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LETTER TO THE EDITOR

Coulomb gap and low temperature conductivity of disordered systems

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Abstract. The Coulomb interaction between localized electrons is shown to create a 'soft' gap in the density of states near the Fermi level. The new temperature dependence of the hopping DC conductivity is the most important manifestation of the gap. The form of the density of states within the gap is discussed.

We consider a disordered system the electronic states of which are localized close to the Fermi level. For example the system could be an amorphous or a doped crystalline semiconductor. The derivation of the Mott law $\ln\sigma \propto T^{-1/4}$ for the DC conductivity of such a system is based upon the assumption that the density of states near the Fermi level is constant. Pollak (1970) and Ambegaokar *et al* (1971) pointed out that actually electron–electron Coulomb interaction should reduce the density of states near the Fermi level. Srinivasan (1971) considered the energy dependence of the density of states in the vicinity of the Fermi level, but his results contradict ours.

We assume that the quantum localization length is much smaller than the distance between the centres and the overlap between the wavefunctions is negligible. So the energy of the system can be written in the form

$$H = \sum \psi_i n_i + \tfrac{1}{2} \sum_{i \neq j} e_{ij} n_i n_j \tag{1}$$

where ψ_i is the energy of the electronic state i not taking into account the contribution of electron–electron interaction, $e_{ij} = e^2/\kappa r_{ij}$ is the energy of electron–electron interaction, $r_{ij} = |r_i - r_j|$ is the distance between the states i and j, κ is the dielectric constant and n_i is the occupation number ($n_i = 0,1$). Let us introduce the energies of one-particle excitations

$$E_i = \psi_i + \sum_j e_{ij} n_i. \tag{2}$$

At temperature $T = 0$, $n_i = 1$ for $E_i < \mu$ and $n_i = 0$ for $E_i > \mu$, where μ is the Fermi level. The ground state of the system should also satisfy another condition. Let us consider two states i and j, which in the ground state are occupied and vacant respectively. The transfer of an electron from state i to state j should increase the energy of the system. Using equation (1) we find that the energy increase is

$$\Delta H(i \to j) = E_j - E_i - e_{ij} > 0. \tag{3}$$

The last term in equation (3) describes 'the exitonic effect', ie the Coulomb interaction of

the created electron–hole pair. So in the ground state any two energies E_i and E_j separated by the Fermi level should satisfy the inequality (3). Now we can show that the density of states $g(E)$ should vanish at the Fermi level. We assume $g(\mu) = g_0$ and consider an energy interval of small width ϵ centred at the Fermi level. For this interval a mean distance R between the states is determined by the condition $g_0 R^3 \epsilon \simeq 1$ and equals $(g_0\epsilon)^{-1/3}$. If $\epsilon \ll \Delta \equiv e^3 g_0^{1/2}/\kappa^{3/2}$ the interaction energy of the states $e^2/\kappa R = (e^2/\kappa)(g_0\epsilon)^{1/3}$ exceeds ϵ and the inequality (3) inevitability breaks down. Thus a constant density of states contradicts the inequality (3) and $g(E)$ at $|E - \mu| < \Delta$ decreases with $|E - \mu|$ and should vanish at the Fermi level. A selfconsistent density of states near the Fermi level may be found from the condition that for any $\epsilon < \Delta$ the mean interaction energy e_{ij} of the states within the ϵ interval is of the order of ϵ. In other words the mean distance between the states in the ϵ interval has to be of the order of $e^2/\kappa\epsilon$ ie

$$g(\epsilon)(e^2/\kappa\epsilon)^3\epsilon \simeq 1, \qquad g(\epsilon) = \alpha\,\kappa^3\epsilon^2/e^6, \qquad (\epsilon = E - \mu). \tag{4}$$

Here α is an unknown numerical coefficient. The assumption that $g(\epsilon) \propto \epsilon^\nu$, where $\nu < 2$, contradicts the inequality (3). If we assume that $\nu > 2$ then the mean distance between the states in the ϵ interval would be so large that interaction between the states may be neglected and the physical reason for the rapid decrease of $g(\epsilon)$ disappears. That is why $\nu = 2$. For the two-dimensional case the same arguments give

$$g(\epsilon) = \alpha' \frac{|\epsilon|\kappa^2}{e^4}. \tag{5}$$

We point out that if the density of states near the Fermi level does not depend on the unperturbed density of states g_0, equations (4) and (5) give respectively the only possible combinations for one and two dimensions. On the other hand the width of the gap Δ depends on g_0. Equations (4) and (5) are valid when $g(\epsilon) \ll g_0$ and so the width of the gap Δ is given by the equation $g(\Delta) = g_0$.

The Coulomb gap plays an important role in the low temperature DC conductivity. For the three-dimensional case the energy interval of width $\epsilon_M = T^{3/4}/a^{3/4}g_0^{1/4}$ is responsible for the hopping conductivity, which obeys the Mott law (here a is the localization length). The influence of the gap can be neglected if $\epsilon_M \gg \Delta$ ie $T \gg T_c = e^4 a g_0/\kappa^2$, at such temperatures the Mott law is valid. If $T \ll T_c$ the states within the Coulomb gap are particularly important. Using equation (4) and by analogy with the Mott law derivation we obtain

$$\sigma(T) \propto \exp\left[-(T_0/T)^{1/2}\right] \tag{6}$$

where $T_0 = e^2/\kappa a$. The same result is valid for the two-dimensional case.

We point out that the Coulomb gap exists only in the spectrum of energies E_i which corresponds to the withdrawal of one electron or its addition to the system. There are other small-energy excitations in the system. These are the electron–hole pairs with small separation between the electron and hole. The energy of such an excitation is given by $\omega_{ij} = E_j - E_i - e^2/\kappa r_{ij}$. It was shown that the density of states $g(E)$ is small near the Fermi level. Thus, pairs with $\omega_{ij} \ll \Delta$ include states with energies $|E_i - \mu|, |E_j - \mu| \geqslant \Delta$ which lie outside the gap. Then $r_{ij} \geqslant r_0 = e^2/\kappa\Delta$. The density of states of such electron–hole pairs is finite when $\omega \to 0$ and is of the order of g_0. Therefore the temperature dependence of the heat capacity is linear. On the other hand most electron–hole pairs with small excitation energies are very compact and isolated from each other. That is why they cannot contribute to the DC conductivity.

We would like to emphasize that in the three-dimensional case the small energy pairs interact strongly with isolated shallow energy levels. Due to this interaction the ground

state of the system should satisfy the following condition. The occupied state of each pair within a sphere of radius $r_e = (e^2 r_0/\kappa|\epsilon|)^{1/2}$ around an isolated level with energy $\epsilon = |E_t - \mu| < 0$ should be at a shorter distance from the level than the unoccupied one. Otherwise the energy of the system could be reduced by removing an electron from the central shallow state to a large distance and by transferring an electron from an occupied to an unoccupied state of the pair.

The opposite direction 'polarization' of pairs takes place near the shallow level with $\epsilon > 0$. The number of polarized pairs in the vicinity of a level is much larger than unity. The influence of such a polarization 'atmosphere' on the density of shallow levels was not taken into account in the derivation of equation (4). We are not able to do it in a correct form and we cannot exclude the possibility of an additional reduction of the density of states due to this effect. Similar considerations show that in the two-dimensional case the number of the 'polarized' pairs per shallow level is of the order of unity. Then the essential part of the levels is not affected at all. Consequently there seems to be no doubt of the validity of equation (5).

According to Knotek *et al* (1973) for amorphous Ge $g_0 = 1{\cdot}5 \times 10^{18}\,\mathrm{eV^{-1}cm^{-3}}$, $a = 10\,\text{Å}$ and $\kappa = 16$. This gives $\Delta = 12$ K and $T_c = 0{\cdot}15$ K. The resistivity was not measured at such low temperatures. Using the data of Hamilton *et al* (1974) we can see that for amorphous carbon T_c is a hundred times larger than for amorphous Ge. Hamilton *et al* (1974) have observed the dependence close to that of equation (6) in amorphous carbon. This resemblance may be explained as a manifestation of the Coulomb gap.

The energy spectrum of lightly doped and intermediate compensated crystalline semiconductors has a single characteristic energy $e^2N^{1/3}/\kappa$, where N is the impurity concentration. Therefore the dispersion of the impurity levels and the width of the Coulomb gap are of the same order of magnitude and the range of constant density of states does not exist at all. So the range of the validity of the Mott law should not exist. In the cases of the extremely weak or extremely strong compensation such a range may exist. Redfield (1973), Shlimak and Nikulin (1972), Emel'anenko *et al* (1972) reported the temperature dependences of σ close to that of equation (6) in crystalline GaAs and Ge.

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