## Self-consistent description of Coulomb gap at finite temperatures

A. A. Mogilyanskiĭ and M. É. Raĭkh

Ioffe Physicotechnical Institute, USSR Academy of Sciences (Submitted 5 December 1988) Zh. Eksp. Teor. Fiz. **95**, 1870–1879 (May 1989)

The density of states in the vicinity of the Fermi level is investigated in a system of localized electrons at nonzero temperature. A self-consistent equation is proposed for the energy dependence of the density of states, and results of its numerical solution in the two- and three-dimensional cases are given. The kinetics of formation of the Coulomb gap in the density of states at zero temperature is also investigated.

## **1.INTRODUCTION**

It was shown in Refs. 1 and 2 that the density of singleelectron states in a system of localized electrons at zero temperatures (T = 0) vanishes at an energy equal to the Fermi energy. This behavior of the density of states (DOS) is due to Coulomb interaction of the localized electrons (Coulomb gap). For energies close to the Fermi energy, the DOS takes the form

$$g(\varepsilon) = \alpha_2 \frac{\varkappa^2}{e^{\varepsilon}} |\varepsilon|, \quad d=2,$$
 (1a)

$$g(\varepsilon) = \alpha_s \frac{\varkappa^s}{e^{\varepsilon}} \varepsilon^2, \quad d=3,$$
 (1b)

where d is the dimensionality of space,  $\varepsilon$  is the energy measured from the Fermi level,  $\varkappa$  is the dielectric constant, e is the electron charge, and  $\alpha_2$  and  $\alpha_3$  are dimensionless coefficients.

Éfros<sup>2</sup> has proposed for the DOS in the vicinity of the Fermi level the self-consistent equations

$$g(\varepsilon) = g_{\infty} \exp\left[-\frac{\pi e^4}{2\kappa^2} \int_{0}^{\infty} dE \frac{g(E)}{(|\varepsilon|+E)^2}\right], \quad d=2, \quad (2a)$$

$$g(\varepsilon) = g_{\infty} \exp\left[-\frac{2\pi e^{\epsilon}}{3\kappa^{3}}\int_{0}^{\infty} dE \frac{g(E)}{(|\varepsilon|+E)^{3}}\right], \quad d=3. \quad (2b)$$

Here  $g_{\infty}$  is the DOS far from the Fermi level, where the Coulomb interaction is insignificant. The derivation of these equations is based on the following idea. At T = 0 the system is in the ground state. For the system energy to be a minimum it is necessary to satisfy for any pair of sites with energies  $\varepsilon_2 > 0$  and  $\varepsilon_1 < 0$  separated by a distance  $r_{12}$  the condition

$$\Delta_{12} = \varepsilon_2 - \varepsilon_1 - \frac{e^2}{\varkappa r_{12}} > 0, \qquad (3)$$

where  $\Delta_{12}$  is the work needed to transfer an electron from an occupied site 1 to an empty site 2. Consider an occupied site with energy  $\varepsilon < 0$ . It follows from condition (3) that at any distance  $r < e^2/\varkappa |\varepsilon|$  from this site there are no empty sites with energies  $E < e^2/\varkappa r - \delta |\varepsilon|$ . The average number of such sites in an hemispherical layer  $(r, r + \delta r)$  is equal to (for d = 3)<sup>1)</sup>

$$\delta N = 2\pi r^2 \delta r \int_{0}^{\sigma^2/\mathrm{xr} - |\mathfrak{s}|} dEg(E).$$

Their number in the entire hemisphere  $r < e^2/\varkappa |\varepsilon|$  is correspondingly

$$N = 2\pi \int_{0}^{e^{2}/x|e|} drr^{2} \int_{0}^{e^{2}/xr-|e|} dEg(E).$$
(4)

The probability of finding the chosen site occupied is proportional to  $\exp(-N)$ . On the other hand, this probability is proportional to the sought DOS  $g(\varepsilon)$ , from which in fact follows Eq. (2b). From Eqs. (2) we find that the numerical coefficients in (1) are  $\alpha_2 = 2\pi$  and  $\alpha_3 = 3/\pi$ . These values agree well with the values of  $\alpha_2$  and  $\alpha_3$  obtained in Ref. 4 by numerical modeling.

In the one-dimensional case the self-consistent equation takes the form

$$g(\varepsilon) = g_{\infty} \exp\left[-\frac{e^2}{\varkappa} \int_0^{E_M} dE \frac{g(E)}{|\varepsilon| + E}\right], \qquad (5)$$

where  $E_M$  is the Coulomb interaction energy of two sites at the mean distance between them. A solution of (5) was obtained in Ref. 5:

$$g(\varepsilon) = g_{\infty} \left/ \left[ 1 + \frac{g_{\infty}e^2}{\varkappa} \ln\left(\frac{E_{\mathbf{M}}}{|\varepsilon|}\right) \right].$$
(6)

Clearly, in the case of nonzero temperature the Coulomb gap is filled at  $\varepsilon \sim T$ . The behavior of the DOS in this case can be represented in the form

$$g(\varepsilon) = \frac{\varkappa^2}{e^4} TF_2\left(\frac{\varepsilon}{T}\right), \quad d=2,$$
 (7a)

$$g(\varepsilon) = \frac{\varkappa^3}{e^6} T^2 F_s\left(\frac{\varepsilon}{T}\right), \quad d=3,$$
 (7b)

where  $F_2$  and  $F_3$  are certain universal dimensionless functions, and for  $|x| \ge 1$  we have  $F_2(x) \approx 2|x|/\pi$  and  $F_3(x) \approx 3x^2/\pi$ . Expressions (7) can be used if  $T \le w$ , where w is the width of the Coulomb gap. We obtain the value of w by putting in (1)  $g(\varepsilon) = g_x$ :

$$w_2 = g_{\infty} e^4 / \kappa^2, \quad w_3 = (g_{\infty} e^6 / \kappa^3)^{1/2}.$$

The DOS at finite temperature was recently investigated<sup>6</sup> by computer modeling of a disordered system. The results have confirmed the universal character of the functions  $F_2$  and  $F_3$ . It is of interest to obtain a self-consistent description of the DOS at finite temperatures. The Éfros equation cannot be used for finite temperatures for the following reason. For T = 0 the number N of "forbidden" sites included only those to which an electron transfer is energywise favored  $(\Delta_{12} < 0)$ . It was assumed that in the presence of such a forbidden site the electron will go over to it, with unity probability, from the site considered by us. If  $T \neq 0$  an electron can go over, with probability  $\exp(-\Delta_{12}/T)$ , also to a site for which  $\Delta_{12} > 0$ . To calculate the probability of finding the site considered by us occupied, we must add to N the quantity

$$N_{i} = 2\pi \int_{e^{2}/\varkappa|e|}^{\infty} drr^{2} \int_{0}^{\infty} dEg(E) \exp\left(-\frac{E+|e|-e^{2}/\varkappa r}{T}\right).$$
(8)

It is easily seen that  $N_1$  becomes infinite for any  $T \neq 0$ . We obtain thus  $g(\varepsilon) \equiv 0$ . The reason for this result is that in the arguments leading to Eq. (2) account is taken only of the possibility of decreasing the site population via electronelectron interaction, and the possibility of the inverse process is not considered, so that a self-consistent description of the DOS at finite temperatures requires in principle a different approach. Such an approach is proposed in the present paper. In Sec. 2 we derive for T = 0 an equation for the DOS and show that it leads to the same results as the Éfros equation. This equation is generalized in Sec. 3 to include the case of finite temperatures, and results of its numerical solution are given.

## 2. ZERO TEMPERATURE<sup>2)</sup>

It was shown in Ref. 2 that the ground state of the system is realized on satisfaction of a set of conditions requiring that the work to transfer any finite group of electrons from occupied to empty sites is positive. One of the main approximations in the derivation of Eq. (2) is that only constraints connected with the transfer of one electron are taken into account (the condition  $\Delta_{12} > 0$ ). If the system is not in the ground state at the initial instant, the establishment of the ground state can be represented in the framework of this approximation by a sequence of transpositions of individual electrons within pairs of sites 1 and 2 for which  $\Delta_{12} < 0$ . This is precisely how a search is made for the ground state in computer modeling.<sup>4</sup>

Our approach to the description of the ground state is based on classifying the various transpositions by length. When a certain narrow energy band below the Fermi level is tracked, the concentration of sites with energies in this band will be altered by the transpositions. We introduce the density  $f^+(r,\varepsilon)$  of the occupied states of energy  $\varepsilon < 0$  after all the transpositions with lengths shorter than r; for  $\varepsilon > 0$  we have  $f^+(r, \varepsilon) = 0$ . We define similarly the density  $f^-(r, \varepsilon)$  of empty states with energy  $\varepsilon > 0$  after transpositions with lengths shorter than r.

Let us see how these functions are altered by transpositions with lengths ranging from r to  $r + \delta r$ . From the electron-hole symmetry we have

$$f^{+}(r, \varepsilon) = f^{-}(r, -\varepsilon).$$
(9)

We consider, to be specific, the three-dimensional case. The density of the occupied sites with energies in the band ( $\varepsilon$ ,  $\varepsilon + \delta \varepsilon$ ) is  $n_0 = f^+(r, \varepsilon)\delta \varepsilon$ . After effective transpositions of lengths from r to  $r + \delta r$  the electrons from this band will be transferred to empty sites with energies E in the interval  $0 < E < \varepsilon + 1/r$ , since the work  $\Delta = E - \varepsilon - 1/r$  for such

transpositions is negative (we assume that  $\varepsilon < 1/r$ , see Fig. 1). The change  $\delta n_0^-$  produced in the density  $n_0$  by these transpositions is<sup>3)</sup>

$$\delta n_0^- = -n_0 \left[ 2\pi r^2 \delta r \int_{\bullet}^{\bullet} dE j^-(r, E) \right].$$
 (10)

In addition, the transpositions will cause some of the empty sites to be occupied by electrons, and their energies will go over to the band  $(\varepsilon, \varepsilon + \delta \varepsilon)$  from the energy band  $(\varepsilon + 1/r, \varepsilon + 1/r + \delta \varepsilon)$  Fig. 1). The corresponding change of the density  $n_0$  is

$$\delta n_0^+ = f^-(r, \varepsilon + 1/r) \,\delta \varepsilon \\ \times \left[ 2\pi r^2 \delta r \int dE f^+(r, E) \right]. \tag{11}$$

The total change of the density  $n_0$  is

 $\delta n_0 = \delta n_0^+ + \delta n_0^- = \delta f^+(r, \epsilon) \delta \epsilon.$ 

Using (10) and (11) we get

$$\frac{\partial f^{+}(\boldsymbol{r},\boldsymbol{\varepsilon})}{\partial \boldsymbol{r}}$$

$$=-2\pi r^{2} \left[ f^{+}(\boldsymbol{r},\boldsymbol{\varepsilon}) \int_{\boldsymbol{\varepsilon}}^{\boldsymbol{\varepsilon}+1/\boldsymbol{r}} dE f^{-}(\boldsymbol{r},E) -f^{-}(\boldsymbol{r},\boldsymbol{\varepsilon}+1/\boldsymbol{r}) \int_{\boldsymbol{\varepsilon}}^{\boldsymbol{\varepsilon}} dE f^{+}(\boldsymbol{r},E) \right]$$

$$\times \boldsymbol{\theta}(-\boldsymbol{\varepsilon}) \boldsymbol{\theta}(\boldsymbol{\varepsilon}+1/\boldsymbol{r}), \qquad (12)$$

where  $\theta(x) = 0$  for x < 0 and  $\theta(x) = 1$  for x > 0. The electron-hole symmetry condition (9) makes it possible to obtain an equation in closed form for the function  $f^+$ . For a space with dimensionality d we have

$$\frac{\partial f^{+}(r,\varepsilon)}{\partial r} = -v_{d}r^{d-1} \left[ f^{+}(r,\varepsilon) \int_{-\varepsilon-1/r}^{0} dE f^{+}(r,E) -f^{+}(r,-\varepsilon-1/r) \int_{\varepsilon}^{0} dE f^{+}(r,E) \right] \theta(-\varepsilon) \theta(\varepsilon+1/r), \quad (13)$$



FIG. 1. Diagram illustrating the establishment of the ground state in a system by successive transposition of electrons, corresponding to departure of an electron from the band  $(\varepsilon, \varepsilon + \delta \varepsilon)$  (1) and arrival of an electron in band  $(\varepsilon, \varepsilon + 1/r + \delta \varepsilon)$  (2).

where

$$v_d = \begin{cases} 1, & d = 1, \\ \pi, & d = 2, \\ 2\pi, & d = 3. \end{cases}$$
(14)

The sought DOS  $g(\varepsilon)$  in the ground state of the system corresponds to the limit  $f^+(r, \varepsilon)$  as  $r \to \infty$ .

Note that Eq. (13) leads to the relation

$$\frac{d}{dr}\int_{-\infty}^{0} dE f^{+}(r,E) = 0, \qquad (15)$$

the meaning of which is obvious: the total number of occupied sites is not changed by the transpositions.

Let us show that a solution of Eq. (13) leads to the same results (1) and (6) obtained by solving Eqs. (2) and (5). It is easiest to solve (13) in the one-dimensional case. With the aid of the substitutions

$$r = \frac{1}{E_{\rm M}} e^{v/g_{\infty}}, \quad \varepsilon = -E_{\rm M} e^{-u/g_{\infty}}, \quad \Phi = f^+/g_{\infty} \tag{16}$$

and with allowance for the condition  $g_{\infty} \ll 1$  ( $g_{\infty}$  is measured in units of  $\varkappa/e^2$ ) it reduces to the equation

$$\frac{\partial \Phi(v, u)}{\partial v} = -\Phi(v, u)\Phi(v, v)\theta(u-v), \qquad (17)$$

the solution of which is

$$\Phi(v, u) = \begin{cases} 1/(1+u), & u < v, \\ 1/(1+v), & u > v. \end{cases}$$
(18)

Substituting (16) in (18) we obtain

$$f^{+}(r,\varepsilon) = \begin{cases} g_{\infty} / \left[ 1 + g_{\infty} \ln\left(\frac{E_{\mathtt{M}}}{|\varepsilon|}\right) \right], & |\varepsilon| > 1/r, \\ g_{\infty} / \left[ 1 + g_{\infty} \ln\left(E_{\mathtt{M}}r\right) \right], & |\varepsilon| < 1/r. \end{cases}$$
(19)

As  $r \to \infty$ , Eq. (19) goes over into (6).

In the case d = 2 or 3 Eq. (13) has a self-similar solution in the form

$$f^{+}(r, \varepsilon) = |\varepsilon|^{d-1} K(\varepsilon r).$$
<sup>(20)</sup>

Substituting (20) in (13) we obtain an equation for the function K(z):

$$\frac{dK}{dz} = -\frac{\nu_d}{|z|^d} \left[ z^{d-1}K(z) \int_{-1-z}^{0} dt t^{d-1}K(t) -(-1-z)^{d-1}K(-1-z) \int_{z}^{0} dt t^{d-1}K(t) \right] \theta(-z) \theta(1+z),$$
(21)

where  $z = \varepsilon r$ . For z < -1 we have dK/dz = 0, so that

$$f^{+}(r, \epsilon) = K(-1) |\epsilon|^{d-1}, \quad \epsilon < -1/r.$$
(22)

We show now that from (1) we get  $K(-1) = d/\pi$ . To this end we introduce, on the interval -1 < z < 0, the function

$$\varphi(z) = \int dt |t|^{d-1} K(t), \qquad (23)$$

so that  $K(-1) = -\varphi'(-1)$ . The equation for the function  $\varphi(z)$  is

$$z\varphi'(z) = \varphi(z) [d - v_d \varphi(-1 - z)].$$
 (24)

From the fact that the DOS does not vanish at  $\varepsilon = 0$  if r is finite it follows that as  $z \rightarrow 0$  the function  $\varphi(z)$  varies like  $\lambda z$ , where  $\lambda$  is a certain constant. Substituting  $\varphi(z) = \lambda z$  in (14) and letting z tend to zero, we obtain the relation

$$1 = d - v_d \varphi(-1).$$
 (25)

On the other hand, putting z = -1 in (24), we have

$$-\varphi'(-1) = d\varphi(-1).$$
 (26)

From (25) and (26) we get

$$K(-1) = -\varphi'(-1) = d\varphi(-1) = d(d-1)/\nu_d = d/\pi.$$

We have thus shown that the solution of Eq. (13) describes, as  $r \to \infty$ , the Coulomb gap (1). For finite *r*, however, the DOS differs from (1) in the energy region  $|\varepsilon| < 1/r$ :

$$f^{+}(r,\varepsilon) = \frac{1}{r^{d-1}} G_{d}(\varepsilon r), \quad -1/r < \varepsilon < 0, \quad (27)$$

where the dimensionless function  $G_d(z)$  is expressed in terms of the function  $\varphi(z)$ :

$$G_d(z) = -\varphi'(z). \tag{28}$$

The functions  $G_d(z)$  with d = 2 and 3 were obtained by numerically solving Eq. (24). The results are shown in Fig. 2.<sup>4)</sup> The DOS for  $\varepsilon = 0$  were found to be 0.073/r for d = 2 and  $0.0083/r^2$  for d = 3, i.e., to be anomalously small. For comparison, we have solved the Éfros equation, choosing the electron interaction in the form

$$V(r) = \begin{cases} 1/r, & r < r_{\bullet}, \\ 0, & r > r_{\bullet}. \end{cases}$$
(29)

The general form of the solution of the Éfros equation with the interaction (29) is

$$g(\varepsilon) = \frac{1}{r_s^{d-1}} \tilde{G}_d(\varepsilon r_s). \tag{30}$$

Plots of  $\tilde{G}_2(z)$  and  $\tilde{G}_3(z)$  are also shown in Fig. 2. Their values at zero are  $\tilde{G}_2(0) = 0.145$  and  $\tilde{G}_3(0) = 0.028$ , i.e., are also small. In addition, the Éfros equation was solved in Ref. 7 for the case of a screened Coulomb interaction:

$$V(r) = (1/r) \exp(-r/r_s)$$
 for  $d=3$ 

The DOS for  $\varepsilon = 0$  was found to be  $g(0) = 0.1/r_s^2$ .

Note that the foregoing results permit a description of the kinetics of Coulomb-gap formation at T = 0. Assume that at the instant t = 0 the system was taken out of the ground state (say by illumination or by applying a voltage pulse). The return to the ground state will be via electron hops from occupied to empty sites, accompanied by phonon emission. The probability of a hop of given length r per unit time is

$$p(r) = \frac{1}{\tau_0} e^{-2r/a},$$
 (31)

where  $\tau_0^{-1}$  is the electron-phonon collision frequency and *a* is the wave-function radius of an electron localized on a site. After a time *t*, hops take place with lengths  $r < r_i$ , where

$$\mathbf{r}_t = \frac{\mathbf{a}}{2} \ln \left( t / \tau_0 \right). \tag{32}$$



The time dependence of the DOS is given in this case by

$$g(\varepsilon) = \begin{cases} \frac{d}{\pi} |\varepsilon|^{d-1}, & |\varepsilon| > 1/r_t, \\ \frac{1}{r_t^{d-1}} G_d(\varepsilon r_t), & |\varepsilon| < 1/r_t. \end{cases}$$
(33)

This expansion is valid for long enough times t, when  $1/r_t \ll w$ , where w is the Coulomb-gap width.

## **3. FINITE TEMPERATURES**

For nonzero temperatures, the assumption of an equilibrium state by the system can also be represented as successive transpositions of individual electrons within site pairs. It must be recognized here that at  $T \neq 0$  it is possible to have, in addition to transpositions with negative work  $\Delta_{12}$ , also transpositions that require positive work  $\Delta_{12} > 0$ . The probability of such a rearrangement is  $\exp(-\Delta_{12}/T)$ .

For  $T \neq 0$  the density of occupied states differs from zero at positive energies. Similarly, the density  $f^{-}(r, \varepsilon)$  of empty states differs from zero at  $\varepsilon < 0$ . The electron-hole symmetry property (9) remains naturally in force at  $T \neq 0$ .

Generalization of the above self-consistent description of the DOS to include finite temperatures reduces to the following. After transpositions with length from r to  $r + \delta r$ , electrons go over with unity probability from band ( $\varepsilon$ ,  $\varepsilon + \delta \varepsilon$ ) to empty sites with energies  $\varepsilon' < \varepsilon + 1/r$ , and with probability

$$\exp\left(-\frac{\varepsilon'-\varepsilon-1/r}{T}\right)$$

to empty sites with energies  $\varepsilon' > \varepsilon + 1/r$ . Entry of occupied sites into the band  $(\varepsilon, \varepsilon + \delta \varepsilon)$  is similarly effected by electrons going over from occupied sites with energies  $\varepsilon''$  to empty sites in the band  $(\varepsilon + 1/r, \varepsilon + 1/r + \delta \varepsilon)$ . The probability of such transitions is unity for  $\varepsilon'' > \varepsilon$  and  $\exp[-(\varepsilon - \varepsilon'')/T]$  for  $\varepsilon'' < \varepsilon$ . As a result we obtain the equation

$$\frac{\partial f^{+}(r,\varepsilon)}{\partial \varepsilon} = -v_{d}r^{d-1} \bigg[ f^{+}(r,\varepsilon) \bigg\{ \int_{-\infty}^{\varepsilon+1/r} d\varepsilon' j^{-}(r,\varepsilon') \\ + \int_{\varepsilon+1/r}^{\infty} d\varepsilon' j^{-}(r,\varepsilon') \exp\bigg(-\frac{\varepsilon'-\varepsilon-1/r}{T}\bigg) \bigg\} \\ -j^{-}(r,\varepsilon+1/r) \bigg\{ \int_{\varepsilon}^{\infty} d\varepsilon' f^{+}(r,\varepsilon') \\ + \int_{-\infty}^{\infty} d\varepsilon' f^{+}(r,\varepsilon') \exp\bigg(-\frac{\varepsilon-\varepsilon'}{T}\bigg) \bigg\} \bigg].$$
(34)

FIG. 2. Dimensionless density of occupied states at T = 0, after transpositions with lengths r, as a function of the energy (in units of 1/r) for the cases d = 2 (a) and d = 3 (b). The insets show the initial sections of these plots in larger scale, and also the result of solving the Efros equation for an electron-interaction law (29).

It is easy to see that as  $T \rightarrow 0$  Eq. (34) is transformed into (1). By analogy with the case T = 0, this equation can be made closed with respect to the function  $f^+(r, \varepsilon)$  by using Eq. (9).

The sought DOS  $g(\varepsilon)$  is expressed in terms of the function  $f^+$  as follows:

$$g(\varepsilon) = f^{+}(\infty, \varepsilon) + f^{+}(\infty, -\varepsilon).$$
(35)

As  $r \to \infty$  the left-hand side of (34) tends to zero. The general form of the function  $f^+(\infty, \varepsilon)$ , which makes the right-hand side equal to zero as  $r \to \infty$ , is

$$f^{+}(\infty,\varepsilon) = \frac{\Lambda(\varepsilon)}{e^{\varepsilon/T} + 1},$$
(36)

where  $\Lambda(\varepsilon)$  is a certain even function of  $\varepsilon$ . Comparing (36) and (35) we get  $\Lambda(\varepsilon) = g(\varepsilon)$ . From (36) follows also the relation

$$f^{+}(\infty, -\varepsilon) = f^{+}(\infty, \varepsilon) e^{\varepsilon/T}.$$
(37)

It is convenient to change in (34) to the dimensionless variables

$$R = rT, \quad E = \varepsilon/T, \quad f^+ = T^{d-1}F_d^+(R, E),$$
 (38)

in which it takes the form

$$\frac{\partial F_{d}^{+}}{\partial R} = -\nu_{d} R^{d-1} [F_{d}^{+}(R, E) Q_{d}(R, -E - 1/R) - F_{d}^{+}(R, -E - 1/R) Q_{d}(R, E)], \qquad (39)$$

where

$$Q_{d}(R,E) = \int_{-\infty}^{\infty} dE' F_{d}^{+}(R,E') \psi(E'-E), \qquad (40)$$

$$\psi(x) = \begin{cases} 1, & x > 0, \\ e^x, & x < 0. \end{cases}$$
(41)

The functions

$$F_d(E) = F_d^+(\infty, E) + F_d^+(\infty, -E)$$

coincide here at d = 2 and 3 with the functions  $F_2$  and  $F_3$  that determine the form of the density of states in expressions (7a) and (7b).



FIG. 3. Dimensionless density of occupied states at nonzero temperature as a function of energy (in units of T) for the cases d = 2 (a) and d = 3 (b).

Equation (39) was solved with a computer in the following manner. As the zeroth approximation we chose the solution (27) of Eq. (13) for  $R = R_i = 0.004$ . As R was increased, the increment  $\delta F_d^+(R, E)$  was obtained by multiplying the right-hand side of (39) by  $\delta R$ , with the condition  $\delta R < R / 500$  preserved. The iteration procedure diverged for large  $\delta R$ . The final values of R were  $R_f = 2$  for d = 2 and  $R_f = 0.7$  for d = 3. At these values, the functions  $F_d^+(R, E)$ ceased to depend on R. Equation (37) for  $R = R_f$  was satisfied accurate to 10%. The calculation results for the functions  $F_d^+(\infty, E)$  are shown in Fig. 3. Figure 4 shows the dimensionless DOS  $F_d(E)$  for d = 2 and 3. The same figures show for comparison the numerical modeling results in Ref. 6.

Figure 4a shows for  $F_2(0)$  a value 0.84, somewhat lower than the value  $1.24 \pm 0.16$  given in Ref. 6. On the whole, however, the  $F_2(E)$  curves obtained by modeling and by solving Eq. (39) are quite close. Numerical modeling of a two-dimensional system of localized electrons at finite temperature was carried out also in Ref. 8. The value of  $F_2(0)$  obtainable from the curves of Ref. 8 is 0.8, close to ours.

An appreciable difference from the results of Ref. 6 occurs in the three-dimensional case. As seen from Fig. 4b, the solution of Eq. (39) give  $F_3(0) = 4.1$ , as against 10 in Ref. 6. The modeling error for d = 3 was not estimated in Ref. 6, for owing to the long program running time a DOS was obtained only for one realization of a random spread of the bare energies of the sites. We call attention also to another<sup>9</sup> numerical modeling of the DOS at finite temperatures at d = 3. The results of Ref. 9 give  $F_3(0) \approx 2$ , but the accuracy with which  $F_3(0)$  can be obtained from the curves there is quite low.

In conclusion, we thank A. L. Efros and B. I. Shklovskiĭ for a number of very helpful suggestions and discussions, E. M. Levin for a discussion of the modeling errors in Ref. 6, and also V. L. Nguen for taking part in initial stage of the study.



FIG. 4. Dimensionless density of states determined by expressions (7a) and (7b) versus energy (in units of T) in the two-dimensional (a) and threedimensional (b) cases; dashed curves—the functions  $2|\varepsilon|/\pi$  (a) and  $3\varepsilon^2/\pi$  (b); points—results of numerical modeling in Ref. 6.

- <sup>3)</sup>The numerical coefficient  $2\pi$  is used in this expression in place of  $4\pi$  for the same reason as in expression (4). Otherwise the transposition of an electron within one and the same pair of sites would be taken into account twice.
- <sup>4)</sup>The asymptotic behavior of the functions  $G_d(z)$  as  $z \rightarrow 0$  can be found from Eq. (24):  $G_d(z) = G_d(0) [1 - 2d(d-1)z].$
- <sup>1</sup>A. L. Éfros and B. I. Shklovskiĭ, J. Phys. C 8, L49 (1975).
- <sup>2</sup>A. L. Éfros, *ibid*. C 9, 2021 (1976).
- <sup>3</sup>S. D. Baranovskiĭ, B. I. Shklovskiĭ, and A. L. Éfros, Zh. Eksp. Teor. Fiz.

78, 395 (1980) [Sov. Phys. JETP 51, 199 (1980)].

- <sup>4</sup>S. D. Baranovskii, A. L. Éfros, B. L. Gelmont, and B. I. Shklovskii, J. Phys. C. 12, 1023 (1979).
- <sup>5</sup>M. É. Raĭkh and A. L. Éfros, Pis'ma Zh. Eksp. Teor. Fiz. 45, 225 (1987) [JETP Lett. 45, 380 (1987)]. <sup>6</sup>E. I. Levin, V. L. Nguen, B. I. Shklovskiĭ, and A. L. Éfros, Zh. Eksp.
- Teor. Fiz. 92, 1499 (1987) [Sov. Phys. JETP 65, 842 (1987)].
- <sup>7</sup>V. L. Nguen, M. É. Raĭkh, and A. L. Éfros, Fiz. Tverd. Tela (Leningrad) 28, 2019 (1986) [Sov. Phys. Solid State 28, 1129 (1986)]
- <sup>8</sup>J. H. Davies, P. A. Lee, and T. M. Rice, Phys. Rev. Lett. 49, 758 (1982). <sup>9</sup>S. Summerfield, J. A. McInnes, and P. N. Butcher, J. Phys. C 20, 3647 (1987).

Translated by J. G. Adashko

<sup>&</sup>lt;sup>1)</sup>The reason why a hemispherical layer should be chosen rather than a spherical one discussed in detail in Ref. 3. <sup>2)</sup>For convenience, we put herefter  $e^2/\varkappa = 1$ .