean value of the exponential appearing here is the relevant characteristic of the random field. In order to illustrate the essence of the situation it is sufficient to consider a gaussian field (which however is frequently realized in

Table 1

Values of A(β) for c = 1

β	A(β)	$\frac{A(\beta)}{A(1)}$	exp (β − 1)	exp($\beta^{0,8}$ − 1)	exp($\beta^{0,5}$ − 1)
1,00	7,00	1,00	1,00	1,00	1,00
1,10	7,03	1,004	1,11	1,08	1,05
1,25	7,20	1,03	1,28	1,22	1,13
1,50	7,56	1,08	1,65	1,47	1,25
1,75	9,44	1,35	2,12	1,76	1,38
2,00	10,4	1,49	2,72	2,10	1,51

Table 2

Values of A(β) for c = 0.5

β	A(β)	$\frac{A(\beta)}{A(1)}$	exp (β − 1)	exp($\beta^{0,8}$ − 1)	exp($\beta^{0,5}$ − 1)
1,00	4,64	1,00	1,00	1,00	1,00
1,25	4,89	1,05	1,28	1,22	1,12
1,50	5,38	1,16	1,65	1,47	1,25
1,75	5,86	1,26	2,18	1,76	1,38
2,00	6,56	1,41	2,72	2,10	1,51
2,50	8,76	1,89	4,48	2,95	1,79
3,00	11,2	2,41	7,39	4,09	2,08

situations of experimental interest). Then the distribution $\mathscr{P}(\nabla U)$ for the vectors ∇U is given by [3]

$$\mathscr{P}(\mathbf{E}) = \left(\frac{3}{4\pi\psi_2}\right)^{3/2} \exp\left[-\frac{3(\nabla U)^2}{4\psi_2}\right],$$

where

$$\psi_2 = \frac{1}{2}\langle(\nabla U)^2\rangle \tag{19}$$

is one of the basic parameters characterizing the field (the definition of (19) differs from that of [3] by the factor 1/2). Then

$$B(p) = \frac{\exp\left(\frac{4\psi_2}{3} p^2 \frac{V^2}{L^2}\right)}{\left(1 - \frac{4}{3}\psi_2 p\right)^{3/2}}. \tag{20}$$

We introduce the dimensionless parameters β, λ, and c and the dimensionless variables of integration z and τ by putting

$$\beta = V/LE_0, \quad \lambda = \frac{4\psi_2 L^2}{3V^2} = c\beta^{-2};$$
$$p = i\frac{V^2}{L^2} z + \sigma, \quad t = \tau\frac{V^2}{L^2}. \tag{21}$$

We get

$$j \sim \int_0^\infty d\tau J(\tau) e^{\beta\sqrt{\tau}}, \tag{22}$$

where

$$J(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dz \frac{\exp[-\lambda z^2 + iz(1-\tau)]}{(1-i\lambda z)^{3/2}}. \tag{23}$$

For $\lambda \to 0$ (no random field) formulas (22) and (23) give as would be expected that

$$j \sim \exp(V/LE_0). \tag{24}$$

On the other hand, for $\lambda \gg 1$ (very weak external field) the exponential dependence vanishes and our formulation becomes of no interest. We deliberately restrict consideration to the case $\lambda \ll 1$, and then, in contrast to the case $\lambda \gg 1$, the singular point under the integral in (23) plays no role, and the function $(1-i\lambda z)^{3/2}$ may be considered as comparatively slowly varying, and with exponential accuracy

$$j \sim \int_0^\infty d\tau \exp\left\{\beta\left[\sqrt{\tau} - \beta\frac{(\tau-1)^2}{4c}\right]\right\} \equiv A(\beta). \tag{25}$$

The integral on the right in (25) has to be calculated numerically. However, without calculation it is clear that the random field weakens the field dependence of the current density relative to (24).

Tables 1 and 2 give values for $A(\beta)$ derived by numerical integration for two values of c, and comparison is also made of $A(\beta)$ for various values of β with the result that would be obtained from the exponential formula (24), and also from the empirical formula sometimes used [4] $j \sim \exp[V/V_0^m)], V_0 = \text{const}, 0 < m < 1$. We see that the field dependence of ln j given by (25) is close to the square-root in type for $\beta \leqslant 2$ and c = 1 or c = 0.5. It is likely that appropriate fitting of c would give a value of m close to 0.8 (in accordance with the results of [4]). However, as the above assumptions are of model character we refrain from such adjustment and merely make the above conclusion of nonmodal character. Also, this still applies for various nongaussian random fields, e.g., for the regular random field of general form [5].

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