

# Temperature-induced smearing of the coulomb gap: experiment and computer simulation

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## Temperature-Induced Smearing of the Coulomb Gap: Experiment and Computer Simulation

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We present the first verification of the theoretically predicted effect of temperature-induced smearing of the Coulomb gap. Measurements of the variable-range-hopping conductivity (VRH) in samples of ion-implanted Si:As and computer simulation are used to study the density of states (DOS) near the Fermi level (FL) in the impurity band. The VRH is determined by the DOS integrated over some energy range that depends on temperature  $T$  and on the magnetic field  $B$ . Using the interplay between  $T$  and  $B$  we find that the DOS in the vicinity of the FL increases with increasing  $T$ .

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The temperature dependence of the resistance  $R(T)$  of an Anderson insulator at low temperatures follows Mott's variable-range-hopping (VRH) law [1],

$$R(T) = R_0 \exp[(T_p/T)^p], \quad (1)$$

with  $p = 1/4$  in a three-dimensional system for the constant density of states (DOS)  $g(\varepsilon) = g_F$ , where  $g_F$  is the DOS at the Fermi level (FL). In this case  $T_{1/4} \equiv T_M = 21/g_F a^3$ , where  $a$  is the localization radius. Pollak [2] and Efros and Shklovskii (ES) [3,4] have predicted that long-range electron-electron interaction reduces the DOS at the FL, forming the so-called Coulomb gap (CG), for which  $g(\varepsilon) = g_0 \varepsilon^2$ , where  $g_0 = (3/\pi)(e^2/\kappa)^{-3}$ , the energy  $\varepsilon = E - E_F$  is measured from the Fermi energy  $E_F$ , and  $\kappa$  is the dielectric constant. This form for  $g(\varepsilon)$  leads to a different VRH law [4] in which  $p = 1/2$  and  $T_{1/2} \equiv T_{ES} = 2.8e^2/\kappa a$ .

Experimental evidence for the "CG behavior" of VRH conductivity was demonstrated on different materials [4]. A "crossover" between these two regimes is expected as  $T$  increases because the Coulomb interaction influences the DOS only near the FL. Far from the FL the DOS has its unperturbed value, which is approximately equal to  $g_F$ . Hence, the half-width  $\Delta$  of the CG can be roughly determined from  $g_0 \Delta^2 = g_F$ , yielding

$$\Delta = (g_F/g_0)^{1/2} \approx [(T_{ES})^3/T_M]^{1/2}. \quad (2)$$

In contrast to the nearest-neighbor hopping conductivity, the VRH mechanism involves only some of the localized states around the FL, the so-called "optimal band,"

whose half-width  $E_c$  is given by [1]

$$E_c = T \xi_c \propto T^{1-p}, \quad (3)$$

where  $\xi_c(T) = (T_p/T)^p$  is the critical percolation parameter, which can be obtained from the experimental data:  $\xi_c(T) = \ln[R(T)/R_0]$  from Eq. (1). It is believed that for  $E_c \ll \Delta$ , the ES law ( $p = 1/2$ ) should be observed, while for  $E_c \gg \Delta$ , the Mott law ( $p = 1/4$ ) is valid. For  $E_c \approx \Delta$ , a crossover should take place between these two regimes.

For a given sample with a fixed concentration of impurities one can increase the value  $E_c$  by increasing  $T$  or by applying a strong magnetic field  $B$ ; in the latter case  $\xi_c(T)$  must be replaced by  $\xi_c(B, T) = \ln[R(B, T)/R_0]$ , which increases with  $B$  due to the positive magnetoresistance.

Recently a number of papers devoted to the experimental investigation of the crossover phenomenon have been published (see, for example, [5,6] and references therein). In [6,7] the variation of  $E_c$  was achieved by increasing  $\xi_c$  in a strong magnetic field, whereas in other studies  $E_c$  was increased by increasing  $T$ . It has been shown theoretically that an increase of  $T$  not only increases  $E_c$  but also modifies considerably the DOS in the region of the CG: The weakening of the gap has been predicted due to the filling in by localized states. This was demonstrated by computer simulations on the lattice model [8–10], on the Coulomb glass model [11], and on the random model [12] of the impurity band, as well as by analytical calculations based on the self-consistent equation for the CG [13]. We will refer to this effect as the temperature-induced smearing of the CG.

We are not aware of any experimental verification of this effect and suggest here a method to study the effect qualitatively. It was shown recently [7] that one can determine the integrated DOS in the optimal band

$$I(E_c) = \int_{-E_c}^{E_c} g(\varepsilon) d\varepsilon \quad (4)$$

from experimental measurements of the VRH resistance in different magnetic fields  $B$ . We suggest using the interplay between  $T$  and  $B$  to determine the values of  $I(E_c)$  at different temperatures.

Our measurements of the VRH conductivity on samples of ion-implanted Si:As show that  $I(E_c)$  in the vicinity of the FL increases with increasing  $T$ . This can be considered as experimental verification of the temperature-induced smearing of the CG. Computer simulations confirm this conclusion.

The hopping magnetoresistance of two samples of ion-implanted Si:As with impurity concentration approximately 10% below the metal-insulator transition has been measured for temperatures down to 0.1 K and in magnetic fields up to 11 T. The conductivity of these samples without the magnetic field had been measured earlier [14], where all details about sample preparation and contact fabrication are described. Our measurements in zero magnetic field agree well with these previous data.

In Fig. 1 we present the results of the resistance measurements as a function of temperature in different magnetic fields for one of the samples. The key point of our analysis is the assumption that the ES law in the VRH conductivity is only reached at the lowest temperatures,  $T < 200$  mK. From the slope of the straight line shown in Fig. 1, we obtain  $T_{ES} = 11.2$  K; the intercept gives  $R_0 = 26.7 \Omega$ . The deviation of the resistance above the straight line with increasing  $T$  is interpreted as the crossover regime. Taking into account that for this

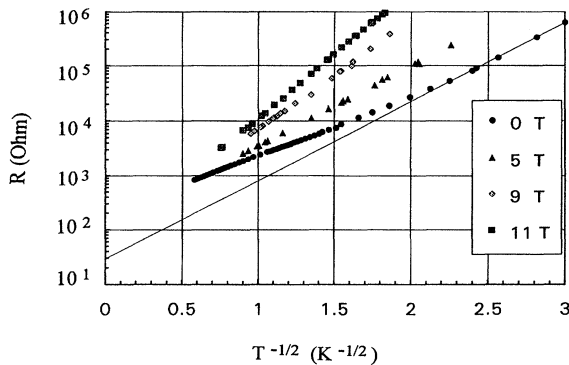


FIG. 1. The resistance of one sample of ion-implanted Si:As in the VRH regime in zero magnetic field and in magnetic fields of 5, 9, and 11 T. The solid line shows the fit to the  $T^{-1/2}$  law in the low-temperature limit; the intercept gives the value  $R_0 = 26.7 \Omega$ .

sample  $T_M = 420$  K [14], one can obtain from (2) the value  $\Delta = 1.8$  K.

It was suggested in [14] that in zero magnetic field the ES law is obeyed at higher temperatures,  $T > 200$  mK, with  $R_0 = 200 \Omega$  and  $T_{ES} = 5.4$  K. In this case, the deviation of higher resistance with decreasing  $T$  below 200 mK could be explained by the appearance of a rigid gap at the Fermi level because of the spin-spin interaction [15]. However, this value of  $T_{ES}$  leads to the smaller width  $\Delta$  of the CG determined from (2),  $\Delta = 0.6$  K, and thus ES law would be observed at  $T \geq \Delta$ , which is doubtful. Moreover, according to the model [15], a significant negative magnetoresistance must be observed because of restoration of the ES law in magnetic field. We measured the magnetoresistance at different fixed temperatures, sweeping the magnetic field. No negative effect was observed even at small fields, where the positive component of magnetoresistance caused by the shrinkage of the electron wave function is negligible. This also supports our assumption.

Let us now turn to the determination of the DOS from the experimental data. The integrated density of localized states in the optimal band  $I(E_c)$  determines the mean hopping length  $r(T) = [I(E_c)]^{-1/3}$ , on the other hand,  $r(T) = a\xi_c/2$  [4] and the average hopping volume around each site

$$V(\xi_c) = (4\pi/3) (a\xi_c/2)^3. \quad (5)$$

A percolation path forms where the number of states in the average volume reaches the critical value  $n_c = I(E_c)V(\xi_c) = 7.66$  [4]. Therefore

$$I(E_c) = \frac{6n_c}{\pi} \frac{1}{a^3[\xi_c(T)]^3} \equiv \frac{A}{[\xi_c(T)]^3}. \quad (6)$$

In strong magnetic fields, Eq. (5) has to be modified because of the shrinking of the electronic wave function and changing its shape from a sphere to a double paraboloid,

$$V(\xi_c) = \frac{4\pi}{3} \left[ \frac{a\xi_c(B, T)}{2} \right]^3 X(s), \quad (7)$$

where  $\xi_c(B, T) = \ln[R(B, T)/R_0]$  and  $s = (\pi e/h)a^2 \times B\xi_c(B, T)$ . In Ref. [7] a plot is given of the function  $X(s)$ . Consequently,

$$I(E_c) = \frac{6n_c}{\pi a^3} \frac{1}{[\xi_c(B, T)]^3 X(s)}. \quad (8)$$

We have calculated the normalized integrated DOS  $I^*(x) = I(x)[(2/3)g_0\Delta^3]^{-1}$ , where  $x = E_c/\Delta$  is the dimensionless energy. We used the value  $a = 16$  nm, which is quite reasonable for given impurity concentration [16]; this is the only adjustable parameter. The quantities  $\xi_c(T)$  and  $\xi_c(B, T)$  were both determined from the

experimental data, assuming that  $R_0$  is constant and independent of magnetic field. The width of the CG,  $\Delta = 1.8$  K, was obtained from (2) using  $T_{ES} = 11.2$  K and  $T_M = 420$  K [14].

The results are shown in Fig. 2. The dotted curve corresponds to the cubic dependence  $I^*(x) = x^3$  for the pure parabolic gap, the dot-dashed line shows the linear dependence  $I^*(x) = x$  for the constant DOS without gap. One can see that at fixed  $E_c$ , for lower magnetic fields (i.e., for higher  $T$ ),  $I(E_c)$  is larger. These results clearly demonstrate the increase of the DOS with increasing  $T$  in the vicinity of the FL.

This means that the deviation of the resistance above the straight line with increasing  $T$  in zero magnetic field (Fig. 1) is caused by temperature-induced smearing of the Coulomb gap rather than by a crossover from the ES to the Mott law. It can hardly be explained in the framework of the "pure" theory because the temperature changes the DOS in the interval of  $\alpha T$ , where  $\alpha = \text{const}$ , while the width of the optimal band is equal  $E_c = (T_{ES}T)^{1/2}$ . Therefore  $E_c/T = \xi_c = \sqrt{T_{ES}/T} \gg 1$ , and so it would seem that the temperature cannot influence the VRH conductivity. However,  $\alpha$  is relatively large ( $\alpha \approx 3$  [9]), of order of  $\xi_c$ , which makes it possible to observe the effect of temperature-induced smearing.

We note that the information on the DOS was obtained indirectly via the integrated DOS. Therefore, the smearing of the CG is given only qualitatively. However, this seems to be the first experimental verification of the effect.

One can also argue that the integrated DOS is essentially the concentration of localized states. If so, how can it depend on temperature? Indeed, the DOS integrated over the entire energy range is just the concentration of the localized states in the impurity system. However, not all energy states, but only those inside the optimal band of width  $2E_c$ , contribute to the VRH conductivity that was investigated. Therefore, the question is how the states

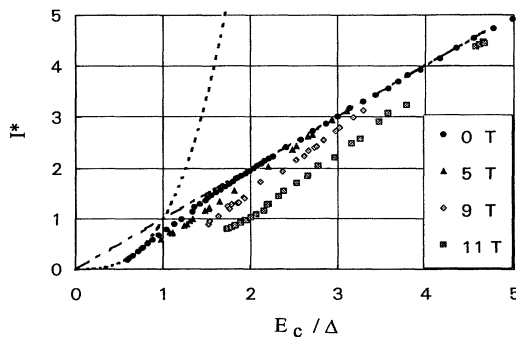


FIG. 2. The normalized integrated DOS  $I^*(x)$  determined from experimental data in magnetic fields 0, 5, 9, and 11 T. The low-energy approximation for the pure Coulomb gap  $I^*(x) = x^3$  is shown as the dotted curve. The dot-dashed straight line shows the linear dependence  $I^*(x) = x$  in the absence of the Coulomb gap.

are redistributed between different energy ranges with increasing  $T$ . Of course, the above method of "hopping spectroscopy" of the integrated DOS cannot answer this question. In order to study this problem, we have carried out a Monte Carlo computer simulation of the DOS in the CG at different  $T$ .

The algorithm of the simulation was the same as that described in detail in [17]. A random impurity band was studied similar to that in [12], i.e., not the lattice model [8–10]. Most of the previous simulations of the temperature dependence of the DOS in the CG were restricted to the intermediate degree of compensation  $K \approx 0.5$ , because the CG is most pronounced in that case ( $K$  being the ratio of the minority to majority impurity concentration). We have measured samples with low  $K$ , so the aim of the computer simulation was to study the impurity band in the case of low  $K$  as well. We first checked that at  $K = 0.5$  the results of our simulation agree with those obtained previously. Our results for the DOS at  $K = 0.5$  are shown on Fig. 3(a) for different temperatures (the values of  $kT$  as well as other energies are given in the units of  $e^2 N^{1/3} / \kappa$ ,  $N$  being the

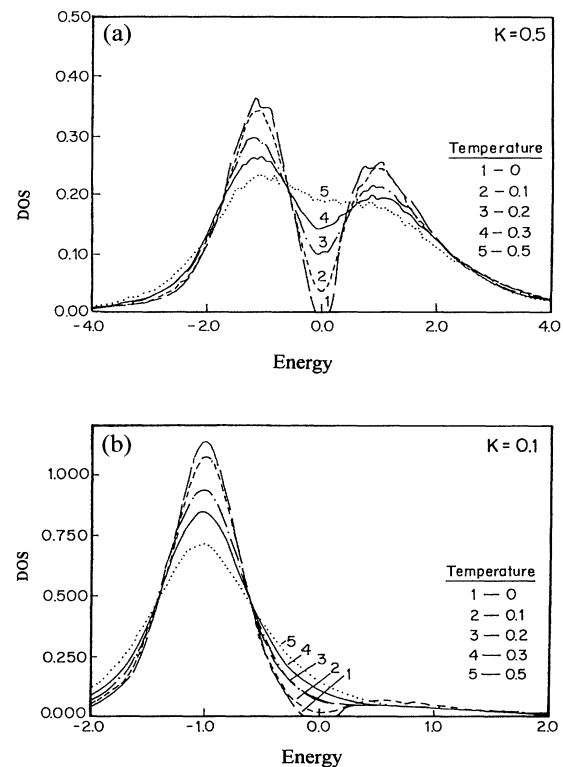


FIG. 3. The computer simulation of the temperature-induced smearing of the Coulomb gap for lightly doped semiconductors with compensation of  $K = 0.5$  (a) and  $K = 0.1$  (b). The temperatures and energies are shown in the units of  $e^2 N^{1/3} / \kappa$ . Curves 1–5 correspond to the temperatures  $T = 0, 0.1, 0.2, 0.3,$  and  $0.5$ .

concentration of majority impurities). The energies are plotted with respect to the Fermi energy  $E_F$ . The value  $E_F \approx 0.490$  was obtained at  $K = 0.5$ , in agreement with the previous calculations [4]. A pronounced CG is seen at  $T = 0$ , which smoothly disappears with a slight increase of  $T$ . The hard gap in the DOS at  $T = 0$  is due to the relatively low size of the simulated array (100 donors). Being interested only in the evolution of the DOS with increasing  $T$ , we did not average the results for the DOS at  $T = 0$  over different arrays to obtain a smooth curve. At nonzero  $T$ , such averaging is provided by the temperature-induced hopping movements of electrons between the sites.

We next carried out the simulation of the low-compensated system having  $K = 0.1$ . The accuracy of the simulation did not allow us to investigate smaller values of  $K$ , which would correspond more closely to the very low degree of compensation of our measured samples. Nevertheless, the simulation results for  $K = 0.1$  presented in Fig. 3(b) give a good impression of the DOS behavior with increasing  $T$  for a low-compensated material. The value  $E_F = 0.968$  was obtained at  $K = 0.1$ , in good agreement with the previous calculation [4]. The main feature of the results shown in Fig. 3(b) is the significant change of the DOS not only in the region of the CG, but near the maximum of the distribution as well at relatively small temperatures, i.e., for  $kT$  much less than the energy distance between the maximum of the distribution at  $\varepsilon \approx -1$  and the position of the CG at  $\varepsilon = 0$ . This allows one to assume that even at low temperatures the redistribution of states between different energy ranges is so effective that some additional states come into the region of the optimal band with increasing  $T$ . This permits the increase of  $I(E_c)$  to be observed experimentally. The above holds until the width of the optimal band  $E_c$  remains small compared to the entire width of the impurity band  $E_{\text{band}}$  ( $\approx 1$  in the units of Fig. 3). Moreover, if  $E_c$  becomes comparable with  $E_{\text{band}}$ , the VRH regime converges into the regime of the hopping conductivity to the nearest neighbor.

We conclude with the statement that the method of "hopping spectroscopy" of the integrated DOS in the optimal band for the VRH conductivity demonstrates

the temperature-induced smearing of the Coulomb gap predicted previously in a number of theoretical investigations [8–13,17].

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