# The fluctuation potential and the structure of impurity bands of a lightly doped and weakly compensated semiconductor

Yu. Ya. Tkach and E. V. Chenskii

Institute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow (Submitted 9 July 1992) Zh. Eksp. Teor. Fiz. **102**, 1683–1692 (November 1992)

We suggest a model for a lightly doped and weakly compensated semiconductor. On the basis of the Markov method we calculate the density of the fluctuation potential as a function of the degree of compensation K of the semiconductor. We show that the dependence of the position of the Fermi level on the degree of compensation is caused by the increase in the amplitude of the fluctuation potential with K. In the region of low compensation degrees we calculate the density of donor and acceptor states and show that both have two peaks when considered as functions of K. The Fermi level for an n-type semiconductor is found to lie between the peaks at the minimum of the donor density, and the acceptor density has a "forbidden" gap with an energy of the order of  $e^2N_d^{1/3}\varepsilon$ , where  $N_d$  is the average volume concentration of donors, and  $\varepsilon$  is the dielectric constant of the semiconductor. We also find that studying the spectral density of absorption from an acceptor level provides theoretically the means for determining the density of the fluctuation potential in weakly compensated semiconductors.

### **1. INTRODUCTION**

When studying doped semiconductors there practically always arises the problem of calculating or estimating the impurity fluctuation potential. As a fairly recent investigation in this field we cite Ridley's paper,<sup>1</sup> which, we believe, lists a clearly overestimated value of the fluctuation potential. On the other hand, such semiconductors have been studied fairly well by numerical modeling.<sup>2,3</sup> These results can be used to test various models for describing the impurity fluctuation potential. Analytical results concerning the position of the Fermi level exist only in the limit of a zero degree of compensation.<sup>2</sup>

In this paper we develop a model of a lightly doped and weakly compensated semiconductor. The model made it possible to calculate the density of the fluctuation potential as a function of the degree of compensation, demonstrate the dependence of the Fermi level on the degree of compensation obtained earlier by numerical modeling in Ref. 3, formulate the physical reasons leading to such a dependence, and calculate the density of donor and acceptor states in the limit of low degrees of compensation. (A similar problem for a strongly compensated semiconductor has been solved by the present authors in Refs. 4 and 5.)

For the sake of definiteness we will consider a semiconductor of the *n*-type doped with shallow donors and acceptors with average volume concentrations  $N_d$  and  $N_a$ . We assume that the conditions of light doping are met, namely  $N_{a,d} \alpha_{a,d}^3 \ll 1$ , where  $a_a$  and  $a_d$  are the respective Bohr radiuses. This inequality makes it possible to speak of donor and acceptor impurity bands in the classical sense, when the shift in a level of an impurity band can be assumed equal to the potential energy of this center generated by the other charged impurities.

Calculations are done for the case of absolute zero and are based on the following qualitative picture. When the degree of compensation is low, all acceptors are negatively charged. Each acceptor is surrounded by many donors, with the result that the closest donor is, as a rule, ionized and the two form a dipole pair, the so-called 1-complex.<sup>2,3</sup> These dipoles are located far from each other (at a distance of the order of  $N_a^{-1/3}$ ) and, therefore, their interaction is weak. There is also a small number of acceptors (about 1.3%) for which the closest donor is located at a distance greater than  $r_{\mu} = 1/\mu$ , where  $\mu$  is the Fermi level energy, with the result that each such acceptor is surrounded only by neutral donors. Such formations are called 0-complexes. Finally, there are what is known as 2-complexes, that is, acceptors near which there is a maximum number (two) of ionized donors.<sup>2,3</sup> By equating the concentrations of 0- and 2-complexes, we ensure the electroneutrality of the sample and find the position of the Fermi level for the case where the degree of compensation of the semiconductor, K, tends to zero. At this stage, as compared to Refs. 2 and 3, we have refined only the expression for the concentration of 2-complexes.

The next step is to apply the Markov method to the system of disordered dipoles (1-complexes) and calculate the density of the fluctuation potential. The presence of a fluctuation potential whose amplitude increases with K changes the concentration of 0- and 2-complexes. Equating their total concentrations, we arrive at the condition of electroneutrality of the sample and the equation specifying the  $\mu$  vs K dependence. This method also provides a way to calculate, as  $K \rightarrow 0$ , the density of donor and acceptor states exactly. It was found that the density of acceptor states exhibits a number of special features (two peaks, among other things) that make it possible, at least in principle, to determine the density of the fluctuation potential of the sample or the sample's degree of compensation by measuring the spectral pattern of absorption.

#### 2. THE FERMI LEVEL FOR $K \rightarrow 0$

To determine the concentration of 0-complexes,  $N_0(\mu)$ , we must count the acceptors for which the closest donor is situated at a distance greater than

$$r_{\mu} = 1/\mu. \tag{1}$$

Here we have employed dimensionless variables for the distance  $\mathbf{r} = \mathbf{r}^*/r_d$ , with  $r_d = (4\pi N_d/3)^{-1/3}$ , and energy  $E = E^*/E_d$ , with  $E_d = e^2/\varepsilon r_d$ , where  $\varepsilon$  is the dielectric constant of the semiconductor, and the asterisk denotes dimensional quantities. The energy was measured from the unperturbed donor state in the conduction band. Assuming that the impurities obey the Poisson distribution, we find the following expression for the concentration of 0-complexes:

$$N_{0}(\mu) = K \exp(-1/\mu^{3}).$$
 (2)

For 2-complexes, the energies of the first and second charged donors positioned at points  $\mathbf{r}_1$  and  $\mathbf{r}_2$  (Fig. 1) are

$$E_{1,2} = \frac{1}{r_{1,2}} - \frac{1}{(r_1^2 + r_2^2 + 2r_1r_2\cos\theta)^{\frac{1}{2}}},$$
(3)

where  $\theta$  is the angle between  $\mathbf{r}_1$  and  $\mathbf{r}_2$ .

Assuming that the donor closest to an acceptor is charged, we can represent the concentration of 2-complexes in the form

$$N_{2}(\mu) = 3K \int_{0}^{1/2\mu} dr_{1}r_{1}^{2} \exp(-r_{1}^{3}) \{1 - \exp[v(r_{1}, \mu)]\}.$$
(4)

The upper limit in the integral corresponds to a symmetric arrangement of the donors in relation to the acceptor, and the last cofactor under the integral sign is found from the condition that at least one donor is inside the volume  $v(r_1,\mu)$  (see Fig. 1) enclosed by the sphere of radius  $r_1$  and the  $\mu$ -surface determined by the equation

$$E_2(\mathbf{r}, r_i) = \mu, \quad |\mathbf{r}| \ge r_i. \tag{5}$$

Employing the fact that the  $\mu$ -surface possesses cylindrical symmetry, we can represent  $v(r_1,\mu)$  as follows:

$$v(r_{i},\mu) = \frac{3}{4i} \int_{x_{\mu}}^{x_{\mu}} y^{2}(x) dx - \frac{1}{2} r_{i}^{3} + \frac{3}{4} r_{i}^{2} x_{\mu} - \frac{1}{4} x_{\mu}^{3}.$$
(6)

Here  $x_{\mu}$ ,  $r_{2\mu}$ , and y(x) (see Fig. 1) are given by the following relations:  $x_{\mu} = r_1 \cos \theta_{\mu}$ , where  $\theta_{\mu}$  is determined by the condition that  $E_2(r_1, r_2 = r_1, \theta_{\mu}) = \mu$ , as a result of which we get



FIG. 1. The spatial cross section of the structure of a 2-complex along the rotation axis x.

$$x_{\mu} = r_{i} \left[ \frac{1}{2(1-\mu r_{i})^{2}} - 1 \right], \tag{7}$$

 $r_{2\mu}$  is found from the equation  $E_2(r_1, r_{2\mu}, \theta = 0) = \mu$  and has the form

$$r_{2\mu} = \frac{r_1}{2} \left[ \left( 1 \pm \frac{4}{r_1 \mu} \right)^{\prime h} - 1 \right], \tag{8}$$

and, finally,  $y(x,\mu,r_1)$  is specified by the formula

$$\mu = \frac{1}{(x^2 + y^2)^{\frac{1}{1}}} - \frac{1}{[(r_1 + x)^2 + y^2]^{\frac{1}{1}}}.$$
(9)

The dependence of the concentrations of 0- and 2-complexes on the position of the Fermi level is depicted in Fig. 2. The point where the two curves intersect corresponds to an electroneutral sample, that is, this condition fixes the position of the Fermi level  $\mu_0$  as  $K \rightarrow 0$ . Note that the more accurate value  $\mu_0 \approx 0.607$  that we obtained does not fall outside the limits of the spread of values listed in Ref. 3.

#### 3. THE DENSITY OF THE FLUCTUATION POTENTIAL

To find the density of the fluctuation potential in the semiconductor we assume, because of low concentrations of the 0- and 2-complexes, that the potential is generated by 1-complexes, and the donor closest to the acceptor is the charged one. This approximation has been substantiated and used in calculating the distribution function for the electric field in a weakly compensated semiconductor.<sup>6</sup> Using the Markov method,<sup>7</sup> we can write the probability density of potential V as follows:

$$P(V) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[i\rho V - KC(\rho)] d\rho,$$
  

$$C(\rho) = \frac{9}{2} \int_{0}^{\infty} r_{1}^{2} dr_{1} \int_{0}^{\infty} r_{2}^{2} \exp(-r_{2}^{3}) dr_{2} \int_{-1}^{1} d\xi \left\{ 1 - \exp\left[i\rho\left(\frac{1}{r_{1}} - \frac{1}{(r_{1}^{2} + r_{2}^{2} + 2r_{1}r_{2}\xi)^{\frac{1}{2}}\right)^{\frac{1}{2}}\right] \right\}, \quad (10)$$

where  $r_1$  is the distance to the acceptor,  $r_2$  the distance between the acceptor and the closest donor, and  $\xi = \cos \theta$ , with  $\theta$  the angle between  $\mathbf{r}_1$  and  $\mathbf{r}_2$ .



FIG. 2. Concentrations of 0-complexes (curve 1) and 2-complexes (curve 2) as functions of the position of the Fermi level.

Formula (10) can be simplified by replacing the potential with the commonly used point-dipole approximation  $(r_2 \ll r_1)$  (Ref. 6). Integrating over the angle and introducing the notation  $y = r_2^3$  and  $z = \rho r_2/r_1$ , we find that

$$C(\rho) = \frac{3}{2} |\rho|^{\frac{y_1}{y_2}} \int_{0}^{\infty} y^{\frac{y_2}{y_2}} e^{-y} dy \int_{0}^{\infty} \left(1 - \frac{\sin z}{z}\right) \frac{dz}{z^{\frac{y_1}{z_2}}} = \alpha |\rho|^{\frac{y_2}{z_2}},$$
(11)

where  $\alpha = \frac{3}{2}\pi^{1/2}C_1$ , with  $C_1 \approx 0.666$  the value of the second integral, that is,  $\alpha = 1.769$ .

Substituting (11) into (10), we can easily verify that the density of the fluctuation potential in the point-dipole approximation for any degree of compensation is expressed in terms of the universal function  $P_d(x)$ :

$$P(V,K) = \frac{1}{(\alpha K)^{\frac{n}{2}}} P_d\left(\frac{V}{(\alpha K)^{\frac{n}{2}}}\right), \qquad (12)$$

where

$$P_{d}(x) = \frac{1}{\pi} \int_{0}^{\infty} \cos(tx) \exp(-t^{t_{0}}) dt.$$
 (13)

The shape of the function  $P_d(x)$  obtained by numerical integration is depicted in Fig. 3.

The results of computer calculations using the more exact formulas (10) demonstrate that on the same scale the expression for P(V,K) in the case of a dipole interaction with a finite "arm" is approximately given by formula (12) but with a different characteristic function  $P_c(x)$ . Its shape is depicted in Fig. 3. As one would expect, in comparison to  $P_d(x)$  this function has a sharper peak as  $V \rightarrow 0$  and falls off more rapidly as V increases.

# 4. THE POSITION OF THE FERMI LEVEL AS A FUNCTION OF THE DEGREE OF COMPENSATION

To find  $\mu(K)$  we employ the fact that on the average the dipoles are at a distance  $N_a^{-1/3}$  from 0- and 2-complexes and, hence, the characteristic spatial scale of fluctuation-potential variations is also  $N_a^{-1/3}$ . The characteristic size of 0- and 2-complexes, however, is of the order of  $N_d^{-1/3}$ , that



$$\int_{-\infty}^{\infty} N_{20}(\mu - V) P(V, K) dV = 0,$$
 (14)

where  $N_{20}(\mu - V) = N_2(\mu - V) - N_0(\mu - V)$ . Using a scaling transformation similar to (12) and the calculated function  $P_c(x)$ , we can write the electroneutrality condition (14) as

$$\int_{-\infty}^{\infty} N_{20}(\mu - V) P_c\left(\frac{V}{(\alpha K)^{\eta_a}}\right) dV = 0.$$
(15)

For moderate values of K the principal contribution to the integral is provided by the small values of the potential,  $|V| \leq \mu$ , and the value of the Fermi level differs little from  $\mu_0$ , or  $|\mu - \mu_0| \leq \mu_0$ . Using these inequalities and performing an expansion in (15), we find that

$$\mu(K) = \mu_0 - \frac{(\alpha K)^{4/2}}{2} \frac{N_{20}''(\mu_0)}{N_{20}'(\mu_0)} \langle V_c^2 \rangle, \qquad (16)$$

where

$$\langle V_c^2 \rangle = \int_{-\infty}^{\infty} x^2 P_c(x) dx.$$

Carrying out numerical calculations, we get the following values:  $N'_{20}(\mu_0) = -0.368$ ,  $N''_{20}(\mu_0) = -0.374$ , and  $\langle V_c^2 \rangle = 1.10$ . Substituting these values into (16), we find that

$$\mu(K) \approx 0.607 - 1.196 K^{\prime\prime}. \tag{17}$$

This dependence coincides with the results of numerical modeling<sup>2,3</sup> (Fig. 4). The remarkable thing here is that this agreement occurs within a broad range of degrees of compensation,  $0 \le K < 0.6$ .



FIG. 3. The probability density of the potential for the dipole approximation. Curve I corresponds to the potential of a point dipole, and curve 2 to the potential of a dipole with a finite moment.



FIG. 4. The position of the Fermi level versus the degree of compensation (the points stand for the results of numerical modeling taken from Ref. 3).

Thus, locally the fluctuation potential of 1-complexes changes the number of 0- and 2-complexes and in this way lowers the Fermi level as the degree of compensation of the semiconductor increases.

If the integral equation (15) is solved numerically, already at K = 0.01 there is a deviation from the dependence specified by (16) ( $\mu$  increases with K). The reason is that as K and, hence, V increase, formula (15) begins to overestimate the value of the concentration of 2-complexes. Since with an increase in V the spatial size of 2-complexes also increases, the potential cannot be assumed constant within a 2-complex. For 0-complexes the opposite is true: as V grows, the 0-complexes become smaller. Hence, the fact that the  $\mu$ vs K dependence specified by (17) coincides with the results of numerical modeling<sup>3</sup> suggests that formula (15) provides correct values for the concentration of 0-complexes within a broad range of compensation degrees.

## 5. THE DENSITIES OF DONOR AND ACCEPTOR STATES

To find the density of donor states one must determine the probability density of the potential near each acceptor and sum over all acceptors. Here the normalization volume  $\Omega$  is the volume per acceptor (in dimensionless units we have  $\Omega = \Omega^*/r_d^3 = 4\pi/3K$ ). The density of charged donors is determined by all the donors in the 1- and 2-complexes, while neutral donors are also in 0-complexes.

Near acceptors forming 0-complexes there are only neutral donors with energies E satisfying the inequalities  $\mu > E > K^{1/3}$ . The contribution of the neutral donors to the density of donor states is

$$N_{0}(\mu) \frac{1}{K\Omega} \int_{0}^{K^{-1/s}} \delta(E - E(r)) 4\pi r^{2} dr.$$
 (18)

Substituting formula (2) that expresses the concentration of 0-complexes and employing the fact that the neutral donors in the 0-complexes are in a potential equal to 1/r, we find after calculations that

$$N_{d0}(E) = K(3/E^4) \exp(-1/\mu^3), \ \mu > E > K^{\nu_1}.$$
(19)

The distribution of 1-complexes along the arm of a dipole,  $r_1$ , which in what follows will be denoted by  $N_1(r_1,\mu)$ , is

$$N_{i}(r_{i}, \mu) = 3Kr_{i}^{2} \exp\left[-r_{i}^{3} - v(r_{i}, \mu)\right].$$
(20)

Here  $v(r_1,\mu)$  is determined by (6), and its appearance in the exponential in (20) is the reflection of the requirement that nrear the given acceptor no 2-complex forms [see Eq. (4)]. Allowing for the fact that a charged donor is in a potential equal to  $1/r_1$  and doing calculations similar to (18), we arrive at the following formula for the density of charged donors in 1-complexes:

$$N_{d_1}(E) = K(3/E^4) \exp\{-E^{-3} - v(1/E, \mu)\}, E > \mu.$$
(21)

Neutral donors that are close to 1-complexes find themselves in the dipole potential  $E(r_1, r, \theta)$  of the type (3) in which  $r_2$  must be replaced by the current coordinate **r**. Combining (3) and (18) and calculating, for a 1-complex with an arm  $r_1$  we find that

$$N_{di}(r_{i}, E) = \frac{3K}{2r_{i}E^{5}} \left[ \frac{1}{2(1-Er)^{2}} - \frac{4}{1-Er} - \ln(1-Er) + 4(1-Er) - \frac{(1-Er)^{2}}{2} \right] \Big|_{r=r_{i}}^{r=r_{mE}},$$
(22)

where  $r_{mE} = \min(r_E, K^{-1/3})$ , with

$$r_{E} = \frac{r_{i}}{2} \begin{cases} \left[ -1 + \left( 1 + \frac{4}{Er_{i}} \right)^{\frac{1}{2}} \right], & \mu > E > 0, \\ \left[ 1 + \left( 1 - \frac{4}{Er_{i}} \right)^{\frac{1}{2}} \right], & E < 0. \end{cases}$$
(23)

The total density of neutral donors can be obtained by integrating over all 1-complexes:

$$N_{di}(E) = 3 \int_{0}^{r_{i}^{2}} \exp[-r_{i}^{3} - v(r_{i}, \mu)] N_{di}(r_{i}, E) dr_{i}. \quad (24)$$

Here  $r_{1m}$  is the maximum value of  $r_1$  at which the energy of neutral donors in 1-complexes still reaches E (note that the neutral donors are at a distance from the acceptor greater than  $r_1$ ):

$$r_{im} = \begin{cases} \min(1/2E, 1/\mu), & \mu > E > 0, \\ 1/\mu, & E < 0. \end{cases}$$
(25)

For the charged donors in 2-complexes one must calculate separately the density of states due to the first charged donor (closest to the acceptor) and that due to the second charged donor, since the different energies of these donors [see Eq. (3)] lead to different limits of integration when calculating  $N_{d2}(E)$ .

The concentration of 2-complexes in which the first donor is inside the spherical layer between  $r_1$  and  $r_1 + dr_1$  and the second donor inside the spherical layer between  $r_2$  and  $r_2 + dr_2$  is given by the following expression:

$$N_{42}(r_1, r_2, \xi) dr_1 dr_2 d\xi$$
  
=  $\frac{9}{2r_1^2} \exp(-r_1^3) dr_1 r_2^2 dr_2 \exp[-v(r_1, E_2)] d\xi.$  (26)

Here,  $\xi = \cos \theta$ , with  $\theta$  the angle between  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , and  $v(r_1, E_2)$  is specified by Eq. (6) where  $\mu$  must be replaced with  $E_2$  given by formula (3).

The density of charged donor states from 2-complexes is

$$N_{d2}(E) = \int \int \int \left[ \delta(E - E_1(r_1, r_2, \xi)) + \delta(E - E_2(r_1, r_2, \xi)) \right] \\ \times N_{d2}(r_1, r_2, \xi) dr_1 dr_2 d\xi.$$

(27)

Here the first and second terms in square brackets correspond, respectively, to the first and second charged donors in a 2-complex. Integrating over  $\xi$ , we get

$$N_{d2}(E) = \int_{1/2E}^{r_{1E}} \int_{r_{2E_{1}}}^{r_{2E}} dr_{1} dr_{2} N_{d2}(r_{1}, r_{2}, \xi_{E_{1}}) \frac{(r_{1}^{2} + r_{2}^{2} + 2r_{1}r_{2}\xi_{E_{1}})^{\eta_{1}}}{r_{1}r_{2}} + \int_{0}^{1/2\mu} \int_{r_{1}}^{r_{1E_{2}}} dr_{1} dr_{2} N_{d2}(r_{1}, r_{2}, \xi_{E_{2}}) \frac{(r_{1}^{2} + r_{2}^{2} + 2r_{1}r_{2}\xi_{E_{2}})^{\eta_{1}}}{r_{1}r_{2}},$$
(28)

where

$$\xi_{E_1} = \frac{Er_1^2(2-Er_1)}{2r_2(1-Er_1)^2} - \frac{r_2}{2r_1}, \quad \xi_{E_1} = \frac{Er_2^2(2-Er_2)}{2r_1(1-Er_2)^2} - \frac{r_1}{2r_2}.$$

Here the limits of integration are found from the condition that there exists a charged donor with the given energy E in a 2-complex and are equal to (see Fig. 1)

$$r_{2E_{1}} = \frac{Er_{1}^{2}}{1 - Er_{1}}, \quad r_{2\mu E} = \left(-E + \mu + \frac{1}{r_{1}}\right)^{-1},$$
  
$$r_{1E} = \frac{1}{E + (E\mu)^{\nu_{1}}}, \quad r_{2E_{2}} = \frac{r_{1}}{2} \left[-1 + \left(1 - \frac{4}{Er_{1}}\right)^{\nu_{2}}\right].$$
  
(29)

The total density of donor states is depicted in Fig. 5. What is important and not obvious here is that the Fermi level is in close connection with the minimum in the density of states and that the density of states is continuous at the Fermi level. The continuity of  $N_d(E)$  with decreasing E is achieved because of the continuous transition of the density of charged (second) donors from 2-complexes to the density of neutral donors from 1-complexes and the density of charged donors from 1-complexes to the density of charged donors from 1-complexes to the density of neutral donors from 1-complexes to the density of neutral donors from 0-complexes. Note that here we have ignored the small density of neutral donors in 2-complexes that appears at E < 0 and has practically no effect on  $N_d(E)$ . We have also ignored the possible features that are associated with the dipole interaction near the Fermi level and lead to a Coulomb gap.<sup>2</sup>

Similar calculations can easily be done for acceptor states. All acceptors in 0-complexes have a zero energy and form, in the limit of  $K \rightarrow 0$ , a delta-like peak in the density of states (for acceptors the origin from which energies are measured is shifted downward by  $\Delta E_{d,a}$ , the difference between the unperturbed energies of donor and acceptor centers). This peak is separated from the rest of the density of states,

equal to  $\mu_0$ , and its height is equal to the concentration of 0complexes and is given by Eq. (2).

The contribution to the density from 1-complexes is equal to the donor density (21) provided that we change the origin from which energies are measured (E is replaced with -E) and (21) use |E| instead of E.

For 2-complexes the acceptor potential is

$$E_a = -\frac{1}{r_1} - \frac{1}{r_2}.$$
 (30)

This is the relation that should be used in (27) when calculating the acceptor density. Integrating once via the delta function, we find that

$$N_{a2} = \frac{9}{2} K \int_{-1/2E}^{r_{1,max}} dr_{1}r_{1}^{2} \exp(-r_{1}^{2}) r_{2E}^{4} \int_{L_{min}}^{1} \exp[-v(r_{1}, E_{2})] d\xi,$$
(31)

where  $r_{2E}$  can be found from (30) by replacing  $E_a$  by the current energy E, and

$$r_{1,max} = [-E + (-E\mu)^{\frac{1}{2}}]^{-1},$$
  
$$\xi_{min} = -\frac{r_1^2 (E + \mu) [2 + (E + \mu)r_1]}{2r_2 [1 + (E + \mu)r_1]^2} - \frac{r_2}{2r_1}.$$

The results of calculations are depicted in Fig. 6. An unexpected though easily explained feature is the presence of two peaks in the distribution  $N_a(E)$  for the initial monoenergetic acceptor level. The presence of a delta-like peak separated by a broad Coulomb gap from the rest of the distribution, can, apparently, be discovered in the spectral dependence of optical absorption from an acceptor to the conduction band. The study of such absorption may at the same time serve as a measurement of the degree of compensation of the semiconductor, since from the  $\mu$  vs K dependence established above and the probability density of the fluctuation potential (10) one can easily determine the position and spread of the density of acceptor states corresponding to 0-complexes. And vice versa, if the degree of compensation of a semiconductor is known, the spectral dependence of absorption makes it possible to establish the density of the fluctuation potential.



FIG. 5. The density of donor states in the limit of  $K \rightarrow 0$ : (a) the general shape of the  $N_a(E)/K$  vs *E* dependence (the maximum at zero is proportional to  $K^{-1/3}$  and is cut off in the figure); (b)  $N_d(E)/K$  near the Fermi level (0, 1, and 2 correspond to densities created by 0-, 1-, and 2-complexes and 3 corresponds to the total density  $N_d(E)/K$ ).



FIG. 6. Density of acceptor states.

#### **6. CONCLUSION**

The suggested model is based on the possibility of carrying out analytical calculations of the structure of the impurity band as  $K \rightarrow 0$ . At small compensation degrees the dipole interaction potential is weak and is characterized by a large spatial scale  $(N_d K)^{-1/3}$ . Hence, the total concentration of 0- and 2-complexes can be established by calculating the density of the fluctuation potential. In the limit of small values of K this agrees well with the situation in a real semiconductor (i.e., the experiment in numerical modeling<sup>2,3</sup>), while the expansion for small K describes correctly the  $\mu$  vs K dependence for 0 < K < 0.6. However, the numerical solution of the nonlinear integral equation (15) obtained on these assumptions changes this dependence quite rapidly (for K > 0.01). The reason is that the size of 0- and 2-complexes is ignored in Eq. (15), while the characteristic size of 2-complexes increases with the compensation degree.

We wish to stress once more the special features of the calculated densities of donor and acceptor states. For donor states the Fermi level is closely connected with the minimum in the density of states, and the density of states is continuous near the Fermi level owing to the jump-like transition between densities from different complexes (Fig. 5b). A characteristic feature of the acceptor density of states is the presence of a delta-like peak separated from the rest of the density by a broad Coulomb gap equal to  $\mu$ . Studies of optical transitions, for instance, optical absorption from an acceptor impurity to the conduction band, may provide easily interpreted information about the degree of compensation of a semiconductor or, for a known K, about the density of the fluctuation potential.

Translated by Eugene Yankovsky

<sup>&</sup>lt;sup>1</sup>B. K. Ridley, Semicond. Sci. Technol. 3, 286 (1988).

<sup>&</sup>lt;sup>2</sup>B. I. Shklovskiĭ, and A. L. Éfros, Fiz. Tekh. Poluprovodn. **14**, 825 (1980) [Sov. Phys. Semicond. **14**, 487 (1980)].

<sup>&</sup>lt;sup>3</sup>A. L. Éfros, Nguen Van Lien, and B. I. Shklovskiĭ, J. Phys. C 12, 1869 (1979).

<sup>&</sup>lt;sup>4</sup>E. V. Chenskiĭ, Zh. Eksp. Teor. Fiz. 77, 155 (1979) [Sov. Phys. JETP 50, 79 (1979)].

<sup>&</sup>lt;sup>5</sup>Yu. Ya. Tkach, Zh. Eksp. Teor. Fiz. 101, 203 (1992) [Sov. Phys. JETP 74, 109 (1992)].

<sup>&</sup>lt;sup>6</sup>Sh. M. Kogan, Nguen Van Lien, and B. I. Shklovskiĭ, Zh. Eksp. Teor. Fiz. **78**, 1933 (1980) [Sov. Phys. JETP **51**, 971 (1980)].

<sup>&</sup>lt;sup>7</sup>S. Chandrasekhar, Rev. Mod. Phys. 15, 1 (1943).