ON THE INCEPTION OF A SMOOTH RANDOM FIELD IN A DISORDERED SEMICONDUCTOR

V. L. Bonch-Bruevich

Vestnik Moskovskogo Universiteta. Fizika,
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Conditions under which one should expect the inception of a smooth random field in a disordered (amorphous or alloyed crystalline) semiconductor are examined. It is shown that such a field may arise in not too well prepared specimens.

The model of a smooth random field, suggested by the present author [1] made it possible to present an analytic treatment of a number of phenomena observed in disordered semiconductors [2-15]. In particular, this makes it possible to explain the origin of the "tail" of the light absorption coefficient at low temperatures ("Aurbach's rule"). The convenience of this model consists in the fact that the smoothness of the field validates the quasi-classical method of calculation of the density of states, the complex electrical conductivity, etc., with the properties of the random field characterized by only a small number of parameters. Thus, in a macroscopically isotropic and homogeneous Gaussian field there are only two such parameters: $\psi_1 = \langle V^2 \rangle$ and $\psi_2 = \frac{1}{2}\langle (\nabla V)^2 \rangle$. Here the angular parentheses designate averaging over the random field, V is the potential energy of the electron in it, normed in such a manner that $\langle V \rangle = 0$. The situation in non-Gaussian fields is analogous [16].

The nature of a smooth field can be treated in two ways. Firstly, it can be due directly to sources of a given type; secondly, this can be a "secondary" field, reflecting the inevitable presence in such systems of a smooth random curving of zones [16,17]. To a certain extent this difference is arbitrary, because this curving of zones is due simply to the long-wave part of the total random field in the specimen. However, it is convenient to consider these two possibilities separately. The point is that the concept of "smoothness" of the distortion of zones has a precise meaning only with respect to a given specific problem (the field should, on the average, differ little over some characteristic length). On the other hand, a smooth field is defined by requiring an increasing (on the average) smallness of derivatives of V with an increase in their order:

$$\frac{\hbar^2 \psi_2}{4m \psi_1^{3/2}} \ll 1, \qquad (1)$$

where m is the effective mass of the charge carrier, corresponding to the auxiliary problem with a periodic field [1]. Analogous relationships also relate the mean values of higher-order derivatives.

It is clear a priori that a smooth (in the sense of Eq. (1)) field can, in

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general, arise only under conditions when there exists a systematic factor ensuring smallness of short-wave Fourier components of function V. Such, for example, is the case in the interaction of charge carriers with an ensemble of acoustic waves having random amplitudes and phases [8]. However, the case of a system with long-range (Coulomb) forces is also of interest; as is known (see, for example the author's paper [3]), condition (1) is not realized in a system of point charges, since parameter ψ_2 diverges due to the Coulomb singularity at short distances. This served as a basis for the assertion that the concept of a smooth field does not at all apply to physically interesting situations. We note in conjunction with this that examples of nonrandom smooth Coulomb-type force fields are well known; it suffices to mention the curving of zones near various kinds of contacts with a not too small screening radius. The essence of the matter is evident: a smooth (including a random) field may arise in a system with Coulomb forces provided that the ensemble of point charges can be replaced by a continuous distribution of charge density. In other words, we are concerned with conditions under which the approach of macroscopic electrodynamics is valid. This is the case, for example, in considering relatively large-scale ("semimacroscopic") structure defects, associated with fluctuations in the concentration of charged impurities. Such fluctuations may arise, in particular, as a result of random variations in the temperature and its gradients in the course of specimen preparation [18]. Let the concentration of such defects, their characteristic linear dimension and the characteristic deviation of impurity concentration in it from the mean be respectively N, R and δn_t. Also we designate by r_0 the screening radius, due either to free charges, or to some other factors. The situation of interest is realized, among others, when

$$R^3\delta n_t \gg 1, \quad R < r_0, \quad NR^3 < 1. \qquad (2)$$

The first of these inequalities validates the aforementioned macroscopic approach, the second eliminates the condition of neutrality within the limits of the defect, the third means that the defects (but not the electric fields produced by them!) do not overlap in space.

For illustration we consider a very special case - an ensemble of randomly distributed spherical domains with constant radius R. The role of δn_t in this case is played by fluctuation of the concentration of noncompensated donors, which remains constant within each domain and is equal to zero outside of it. Screening is due to free electrons, the excess concentration of which is $\delta n = n_0 \exp(e\varphi/T)$. Here n_0 is the mean electron concentration, T is the temperature in energy units, e is the absolute magnitude of the electron charge, and φ is the electrostatic potential. We shall assume for simplicity that $e\varphi \ll T$. We note that this approximation, just as the use of the Boltzmann statistic, is not of fundamental importance, and does not affect our principal qualitative conclusion. Under conditions (2) an ensemble of such defects produces a random Poisson field, with the potential of an individual defect being

$$\varphi = \begin{cases} ar_0^2 \left[1 - (r_0/r)\left(1 + \frac{R}{r_0}\right)\exp\left(-\frac{R}{r_0}\right)\operatorname{sh}\frac{r}{r_0}\right], & r \leqslant R, \\ ar_0^3 \left[\frac{R}{r_0}\operatorname{ch}\frac{R}{r_0} - \operatorname{sh}\frac{R}{r_0}\right]\frac{\exp(-r/r_0)}{r}, & r \geqslant R, \end{cases} \qquad (3)$$

where

$$a = \frac{4\pi e}{\varepsilon}\delta n_t, \quad r_0^2 = \frac{4\pi n_0 e^2}{\varepsilon T}.$$

Quantities ψ_1 and ψ_2 are expressed as

$$\psi_1 = N\int d\mathbf{r}\, e^2\varphi^2(\mathbf{r}), \quad \psi_2 = \frac{1}{2}N\int d\mathbf{r}\, e^2(\nabla\varphi)^2.$$

Substituting here $\varphi(\mathbf{r})$ from Eqs. (3), we find, under conditions (2):

$$\psi_1 = \frac{4\pi a^2}{3} r_0^2 R^5 e^2 N, \quad \psi_2 = \frac{4\pi a^2}{15} R^5 e^2 N.$$

Accordingly, Eq. (1) becomes

$$\frac{\varepsilon\hbar^2}{me^2R}\cdot\frac{1}{4\pi R^3\,\delta n_t\,(Nr_0^3)^{1/2}} \ll 1. \qquad (4)$$

According to the problem's meaning, $\varepsilon\hbar^2/me^2R < 1$, and condition (4) is satisfied a priori already at $Nr_0^3 \sim 1$.

In order to apply the results of this illustrative example to real materials, we would have to average over values of R and δn_t and over the shape of volumes under study, and also possibly, make allowance for correlation in their mutual spatial arrangement. Apparently, the large number of model assumptions which inevitably arises here does not validate such a calculation. It should be merely noted that the averaging procedure cannot change the conclusion of smoothness of the field, and results only in replacing the model values of R and δn_t by their characteristic (mean) values. Here quantities ψ_1 and ψ_2 or their analogs in the case of a non-Gaussian field are simplest treated as phenomenological quantities (which was precisely done in the previously cited studies). The above provides a microscopic validation of this.

It is thus seen that one should expect a smooth random field in not too well prepared materials. We note in connection with this that, as was shown experimentally by Pierce and Spicer [19], the Aurbach tail of the absorption coefficient in amorphous silicon films virtually vanishes upon sufficiently prolonged annealing.

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Department of Semiconductor Physics