

Deep tail of the interband coefficient for light absorption in disordered semiconductors

Yu. D. Arbuzov and M. Yu. Kolenkin

All-Union Scientific Research, Design-Construction, and Technological Institute of Current Sources
(Submitted 25 May 1988)

Zh. Eksp. Teor. Fiz. 95, 621–630 (February 1989)

A new method is proposed for calculating the coefficient representing the interband absorption of light in the deep tail region. If the bending of the energy bands differs and the random fields acting on carriers in different bands are positively correlated, the main contribution to the absorption of light in the deep tail region comes from indirect transitions of carriers between states in fluctuation wells and the absorption coefficient then reproduces a convolution of the density of states, exactly as in the case of zero correlation. It is shown that in the case of a nonpositive correlation an allowance for quantum effects reduces considerably the absorption coefficient compared with the semiclassical case.

1. INTRODUCTION: FORMULATION OF THE PROBLEM

The profile of the absorption edge of light in disordered semiconductors depends strongly on the nature of the bending (same or different) of the energy bands by a random field.¹⁻³ In the semiclassical approximation this dependence is explained by postulating that the tail of the interband absorption of light is due to different physical factors in the cases of the same and different bending. When the band bending is the same, i.e., when random potential energies of carriers in the conduction band $V_c(\mathbf{x})$ and in the valence band $V_v(\mathbf{x})$ are equal ($V_c(\mathbf{x}) = V_v(\mathbf{x})$), the local width of the band gap remains constant and the absorption of light is possible only because of quantum effects giving rise to "indirect" transitions.¹ Following the terminology adopted in Ref. 4, the indirect transitions are those interband optical transitions which involve the transfer of an electron to the band gap and subbarrier tunneling to one of the levels in a fluctuation well.

If the energy bands are bent differently ($V_c(\mathbf{x}) \neq V_v(\mathbf{x})$), which is true when a random field is due to the deformation potential or if we allow for the energy dependence of the pseudopotential,^{3,4} then fluctuations of the potential energy give rise to fluctuations of the width of the band gap and the absorption of light may be ensured by "direct" transitions that do not involve tunneling. For this reason the semiclassical description of the absorption of light in semiconductors with bands bent in different ways is simplified by ignoring quantum effects and adopting a purely classical treatment. This approach shows² that the tail of the absorption coefficient considered on the basis of the Gaussian model of a random field is

$$\alpha(\omega) = A \exp\{-(E_g - \hbar\omega)^2 / 2W_k^2\}, \quad (1)$$

where the quantity A depends weakly on the frequency of light, E_g is the renormalized width of the band gap,

$$E_g = E_{g0} + \langle V_c(\mathbf{x}) \rangle - \langle V_v(\mathbf{x}) \rangle, \quad (2)$$

E_{g0} is the width of the band gap of the investigated semiconductor in the absence of a random field, the angular brackets denote here and below (and unless otherwise stated) the process of averaging over the random field, and the characteristic energy W_k is given by

$$W_k^2 = D_{cc}(0) + D_{vv}(0) - 2D_{cv}(0). \quad (3)$$

Here and below we have

$$D_{l_1 l_2}(\mathbf{x}_1 - \mathbf{x}_2) = \langle V_{l_1}(\mathbf{x}_1) V_{l_2}(\mathbf{x}_2) \rangle,$$

where $l_1, l_2 = c, v$ are the correlation functions of the random fields $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$.

The exponential function occurring in Eq. (1) is essentially the probability for such a fluctuation to appear in a semiconductor as a result of which the width of the band gap decreases by an amount equal to the photon energy deficit $\Delta = E_g - \hbar\omega$. However, it should be pointed out that neglect of quantum effects in dealing with the absorption of light in disordered semiconductors under conditions of different band bending is not always justified because—as shown below—within the deep tail the inclusion of these effects is fundamentally essential and in some cases the contribution to the absorption of light in this range is from quantum and not from classical effects.

For example, we shall consider a situation in which a random field displaces the bottom of the conduction band and the top of the valence band in the same directions, as shown in Fig. 1, and these displacements are different at each point in the investigated semiconductor: $V_c(\mathbf{x}) \neq V_v(\mathbf{x})$. The contribution of the indirect transitions to the absorption of light in the region of the tail where $\Delta > 0$ is determined, as is known from Refs. 5–7, by the probability of appearance in the semiconductor of a fluctuation that ensures the absorption of a photon with a given deficit $P[\Delta]$ and by the tunneling probability P_t . We shall assume that as

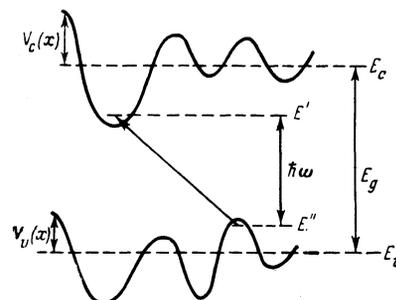


FIG. 1. Band bending in the case of a positive correlation of the random fields $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$.

a result of some fluctuation in one part of the semiconductor the bottom of the conduction band is shifted by $V_c(\mathbf{x})$, whereas elsewhere the top of the valence band is shifted by $V_v(\mathbf{y})$. The absorption of a photon of energy $\hbar\omega < E_g$ is possible if this fluctuation creates fluctuation levels for an electron E' and a hole E'' , which are separated from one another by $\hbar\omega = E' - E''$. It is essential to ensure that the band displacements satisfy the condition

$$V_c(\mathbf{x}) - V_v(\mathbf{y}) + E_g \leq \hbar\omega$$

(we shall ignore here the familiar limitations on the size of the fluctuation wells). The probability for a fluctuation to appear for which this condition is satisfied amounts to

$$P[\Delta] = \langle \theta(V_v(\mathbf{y}) - V_c(\mathbf{x}) - \Delta) \rangle. \quad (4)$$

Here and below the quantity $\theta(x)$ is a unit step function [$\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$].

It follows from Eq. (4) that in the case of large positive values of the photon energy deficit $\Delta \gg W_k$ the probability for a fluctuation ensuring the absorption of a photon to appear is described by

$$P[\Delta] \propto \exp\{-\Delta^2/2[D_{cc}(0) + D_{vv}(0) - 2D_{cv}(\mathbf{r})]\}, \quad (5)$$

where $\mathbf{r} = \mathbf{x} - \mathbf{y}$. The probability of the tunneling of an electron and a hole over a distance of order \mathbf{r} is given by the following expression, which is accurate apart from numerical coefficients in the argument of the exponential function⁵⁻⁷

$$P_t \propto \exp\left\{-\frac{1}{\hbar} (m_c^{1/2}\Delta^{1/2}r + m_v^{1/2}\Delta^{1/2}r)\right\},$$

where m_c and m_v are the effective masses of an electron and a hole, and the photon energy deficit Δ is of the order of magnitude of the ionization energy of the levels at which the electron and the hole are located before tunneling.

In finding the maximum of the product $P[\Delta] \cdot P_t$, which determines the absorption coefficient of light representing the indirect transitions, we shall consider the specific case where

$$D_{cv}(\mathbf{r}) = D_{cv}(0) \exp\{-r^2/L^2\}. \quad (6)$$

This function satisfies all the requirements that must be met by correlation functions and it is frequently used to calculate various characteristics of disordered semiconductors.⁴ It describes a smooth random field which can be differentiated an infinite number of times. We then find that the main contribution to the absorption in the deep tail region comes from the indirect transitions at distances of order

$$r_0 \approx L^2 \ln \frac{D_{cv}(0)\Delta^{1/2}\hbar}{[D_{cc}(0) + D_{vv}(0)]^2 (m_c^{1/2} + m_v^{1/2})L},$$

and the absorption coefficient is given by

$$\alpha(\omega) \sim \exp\{-\Delta^2/2[D_{cc}(0) + D_{vv}(0)] + O(m_{c,v}^{1/2}\Delta^{1/2}r_0/\hbar)\},$$

which shows that the contribution of the indirect transitions to the absorption of light in the deep tail region is exponentially small compared with the contribution of the direct transitions described by Eq. (1). It should be pointed out that tunneling makes a contribution of order of $m_{c,v}^{1/2}\Delta^{1/2}r_0/\hbar$ to the argument of the exponential function in the expression

for the absorption coefficient and the actual form of the mutual correlation function $D_{cv}(\mathbf{r})$ influences only the logarithmic term in the expression for r_0 . Naturally, the relationships obtained above, like the method used to find them, represent only qualitative estimates and the description of the absorption of light in the deep tail region requires a more rigorous theory.

We shall propose a new method for calculating the coefficient representing the interband absorption of light in disordered semiconductors, which will not be based on the assumption that the motion of carriers in the random field is of a semiclassical nature.

We shall consider a model of a disordered semiconductor with a Gaussian random field in which the interaction of carriers with phonons and the exciton effects are ignored. The width of the band gap is assumed to be fairly large, $E_g \gg \Delta$, which makes it possible to use the effective mass method. The unrenormalized dispersion law is selected in the simplest form:

$$W_c(\mathbf{p}) = \frac{\mathbf{p}^2}{2m_c}, \quad W_v(\mathbf{p}) = -E_{g0} - \frac{\mathbf{p}^2}{2m_v}.$$

The absolute temperature of the system is assumed to be zero.

In this model the absorption coefficient of light is given by⁸

$$\alpha(\omega) = -\frac{4\pi e^2 \Gamma}{\omega c \epsilon_1^{1/2}} i \int_{-i\infty+\delta}^{i\infty+\delta} dt e^{(\omega - E_q)t} Z(t), \quad \delta \rightarrow +0, \quad (7)$$

where c is the velocity of light, ϵ_1 is the real part of the permittivity, e is the electron charge, Γ is the square of the matrix element of the velocity operator, and the function $Z(t)$ is

$$\begin{aligned} Z(t) = & \int d\mathbf{r} \int D\mathbf{x}(\tau) \int D\mathbf{y}(\tau) \\ & \times \exp\left\{-\int_0^t \left[\frac{m_c}{2} \dot{\mathbf{x}}^2(\tau) + \frac{m_v}{2} \dot{\mathbf{y}}^2(\tau) \right] d\tau \right. \\ & \left. + \frac{1}{2} \int_0^t \int_0^t d\tau ds [D_{cc}(\mathbf{x}(\tau) - \mathbf{x}(s)) + D_{vv}(\mathbf{y}(\tau) - \mathbf{y}(s)) \right. \\ & \left. - 2D_{cv}(\mathbf{x}(\tau) - \mathbf{y}(s))] \right\}. \quad (8) \end{aligned}$$

In the path integral we shall carry out integration (both here and below) over all the paths satisfying the conditions

$$\mathbf{x}(0) = -\mathbf{r}/2, \quad \mathbf{x}(t) = \mathbf{r}/2, \quad \mathbf{y}(0) = \mathbf{r}/2, \quad \mathbf{y}(t) = -\mathbf{r}/2.$$

We shall use a system of units in which $\hbar = 1$.

A method proposed in Ref. 9 can be used to show that the function $Z(t)$, governed by Eq. (8), where the correlation functions are $D_{l_1 l_2}(\mathbf{x}_1 - \mathbf{x}_2)$ and $l_1, l_2 = c, v$ are assumed to be finite and continuous, is an analytic function of the complex variable t in the final part of the right-hand half-plane $\text{Re } t > 0$ and the frequency dependence of the interband absorption coefficient in the deep tail region is governed by the asymptotic behavior of the function $Z(t)$ at high values of t .

2. ASYMPTOTIC FORM OF THE FUNCTION $Z(t)$

We shall now consider the case where the correlation functions of the random field are finite, can be differentiated the required number of times, and are described by

$$D_{l_1 l_2}(\mathbf{x}_1 - \mathbf{x}_2) = \gamma_{l_1 l_2} f(\mathbf{x}_1 - \mathbf{x}_2), \quad (9)$$

where $\gamma_{l_1 l_2}$ are arbitrary quantities with the dimensions of the square of energy, satisfying the condition

$$\gamma_{cc} + \gamma_{vv} - 2\gamma_{cv} \geq 0,$$

and $f(\mathbf{x}_1 - \mathbf{x}_2)$ is a dimensionless function of the coordinates, but is independent of the energy band number. The corresponding renormalized quantity $\gamma_{l_1 l_2}$ can always be obtained if the condition $f(0) = 1$ is satisfied; and in this case γ_{cc} and γ_{vv} represent the dispersion of scatter of the random fields $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$.

It should be pointed out that the correlation functions of Eq. (9) are encountered in considering a random field due to the deformation potential.^{2,4} In this case the quantities $\gamma_{l_1 l_2}$ are related by

$$|\gamma_{cv}| = \gamma_{cc}^{1/2} \gamma_{vv}^{1/2}.$$

Moreover, the correlation functions of the form (9) can be used as a model of a random field representing the sum of the electrostatic potential $V(\mathbf{x})$, which bends in the same way the bottom of the conduction band and the top of the valence band, and the deformation potential $V_{dl}(\mathbf{x})$; if the correlation functions

$$\langle V(\mathbf{x}_1) V(\mathbf{x}_2) \rangle \text{ and } \langle V_{dl}(\mathbf{x}_1) V_{dl}(\mathbf{x}_2) \rangle$$

have the same coordinate dependences and there is no correlation between the fields $V(\mathbf{x})$ and $V_{dl}(\mathbf{x})$. We then have

$$|\gamma_{cv}| < \gamma_{cc}^{1/2} \gamma_{vv}^{1/2}.$$

Finally, the correlation functions of the form (9) can be used in considering the model of statistically independent fields on the assumption that $\gamma_{cv} = 0$.

We shall now show how we can construct an asymptotic expansion of the function $Z(t)$ in the limit $t \rightarrow \infty$. We shall adopt the canonical representation of the correlation functions¹⁰

$$D_{l_1 l_2}(\mathbf{x}_1 - \mathbf{x}_2) = \gamma_{l_1 l_2} \sum_n a_n(\mathbf{x}_1) a_n(\mathbf{x}_2),$$

where $a_n(\mathbf{x})$ are some basis functions. Introducing auxiliary integration with respect to ξ_n and φ_n , we shall represent the function $Z(t)$ in the form

$$\begin{aligned} Z(t) = & \int d\mathbf{x} \int P[\dots \xi_n \dots, \dots \varphi_n \dots] \prod_n d\xi_n d\varphi_n \int D\mathbf{x}(\tau) \\ & \times \exp \left\{ - \int_0^t \left[\frac{m_c}{2} \dot{\mathbf{x}}^2(\tau) + \sum_n \xi_n a_n(\mathbf{x}(\tau)) \right] d\tau \right\} \int D\mathbf{y}(\tau) \\ & \times \exp \left\{ - \int_0^t \left[\frac{m_v}{2} \dot{\mathbf{y}}^2(\tau) - \sum_n \varphi_n a_n(\mathbf{y}(\tau)) \right] d\tau \right\}, \quad (10) \end{aligned}$$

where

$$\begin{aligned} P[\dots \xi_n \dots, \dots \varphi_n \dots] = & \prod_n [2\pi \gamma_{cc}^{1/2} \gamma_{vv}^{1/2} (1-R^2)^{-1/2}]^{-1} \\ & \times \exp \left\{ - \frac{1}{2(1-R^2)} \left[\frac{\xi_n^2}{\gamma_{cc}} - \frac{2R\xi_n\varphi_n}{\gamma_{cc}^{1/2}\gamma_{vv}^{1/2}} + \frac{\varphi_n^2}{\gamma_{vv}} \right] \right\}. \quad (11) \end{aligned}$$

Here, $R = \gamma_{cv}/(\gamma_{cc}\gamma_{vv})^{1/2}$. The function $P[\dots \xi_n \dots, \dots \varphi_n \dots]$ obviously represents the probability density of normally distributed random quantities ξ_n and φ_n , the correlation moments of which satisfy the relationships

$$\langle \xi_n \xi_k \rangle = \gamma_{cc} \delta_{nk}, \quad \langle \varphi_n \varphi_k \rangle = \gamma_{vv} \delta_{nk}, \quad \langle \xi_n \varphi_k \rangle = \gamma_{cv} \delta_{nk}.$$

The correlation coefficient R , which can have any value, satisfies the condition $|R| \leq 1$, which essentially determines how much the functional relationship between $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$ deviates from linearity. A linear relationship between these fields corresponds to $|R| = 1$, and in this case the exponential function in Eq. (11) reduces to a product of a Gaussian distribution function for ξ_n or φ_n and a delta function representing the existence of a linear relationship between ξ_n and φ_n , and, consequently, between the fields $V_c(\mathbf{x}) = \sum_n \xi_n a_n(\mathbf{x})$ and $V_v(\mathbf{x}) = -\sum_n \varphi_n a_n(\mathbf{x})$.

Representation of the function $Z(t)$ in the form (10) is convenient because, instead of the double integral along the paths in Eq. (8), we are now dealing with a product of two single integrals which, as is easily shown, represent one-particle density matrices $\rho_c(\mathbf{r}/2; -\mathbf{r}/2; t)$ and $\rho_v(-\mathbf{r}/2; \mathbf{r}/2; t)$ whose asymptotic form in the limit $t \rightarrow \infty$ is known¹¹:

$$\rho_l(\mathbf{x}_1, \mathbf{x}_2; t) = e^{-E_{0l}t} \psi_{0l}(\mathbf{x}_1) \psi_{0l}(\mathbf{x}_2). \quad (12)$$

Here, E_{0l} and $\psi_{0l}(\mathbf{x})$ are the energy and the wave function of the ground state of a particle which is in a potential $V_l(\mathbf{x})$, and which are found by solving the appropriate Schrödinger equation. If we now represent the potential $V_l(\mathbf{x})$ in the form

$$V_l(\mathbf{x}) = V_{0l}(\mathbf{x}) + V_{1l}(\mathbf{x}),$$

where

$$V_{0l}(\mathbf{x}) = -\frac{t}{2} [D_{ll}(0) - D_{cv}(t)] + \frac{m_l \omega_l^2}{2} (\mathbf{x} \mp \mathbf{r}/2)^2, \quad (13)$$

$$V_{1l}(\mathbf{x}) = V_l(\mathbf{x}) - V_{0l}(\mathbf{x}).$$

Here and below the upper indices correspond to $l = c$ and the lower ones to $l = v$. The oscillator frequencies are given by the relationship

$$\omega_l^2 = \frac{t}{m_l} \{-D_{ll}''(0) + D_{cv}''(0) [1 - \theta(R)]\}. \quad (14)$$

The dependence of the frequencies ω_l on the correlation coefficient R reflects the circumstance that different values of R correspond to physically different situations. For example, in the positive correlation case ($R > 0$) the bottom of the conduction band and the top of the valence band are bent by the random field in the same direction (Fig. 1). In the negative correlation case ($R < 0$) we can see from Fig. 2 that the bottom of the conduction band and the top of the valence band are shifted in opposite directions. Finally, $R = 0$ corresponds to the situation when the band bending by the random field is statistically independent (Fig. 3).

We shall show that the main contribution to the asymp-

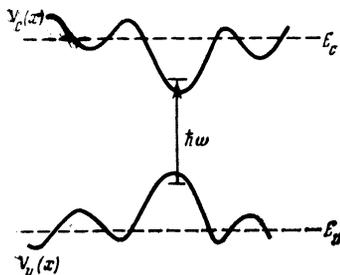


FIG. 2. Band bending in the case of a negative correlation of the random fields $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$.

otic form of the density matrix (12) comes from the potential $V_{0l}(\mathbf{x})$, and the influence of the potential $V_{1l}(\mathbf{x})$ can be allowed for by using perturbation theory. We shall find initially the energy and the wave functions for the potential V_{0l} :

$$E_{0l}^{(0)} = -\frac{t}{2} [D_{ll}(0) - D_{cv}(r)] + \frac{3}{2} \omega_l, \quad (15)$$

$$\Psi_{0l}(\mathbf{x}) = \left(\frac{m_l \omega_l}{\pi}\right)^{3/4} \exp\left\{-\frac{m_l \omega_l}{2} (\mathbf{x} \mp \mathbf{r}/2)^2\right\}. \quad (16)$$

The corrections to the energy of the ground state derived in the first order of perturbation theory in V_{1l} are¹²

$$E_{0c}^{(1)} = \langle 0c | \sum_n \xi_n a_n(\mathbf{x}) - V_{0c}(\mathbf{x}) | 0c \rangle, \quad (17)$$

$$E_{0v}^{(1)} = \langle 0v | -\sum_n \varphi_n a_n(\mathbf{x}) - V_{0v}(\mathbf{y}) | 0v \rangle, \quad (18)$$

where $|0l\rangle = |\Psi_{0l}\rangle$. We shall be interested only in the exponential terms in the absorption coefficient, so that the corrections to the wave functions will be ignored, since they affect only the value of the preexponential factor, which we shall later omit. Using Eqs. (15)–(18) and also the relationship between the path integrals in Eq. (10) with the asymptote of the density matrices of Eq. (12), we find that after integration with respect to ξ_n and φ_n the function $Z(t)$ becomes

$$\begin{aligned} Z(t) = \int d\mathbf{r} \exp \left\{ \frac{t^2}{2} [D_{cc}(0) + D_{vv}(0) - 2D_{cv}(r)] - \frac{3}{2} \omega_c t \right. \\ \left. - \frac{3}{2} \omega_v t + \frac{t^2}{2} \langle 0c0c | D_{cc}(\mathbf{x}_1 - \mathbf{x}_2) | 0c0c \rangle + t \langle 0c | V_{0c} | 0c \rangle \right. \\ \left. + \frac{t^2}{2} \langle 0v0v | D_{vv}(\mathbf{y}_1 - \mathbf{y}_2) | 0v0v \rangle + t \langle 0v | V_{0v} | 0v \rangle \right. \\ \left. - t^2 \langle 0v0c | D_{cv}(\mathbf{y}_1 - \mathbf{x}_2) | 0c0v \rangle - (m_c \omega_c + m_v \omega_v) \mathbf{r}^2 \right\}, \quad (19) \end{aligned}$$

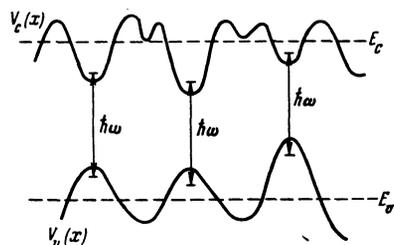


FIG. 3. Band bending in the case of zero correlation of the random fields $V_c(\mathbf{x})$ and $V_v(\mathbf{x})$.

where

$$|0l_1 0l_2\rangle = |\Psi_{0l_1} \Psi_{0l_2}\rangle.$$

It should be noted that in calculation of the matrix elements in Eq. (19) we can use the smallness of the parameter $(m_l \omega_l L^2)^{-1/2}$ in the limit $t \rightarrow \infty$, which represents the ratio of the localization radius of the wave function (16) to the correlation length L of the random field.

It is clear from Eq. (19) that in calculating the integral with respect to the spatial coordinate \mathbf{r} an important role is played by the sign of the correlation function $D_{cv}(\mathbf{r})$. For nonpositive correlations ($R \leq 0$) this correlation function obeys $D_{cv}(\mathbf{r}) \leq 0$ for all values of \mathbf{r} and the important values of the coordinates which determine the integral are of order

$$r^2 \approx [-D_{cv}''(0)t^2 + m_c \omega_c + m_v \omega_v]^{-1}. \quad (20)$$

In the case when the correlation coefficient is positive ($R > 0$) the mutual correlation function obeys $D_{cv}(\mathbf{r}) > 0$ for all values of \mathbf{r} , so that in the case of integration with respect to the coordinates we have to know the actual form of the correlation function $D_{cv}(\mathbf{r})$ for large values of the argument, because—as shown below—the important values of the coordinates are much larger than the correlation length of the random field. We shall assume that at large values of $|\mathbf{r}|$ the mutual correlation function is given by Eq. (6). Then, after integration with respect to \mathbf{r} we find that the important values of the coordinates governing the integral are of order

$$r^2 \approx L^2 \ln \frac{t^2 D_{cv}(0) L^{-2}}{[-m_c D_{cc}''(0)]^{1/2} + [-m_v D_{vv}''(0)]^{1/2}}. \quad (21)$$

After integration with respect to position the function $Z(t)$ can be represented in the form

$$\begin{aligned} Z(t) = \exp \left\{ \frac{t^2}{2} W^2 - \frac{3}{2} t^2 \left[\frac{\Omega_c^{1/2}}{m_c^{1/2}} + \frac{\Omega_v^{1/2}}{m_v^{1/2}} \right] + \frac{21}{2 \cdot 4!} t \left[\frac{D_{cc}^{IV}(0)}{m_c \Omega_c} \right. \right. \\ \left. \left. + \frac{D_{vv}^{IV}(0)}{m_v \Omega_v} \right] + \frac{15t}{4 \cdot 4!} \left[\frac{D_{cv}^{IV}(0)}{m_c \Omega_c} + \frac{D_{cv}^{IV}(0)}{m_v \Omega_v} \right] [1 - \theta(R)] \right. \\ \left. + \frac{27}{2 \cdot 4!} \frac{D_{cv}^{IV}(0)t}{(m_c m_v \Omega_c \Omega_v)^{1/2}} [1 - \theta(R)] + O(t^4) \right\}, \quad (22) \end{aligned}$$

where

$$W^2 = D_{cc}(0) + D_{vv}(0) - 2D_{cv}(0) [1 - \theta(R)], \quad (23)$$

$$\Omega_l = -D_{ll}''(0) + D_{cv}''(0) [1 - \theta(R)]. \quad (24)$$

The following point should be made. The expression (22) was obtained for $R > 0$ on the assumption that the fall of the correlation function at large values of the argument is given by Eq. (6); nevertheless, we can show that it remains valid also when the correlation factor drops off more slowly than exponential. An estimate of the characteristic values of the coordinates naturally changes, but Eq. (21) then plays the role of the lower limit.

Equation (22) was obtained on the assumption that the correlation functions of the random field are related by Eq. (9). We can show that in the case of statistically independent fields, when $D_{cv}(\mathbf{x}) = 0$, Eq. (22) is valid for any form of correlation functions $D_{cc}(\mathbf{x}_1 - \mathbf{x}_2)$ and $D_{vv}(\mathbf{x}_1 - \mathbf{x}_2)$ which satisfy the conditions that they are finite and differentiable the required number of times at the zero.

In calculating the asymptotic form of the function $Z(t)$

we shall include only the first corrections to the ground-state energy. However, we can also find the higher corrections and show that inclusion of these corrections does not alter the estimate of the accuracy of the function $Z(t)$ given by Eq. (22). We shall show that the potentials V_{0c} and V_{0v} should be selected to ensure that these corrections are small.

3. ABSORPTION COEFFICIENT

We shall now calculate the absorption coefficient for light. After integration with respect to t , Eqs. (22) and (7) yield

$$\begin{aligned} \alpha(\omega) = \exp \left\{ -\frac{(E_q - \omega)^2}{2W^2} - \frac{3}{2} \frac{(E_q - \omega)^3}{W^3} \left[\frac{\Omega_c^{1/2}}{m_c^{1/2}} + \frac{\Omega_v^{1/2}}{m_v^{1/2}} \right] \right. \\ \left. - \frac{(E_q - \omega)}{W^2} \left[\frac{81}{32W^2} \left(\frac{\Omega_c^{1/2}}{m_c^{1/2}} + \frac{\Omega_v^{1/2}}{m_v^{1/2}} \right)^2 \right. \right. \\ \left. \left. - \frac{7}{16} \left(\frac{D_{cc}^{IV}(0)}{m_c \Omega_c} + \frac{D_{vv}^{IV}(0)}{m_v \Omega_v} \right) \right] \right. \\ \left. - (1 - \theta(R)) \frac{5}{32} \left(\frac{D_{cv}^{IV}(0)}{m_c \Omega_c} + \frac{D_{vc}^{IV}(0)}{m_v \Omega_v} \right) \right. \\ \left. - (1 - \theta(R)) \frac{9}{16} \frac{D_{cv}^{IV}(0)}{(m_c m_v \Omega_c \Omega_v)^{1/2}} \right\}. \quad (25) \end{aligned}$$

The important values of t which determine the integral are of order

$$t \approx (E_q - \omega)/W^2.$$

Hence, it is clear that an asymptotic expansion of the absorption coefficient should be made in the argument of the exponential function using the powers of $(E_q - \omega)^{-1/2}$. It should be pointed out, however, that although the higher terms of the expansion are smaller than the first, nevertheless they cannot be used in the expansion of the exponential function because they are much greater than unity. This means that all the attempts to obtain an expansion in which only the first term is retained in the argument of the exponential function fail to give the correct result in the deep tail region.

A comparison of Eqs. (3) and (23) shows that in the nonpositive correlation case ($R \leq 0$) we have $W^2 = W_k^2$ and the first term of the expansion of Eq. (25) is identical with the semiclassical result (1) and describes the absorption of light due to fluctuations of the width of the band gap. We can easily see that inclusion of the higher terms of the expansion in Eq. (25) reduces considerably the absorption coefficient compared with the semiclassical result. This is due to the fact that in the case of differences in the band bending all the quantum effects are ignored in the semiclassical approximation and it is assumed that if a fluctuation of the width of the band gap, ensuring the absorption of a photon with a given energy deficit, appears in a semiconductor, then a carrier undergoes a transition between the top of the valence band and the bottom of the conduction band. In fact, because of the quantum effects the transition occurs between states in fluctuation wells separated by a finite energy from the edges of the corresponding bands (Fig. 2). This means that if we allow for the quantum effects, the absorption coefficient should be less than the semiclassical value.

In the positive correlation case ($R > 0$) the first term of the expansion (25) is different from the result of the semiclassical approximation, because for $R > 0$ case we have $W^2 \neq W_k^2$. As shown above, this is due to the fact that in the case of a positive correlation of the random fields the absorption of light in the deep tail region is dominated by the indirect transitions and these are ignored in the semiclassical description.

The expression for the absorption coefficient of light in the case of a positive correlation between the random fields is identical with the expression for the absorption coefficient corresponding to zero correlation. This is to be expected because typical electron tunneling distances are much greater than the correlation length of the random field. At these distances the correlation between the random fields is so weak that they are in fact statistically independent. Moreover, the function $Z(t)$ is identical, within the limits indicated in Eq. (22), with the product of one-particle averaged density matrices.¹³ This means that if $R \geq 0$, the absorption coefficient of light in the deep tail region reproduces, apart from the terms proportional to $(E_q - \omega)$ in the argument of the exponential function, a convolution of the densities of states. The relationship between the absorption coefficient of light and the convolution of the density of states is primarily due to the statistical independence (in the sense defined above) of the random fields V_c and V_v and, secondly, due to the fact that the absorption of light includes contributions of transitions between all the tail states separated from one another by ω on the energy scale (Fig. 3). It should also be pointed out that in the case of the same band bending, when $D_{cv}(\mathbf{x}) = D_{cc}(\mathbf{x}) = D_{vv}(\mathbf{x})$, Eq. (25) is identical with the result obtained earlier in Ref. 14.

We shall now discuss the limits of validity of our results. Representation of the asymptotic limit of the density matrix in the form (12) is justified provided the potential of Eq. (13) includes bound states, i.e., $E_{0l} < 0$, or if

$$\Delta \gg \Omega_l W^2 / m_l \{ D_{ll}(0) - D_{cv}(0) [1 - \theta(R)] \}^2. \quad (26)$$

In finding the asymptotic form of the density matrix we included only the contribution of the ground state, which is justified if

$$\Delta \gg W^2 \left(\frac{m_l}{\Omega_l} \right)^{1/2}. \quad (27)$$

The matrix elements were calculated in Eq. (19) on the assumption that we have $(m_l \omega_l L^2)^{-1/2} \ll 1$, which is valid if

$$\Delta \gg W^2 / m_l \Omega_l L^4. \quad (28)$$

Moreover, the influence of the potential V_{1l} is included using perturbation theory, the condition of validity of which is in this case

$$\Delta \gg W^2 \frac{[D_{l_1 l_2}^{IV}(0)]^2}{m_l \Omega_l^3}. \quad (29)$$

Finally, in calculating the integral with respect to the spatial coordinates in the case of a nonzero correlation of the random fields, we use the steepest-descent method which in this case is justified if

$$\Delta^2 \gg [D_{cc}(0) + D_{vv}(0)]^2 / |D_{cv}(0)|. \quad (30)$$

When the random fields are uncorrelated the integral with

respect to r in Eq. (19) can be carried out exactly, so that there is no need to satisfy the condition (30). Moreover, we can show that in the case of a weak correlation between the random fields, when

$$D_{cv}(0) \ll D_{cc}(0), D_{vv}(0),$$

Eq. (25) is valid also if

$$\Delta^2 \ll [D_{cc}(0) + D_{vv}(0)]^2 / |D_{cv}(0)|. \quad (31)$$

The above conditions are noncontradictory and can be satisfied simultaneously, which determines the conditions for the validity of the asymptotic expansion for the absorption coefficient of Eq. (25).

¹V. L. Bonch-Bruевич, Phys. Status Solidi **42**, 35 (1970).

²E. V. Burtsev, Izv. Vyssh. Uchebn. Zaved. Fiz. No. 4, 121 (1972).

³V. L. Bonch-Bruевич, Usp. Fiz. Nauk **140**, 583 (1983) [Sov. Phys. Usp. **26**, 664 (1983)].

⁴V. L. Bonch-Bruевич, I. P. Zvyagin, R. Kaiper, A. G. Mironov, R.

Enderlein, and B. Esser, *Electronic Theory of Disordered Semiconductors* [in Russian], Nauka, Moscow (1981), Chap. 5.

⁵B. I. Shklovskii and A. L. Éfros, Zh. Eksp. Teor. Fiz. **59**, 1343 (1970) [Sov. Phys. JETP **32**, 733 (1971)].

⁶A. L. Éfros, Usp. Fiz. Nauk **111**, 451 (1973) [Sov. Phys. Usp. **16**, 789 (1974)].

⁷B. I. Shklovskii and A. L. Éfros, *Electronic Properties of Doped Semiconductors*, Springer Verlag, Berlin (1984), §42.

⁸Yu. D. Arbuzov and M. Yu. Kolenkin, Phys. Status Solidi B **138**, 547 (1986).

⁹Yu. D. Arbuzov and M. Yu. Kolenkin, Izv. Vyssh. Uchebn. Zaved. Fiz. No. 6, 46 (1987).

¹⁰V. S. Pugachev, *Theory of Random Functions and Its Application to Control Problems*, Pergamon, Oxford (1965), Chap. 9.

¹¹R. P. Feynman, *Statistical Mechanics: A Set of Lectures*, Benjamin, New York (1972), Chap. 2.

¹²L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 3rd ed., Pergamon Press, Oxford (1977), Chap. 6.

¹³Yu. D. Arbuzov and V. M. Evdokimov, Fiz. Tverd. Tela (Leningrad) **21**, 2099 (1979) [Sov. Phys. Solid State **21**, 1202 (1979)].

¹⁴Yu. D. Arbuzov and M. Yu. Kolenkin, Fiz. Tverd. Tela (Leningrad) **29**, 206 (1987) [Sov. Phys. Solid State **29**, 115 (1987)].

Translated by A. Tybulewicz