Interband light absorption in heavily doped semiconductors in the deep tail region

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(Submitted 28 February 1986)
Zh. Eksp. Teor. Fiz. **92**, 1351–1356 (April 1987)

A new method of computing the coefficient of light absorption in a heavily doped semiconductor is proposed. The method is based on a power series expansion in a found small parameter, which is the ratio of the localization length of the charge-carrier wave function to the correlation length of the random field. It is shown that in the deep tail region, where a significant role is played by the transitions between the highly localized states, the absorption coefficient does not reproduce the density of states, as has been erroneously asserted by Shklovskiĭ and Éfros [Sov. Phys. JETP **32**, 733 (1971); Sov. Phys. Usp. **16**, No. 6 (1974); Electronic Properties of Doped Semiconductors [in Russian], Nauka, Moscow, 1979, p. 364]. The first three terms of the asymptotic series for the absorption coefficient are obtained in their explicit form.

1. INTRODUCTION. FORMULATION OF THE PROBLEM

As is well known, the occurrence of a light-absorption coefficient tail in a heavily doped semiconductor at low temperatures is due to the transitions of the carriers between the fluctuational levels in the forbidden band. Such transitions are usually described with the use of a model according to which the electron moves in the random field produced by the impurity atoms, which are randomly distributed in the sample.[1–3] The interaction of the electrons with the phonons is ignored, and the electron-electron interaction is taken into account only partially, specifically, with the aid of a screened potential. The magnitude of the absorption coefficient is determined by the probability for the appearance of the appropriate fluctuation in the impurity disposition and the tunneling probability. The problem formulated in the title of the present paper is solved for the Gaussian random field within the framework of such a model in Refs. 1–3, where it is found that, in the deep-tail region, the tunneling is insignificant, and the absorption coefficient is virtually determined by only the probability for formation in the semiconductor of a potential well of depth $\Delta = E_g - \hbar\omega$, where E_g is the forbidden band width and ω is the frequency of the absorbed light. This probability turns out to be proportional to the quantity $\exp[-\Delta^2/\gamma^2]$, where γ^2 is the doubled mean square of the potential energy of the charged carrier. On this basis, it is asserted in the indicated papers that, at large positive values of the photon energy deficit Δ, the index of the exponential light-absorption coefficient function coincides with that of the density-of-states exponential function. This result is, as will be shown in the present paper, erroneous. Using the very arguments adduced in these papers, we can easily show that in the deep-tail region, where the tunneling is insignificant, a much greater contribution to the absorption is made by such a fluctuation, as a result of which there is formed in one part of the semiconductor a potential well of depth $\Delta/2$ for the electron, and in the other part a similar well for the hole. In the deep-tail region, where the distance between the wells is greater than the correlation length of the random field, the probabilities for their formation can be considered to be independent of each other; therefore, the resulting probability for such a fluctuation turns out to be proportional to the quantity

$$\exp[-(\Delta/2\gamma)^2]\exp[-(\Delta/2\gamma)^2]=\exp[-\Delta^2/2\gamma^2],$$

which, for $\Delta \gg \gamma$, is exponentially large in comparison with the probability for the appearance of the fluctuation considered in Refs. 1–3. Naturally, these are all just qualitative arguments, which need to be more rigorously substantiated.

In the present paper we propose a new method of computing the coefficient of interband absorption of light in heavily doped semiconductors in the region of photon energies $\hbar\omega$ smaller than the forbidden band width E_g. We consider semiconductors with a sufficiently large forbidden band width $E_g \gg \Delta$. This allows us to use the effective mass method. The bare dispersion law is chosen in the simplest form

$$W_c=\mathbf{p}^2/2m_c, \quad W_v=-E_g-\mathbf{p}^2/2m_v,$$

where the $m_{c,v}$ are the effective masses of the carriers in the conduction and valence bands. The temperature of the semiconductor is assumed to be equal to zero. It is assumed that the random field is described by the Gaussian statistics.

2. BASIC RELATIONS

As is well known,[4] the coefficient of light absorption in disordered semiconductors is given by the relation

$$\alpha(\omega)=\frac{32\pi^2e^2\Gamma}{\omega c\varepsilon_1^{1/2}V_n}\int d\mathbf{x}_1\int d\mathbf{x}_2\int d\omega'[n_F(\omega'-\omega)-n_F(\omega')]\times\langle \operatorname{Im} G_r^v(\mathbf{x}_1,\mathbf{x}_2;\omega'-\omega)\operatorname{Im} G_r^c(\mathbf{x}_2,\mathbf{x}_1;\omega')\rangle, \quad (1)$$

where

$$\Gamma=\tfrac{1}{3}\left|\int d\mathbf{x}\, U_c^*(\mathbf{x})\,(1/im_0)\,\nabla U_v(\mathbf{x})\right|^2,$$

$U_c(\mathbf{x})$ and $U_v(\mathbf{x})$ are the periodic parts of the Bloch functions, c is the velocity of light, ε_1 is the real part of the permittivity, $n_F(\omega)$ is the Fermi function, and e and m_0 are the electron charge and mass. The integration over the coordinates $\mathbf{x}_1$ and $\mathbf{x}_2$ is over the entire volume V_n of the semiconductor. The angle brackets denote averaging over the random field. Here and below we use the system of units in which $\hbar = 1$. By going over to the time representation for the anticommutator retarded Green functions $G_r(\mathbf{x}_1, \mathbf{x}_2; \omega)$, and using the path-integral technique,[5] we can show that, under the conditions of our problem, the expression (1) is

 0038-5646/87/040758-04$04.00

equivalent to the following representation for the absorption coefficient:

$$\alpha(\omega)=-\frac{4\pi e^2\Gamma}{\omega c\varepsilon_1^{1/2}}\,i\int\limits_{-i\infty+\delta}^{i\infty+\delta}dt\,e^{(\omega-E_g)t}Z(t),\qquad \delta\to+0,\qquad (2)$$

where

$$Z(t)=\int d\mathbf{r}\int\limits_{-\mathbf{r}}^{0}D\mathbf{x}(\tau)\int\limits_{\mathbf{r}}^{0}D\mathbf{y}(\tau)\exp\left\{-\int\limits_{0}^{t}\left[\frac{m_c}{2}\dot{\mathbf{x}}^2(\tau)+\frac{m_v}{2}\dot{\mathbf{y}}^2(\tau)\right]d\tau+\frac{1}{2}\int\limits_{0}^{t}\int\limits_{0}^{t}[D(\mathbf{x}(\tau)-\mathbf{x}(s))+D(\mathbf{y}(\tau)-\mathbf{y}(s))-2D(\mathbf{r}+\mathbf{x}(\tau)-\mathbf{y}(s))]\,d\tau\,ds\right\},\qquad (3)$$

$\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$, and $D(\mathbf{x}_1-\mathbf{x}_2)$ is the random field's correlation function, which in heavily doped semiconductors has the form[6]

$$D(\mathbf{x}_1-\mathbf{x}_2)=\tfrac{1}{2}\gamma^2\exp[-\varkappa|\mathbf{x}_1-\mathbf{x}_2|].$$

Here $\varkappa^{-1}$ is the correlation length of the random field.

Let us note that the function $Z(t)$ is analytic in the right half-plane of the complex variable t. We can verify this by expanding the exponential function in the integral over the trajectories in (3) in a series in powers of the correlation function. It turns out here that, if the correlation function is bounded, then this series converges uniformly in the region $\mathrm{Re}\,t>0$ and each one of its terms is an analytic function in the indicated region. Thus, the function $Z(t)$ does not possess singularities in a finite region of the half-plane $\mathrm{Re}\,t>0$, and, consequently, the behavior of the coefficient of interband absorption of light at large positive values of the energy deficit Δ is determined by the asymptotic form of $Z(t)$ for $t\to\infty$.

3. ASYMPTOTIC FORM OF THE AVERAGED DENSITY MATRIX

Let us now show how we can obtain the asymptotic representation of $Z(t)$ for large values of t. Let us use the canonical expansion

$$D(\mathbf{x}_1-\mathbf{x}_2)=\sum_n a_n(\mathbf{x}_1)a_n(\mathbf{x}_2)$$

of the correlation function in terms of some set of functions[7] $a_n(\mathbf{x})$, the specific form of which will not be required below. By introducing an additional integration over the variables ξ_n, we can represent the expression (3) in the form

$$Z(t)=\int d\mathbf{r}\exp[-D(\mathbf{r})t^2]\int\prod_n\frac{d\xi_n}{(2\pi)^{1/2}}\exp\left(-\frac{\xi_n^2}{2}\right)\times\int\limits_{-\mathbf{r}}^{0}\int\limits_{\mathbf{r}}^{0}D\mathbf{x}(\tau)D\mathbf{y}(\tau)\exp\left\{-\int\limits_{0}^{t}\left[\frac{m_c}{2}\dot{\mathbf{x}}^2(\tau)+\frac{m_v}{2}\dot{\mathbf{y}}^2(\tau)+V_{0c}(\mathbf{x}(\tau))+V_{0v}(\mathbf{y}(\tau))\right]d\tau-\int\limits_{0}^{t}\left[\sum_n\xi_n a_n(\mathbf{x}(\tau)+\mathbf{r}/2)-\sum_n\xi_n a_n(\mathbf{y}(\tau)-\mathbf{r}/2)-V_{0c}(\mathbf{x}(\tau))-V_{0v}(\mathbf{y}(\tau))-D(\mathbf{r})t\right]d\tau\right\}.\qquad (4)$$

Here we have introduced the self-consistent potential

$$V_{0l}=-\frac{\gamma^2 t}{4}\int d\mathbf{y}\{2\exp[-\varkappa|\mathbf{x}-\mathbf{y}|]-1\}|\Psi_{0l}(\mathbf{y})|^2,\qquad (5)$$

where $\Psi_{0l}(\mathbf{x})$ is the normalized wave function of the ground state in the potential $V_{0l}(\mathbf{x})$. Below we shall show that the last integral in the index of the exponential function makes a small contribution to the light absorption, and it can be taken into account with the aid of perturbation theory. The remaining integral over the trajectories is a product of density matrices for the particles located in the potentials $V_{0c}(\mathbf{x})$ and $V_{0v}(\mathbf{y})$. The asymptotic form of the density matrix for large values of t can be expressed in a certain way in terms of the ground-state energy and the corresponding wave functions,[5] which should be determined from the Schrödinger equation

$$-\frac{\Delta}{2m_l}\Psi_{0l}(\mathbf{x})-\frac{\gamma^2 t}{4}\Psi_{0l}(\mathbf{x})\times\int d\mathbf{y}\{2e^{-\varkappa|\mathbf{x}-\mathbf{y}|}-1\}|\Psi_{0l}(\mathbf{y})|^2=E_{0l}\Psi_{0l}(\mathbf{x}).\qquad (6)$$

Let us introduce the dimensionless coordinates $z=\lambda_l x$, where $\lambda_l=(m_l\gamma^2 t\varkappa)^{1/3}$, the energy $\Omega=(4m_lE_{0l}+\gamma^2 t m_l)/2\gamma_l^2$ and the wave functions $f(\mathbf{z})=\lambda_l^{-3/2}\Psi_{0l}(\mathbf{z})$. At large t values the problem contains the small parameter $\varkappa/\lambda_l$, and Eq. (6) can be reduced to the dimensionless form

$$-\Delta f(\mathbf{z})+f(\mathbf{z})\int d\mathbf{y}|\mathbf{z}-\mathbf{y}|\,|f(\mathbf{y})|^2=\Omega f(\mathbf{z}),\qquad (7)$$

if we drop the terms of order $\varkappa/\lambda_l$. From this it follows that

$$E_{0l}=-\frac{\gamma^2 t}{4}+\frac{\gamma^{4/3}\varkappa^{2/3}t^{2/3}}{2m_l^{1/3}}\Omega,\qquad (8)$$

where Ω is a number of the order of unity, being the smallest eigenvalue of Eq. (7).

The corrections to the ground-state energy that stem from the terms discarded in (7) and (4) can be found with the aid of standard perturbation theory[8]:

$$E_{0l}^{(1)}=\pm\langle\Psi_{0l}(\mathbf{x})|\sum_n\xi_n a_n\left(\mathbf{x}\pm\frac{\mathbf{r}}{2}\right)\mp\frac{D(\mathbf{r})t}{2}|\Psi_{0l}(\mathbf{x})\rangle-\langle\Psi_{0l}(\mathbf{x})\Psi_{0l}(\mathbf{y})|\frac{\gamma^2\varkappa^2 t}{4}|\mathbf{x}-\mathbf{y}|^2|\Psi_{0l}(\mathbf{x})\Psi_{0l}(\mathbf{y})\rangle.\qquad (9)$$

Here the upper signs correspond to the value $l=c$; the lower signs, to $l=v$. As long as we are interested in the exponential terms in the asymptotic form of the absorption coefficient, the corrections to the wave functions can be ignored, since they affect only the value of the preexponential factor. Therefore, taking account of the first-order correction to the ground-state energy, we obtain

$$Z(t)=\int d\mathbf{r}\exp[-D(\mathbf{r})t^2-E_{0c}t-E_{0v}t]\times\Psi_{0c}(0)\Psi_{0c}(-\mathbf{r})\Psi_{0v}(0)\Psi_{0v}(\mathbf{r})\times\exp\left\{\frac{\gamma^2 t^2}{4}\langle\Psi_{0c}(\mathbf{x})\Psi_{0c}(\mathbf{y})|1-\exp(-\varkappa|\mathbf{x}-\mathbf{y}|)+\varkappa^2|\mathbf{x}-\mathbf{y}|^2|\times\Psi_{0c}(\mathbf{x})\Psi_{0c}(\mathbf{y})|\rangle\right.$$

$$+\frac{\gamma^2 t^2}{4}\langle\Psi_{0v}(\mathbf{x})\Psi_{0v}(\mathbf{y})|1-\exp(-\varkappa|\mathbf{x}-\mathbf{y}|)$$

$$+\varkappa^2|\mathbf{x}-\mathbf{y}|^2|\Psi_{0v}(\mathbf{x})\Psi_{0v}(\mathbf{y})\rangle-\frac{\gamma^2 t^2}{2}\langle\Psi_{0c}(\mathbf{x})\Psi_{0v}(\mathbf{y})$$

$$\times|\exp(-\varkappa|\mathbf{r}+\mathbf{x}-\mathbf{y}|)-e^{-\varkappa|\mathbf{r}|}|\Psi_{0c}(\mathbf{x})\Psi_{0v}(\mathbf{y})\rangle\Big\}. \quad (10)$$

Let us evaluate the integral over the coordinates $\mathbf{r}$, using the asymptotic wave functions, the form of which can be determined from Eq. (6). The important $|\mathbf{r}|$ values that enter into the integral turn out to be of the order of

$$|\mathbf{r}|\sim\varkappa^{-1}\ln(\gamma t^{3/2}\varkappa/2(m_c^{1/2}+m_v^{1/2})),$$

and the asymptotic form of the function $Z(t)$ at large t has the form

$$Z(t)=\exp\left\{\frac{\gamma^2 t^2}{2}-\left(\Omega-\frac{\Pi}{2}\right)\frac{\gamma^{4/3}\varkappa^{2/3}t^{5/3}}{2}(m_c^{-1/3}+m_v^{-1/3})\right.$$
$$\left.+C\frac{\gamma^{2/3}\varkappa^{4/3}t^{4/3}}{8}(m_c^{-2/3}+m_v^{-2/3})+O\left(\frac{\varkappa^2}{m_{c,v}}t\right)\right\}, \quad (11)$$

where C and Π are certain numbers that can be determined from the relations

$$C=2\int d\mathbf{z}\,\mathbf{z}^2|f(\mathbf{z})|^2,$$
$$\Pi=\int\int d\mathbf{z}\,d\mathbf{z}'|f(\mathbf{z})|^2|f(\mathbf{z}')|^2|\mathbf{z}-\mathbf{z}'|.$$

In finding the asymptotic form of $Z(t)$, we limited ourselves to the computation of only the first-order correction to the ground-state energy. It can be shown that allowance for the next orders of the perturbation theory does not change the terms written out in explicit form in (11).

4. THE ABSORPTION COEFFICIENT

Substituting (11) into (2), and evaluating the integral by the method of steepest descent, we obtain for the absorption coefficient the expression

$$\alpha(\omega)=\exp\left\{-\frac{(E_g-\omega)^2}{2\gamma^2}\left[1+\left(\Omega-\frac{\Pi}{2}\right)\frac{\varepsilon_c^{1/3}+\varepsilon_v^{1/3}}{(E_g-\omega)^{1/3}}\right.\right.$$
$$+\frac{25}{36}\left(\Omega-\frac{\Pi}{2}\right)^2\frac{(\varepsilon_c^{1/3}+\varepsilon_v^{1/3})^2}{(E_g-\omega)^{2/3}}-\frac{C}{4}\frac{\varepsilon_c^{2/3}+\varepsilon_v^{2/3}}{(E_g-\omega)^{2/3}}$$
$$\left.\left.+O\left(\frac{\varepsilon_{c,v}}{E_g-\omega}\right)\right]\right\}, \quad (12)$$

where $\varepsilon_{c,v}=\varkappa^2/m_{c,v}$. The important t values that enter into the integral turn out to be of the order of $t\approx\Delta/\gamma^2$.

We assumed in our derivation that the parameter $\varkappa/\lambda_l$ is small. Using the above-presented estimate for t, we easily find that this assumption is justified when

$$\Delta\gg\varepsilon_{c,v}. \quad (13)$$

Let us note that the condition for the existence of bound states in the potential (5) leads to the same inequality. In finding the asymptotic form of the density matrix, we neglected the contributions from the excited states, and this is justified when

$$\Delta\gg\gamma(\gamma/\varepsilon_{c,v})^{1/2}. \quad (14)$$

Furthermore, perturbation theory was used to compute the corrections to the ground state energy. The condition for its applicability in the present case has the form

$$\Delta\gg\gamma[(\gamma/\varepsilon_c)^{1/2}+(\gamma/\varepsilon_v)^{1/2}]^{2/3}. \quad (15)$$

And finally, the integral over the coordinates in (10) was evaluated with the asymptotic wave functions. Their use can be justified in the following manner. The integrand in (10) contains wave functions whose radius of localization is of the order of $1/\lambda_l$ and the distance between the centers of localization is equal to $|\mathbf{r}|$. At large values of the photon energy deficit, specifically, for $\Delta\gg\gamma$, the probability for the formation of wells of depth of the order of Δ is small, and the wells occur with characteristic spacing greater than the correlation length $1/\varkappa$ of the random field. Since in the deep-tail region the ratio $\varkappa/\lambda_l\ll 1$, the dominant contribution to the integral over the coordinates, the value of which is determined by both the probability for the appearance of potential wells at distances $|\mathbf{r}|$ from each other and the overlap of the wave functions, is made by the region of large $|\mathbf{r}|$ values, where the asymptotic representation for $\Psi_{0l}(\mathbf{r})$ is valid. Evaluation of the integrals over the coordinates with the exact and the asymptotic wave functions shows that the use of the asymptotic form for $\Psi_{0l}(\mathbf{r})$ is justified when

$$\Delta\gg\gamma\left[\left(\frac{\gamma}{\varepsilon_c}\right)^{1/2}+\left(\frac{\gamma}{\varepsilon_v}\right)^{1/2}\right]\ln\frac{\Delta^{1/2}}{2\gamma^2(\varepsilon_c^{-1/2}+\varepsilon_v^{-1/2})}. \quad (16)$$

It can be seen from the expression (12) that, in the region of the deep tail defined by the inequalities (13)–(16), the asymptotic series for the absorption coefficient is constructed in the index of the exponential function, and the expansion is in powers of $(E_g-\omega)^{-1/3}$. Although the subsequent terms of the expansion are smaller than the preceding ones, it is necessary to take them into consideration in the index of the exponential function, since they are much greater than unity. Notice that the expression (11) coincides up to terms of the order of $\varkappa^2 t/m_{c,v}$ with the product of the averaged single-particle density matrices,[9] and, as follows from the expression (2), the absorption coefficient in the indicated region is proportional to the convolution of the density of states. This result is explained by the fact that tunneling is unimportant in the present problem, since the terms connected with it make in the index of the exponential function a contribution of the order of $(m_{c,v}\Delta)^{1/2}|\mathbf{r}|$. Consequently, the probability for absorption of a photon is determined only by the probability for the appearance of the requisite fluctuational wells, contributions to the absorption being made by all the transitions between the states on the density-of-states tails whose spacing in energy terms is equal to Δ. But, as follows from the above-presented estimates for t and $|\mathbf{r}|$, the most probable transitions are those between the ground states in the fluctuational wells with depth $\Delta/2$ and characteristic spacing much greater than the correlation length $\varkappa^{-1}$ of the random field. Let us note that the expression relating the absorption coefficient with the convolution of the densities of states has been used in a number of papers (see, for example, Ref. 10), but as pointed out in Ref. 11, it has to date not been rigorously proved.

In conclusion, let us point out that the small parameter that allowed us to construct the asymptotic expansion for the absorption coefficient is the ratio of the radius of localization of the wave function to the correlation length of the

random field. It is natural that the existence of this parameter is not connected with the specific nature of the random impurity field considered by us; therefore, the method proposed in the present paper can find application in the solution of other problems.

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Translated by A. K. Agyei