State density near the Fermi level in 1*D* systems with localized electrons

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The state density in a 1*D* system with localized electrons is calculated near the Fermi level, where the state density has a Coulomb gap. The calculation is carried out by solving a self-consistent equation.

White *et al.*[1] have reported an experimental study of the energy dependence of the state density near the Fermi level in thin wires made of granular aluminum. White *et al.*[1] actually measured the dependence of the conductance of a wire-oxide-(metal electrode) tunnel junction on the applied voltage V. This conductance is proportional to the state density $g(\epsilon)$ in the wire at the energy $\epsilon = eV$. For wires with a large resistivity, White *et al.*[1] observed a sharp (severalfold) decrease in the conductance of the junction at low voltages $eV \lesssim 20$ meV, which they linked with a Coulomb gap due to an interaction of the localized electrons in the 1*D* case. It is therefore interesting to examine theoretically the behavior of the state density in a disordered 1*D* system with a Coulomb interaction.

Following the model proposed in Ref. 2, we assume that the electrons can occupy the sites of a periodic chain, separated from each other by a distance a. The energy of site i, reckoned from the Fermi level, is given by

$$\epsilon_i = \Phi_i + \frac{e^2}{\kappa a} \sum_{j \neq i} \frac{n_j}{|i-j|}, \tag{1}$$

where e is the electron charge, and κ is the dielectric constant of the medium around the chain. The random quantities Φ_i are assumed to be distributed uniformly over the interval from $-A$ to A, and there is no correlation between their values at different sites. These quantities model a nucleating spread of energies of a non-Coulomb nature, so that the nucleating state density is $g_\infty = 1/2aA$. The second term in (1) describes the energy shift of site i due to the potential set up by the electrons localized at neighboring sites. The occupation numbers n_j take on the value 1/2 if a site is occupied or $-1/2$ if the site is vacant. The total number of electrons is assumed to be equal to half the number of sites, so that the chain has an overall electrical neutrality. By virtue of this symmetry with respect to the positive and negative charges, the Fermi energy is zero in this model.

We assume $E_M = e^2/\kappa a \ll A$. In this case the electron-electron interaction will affect the state density only in a narrow strip near the Fermi level. This condition can be written as $g_\infty e^2/\kappa \ll 1$. The self-consistent equation which was derived in Refs. 2 and 3 for the density of one-electron states, $g(\epsilon)$, in the ground state of this system takes the following form in our case:

$$g(\epsilon) = g_\infty e^{-(e^2/\kappa)\int_0^{E_M} \frac{d\epsilon' g(\epsilon')}{(|\epsilon| + \epsilon')}} \tag{2}$$

The integral in the argument of the exponential function is the mean number of electron states for which the inequality $|\epsilon| + |\epsilon'| < e^2/\kappa r$ is violated, where the energies ϵ and ϵ' lie on different sides of the Fermi level, and r is the distance between the corresponding sites. We transform to the new variables

$$G = \frac{g(\epsilon)}{g_\infty}, \quad |\epsilon| = E_M e^{-\kappa z/g_\infty e^2}, \quad \epsilon' = E_M e^{-\kappa z'/g_\infty e^2}. \tag{3}$$

Equation (2) then becomes

$$G(z) = \exp\left\{ -\int_0^\infty dz' G(z') \left[1 + e^{\frac{\kappa(z'-z)}{g_\infty e^2}} \right]^{-1} \right\} \tag{4}$$

As we will see below, the substantial change in the state density occurs at energies $|\epsilon| \ll E_M$, i.e., at $z \gg g_\infty e^2/\kappa$. Here the second factor in the integrand in (4) changes from 1 to 0 in a narrow interval $|z'-z| \sim g_\infty e^2/\kappa \ll 1$, so that it can be replaced by a step. As a result, we find the equation

$$G(z) = \exp\left[-\int_0^z dz' G(z') \right]. \tag{5}$$

A solution of this equation is $G(z) = (1+z)^{-1}$; the final expression for the state density is

$$g(\epsilon) = \frac{g_\infty}{1 + \frac{g_\infty e^2}{\kappa} \ln \frac{E_M}{|\epsilon|}} . \tag{6}$$

It can be seen from (6) that in the $1D$ case the Coulomb gap is exponentially narrow. Its width is $\Delta_1 = E_M \exp(-\kappa/g_\infty e^2) \ll E_M$. At $|\epsilon| \ll \Delta_1$ we have $g(\epsilon) \approx \kappa/e^2 \ln(E_M/|\epsilon|)$, and this state density does not depend on the nucleating energy spread A. At $|\epsilon| \gg \Delta_1$ we have $g(\epsilon) \approx g_\infty$.

In order to discuss the experimental data, we need to analyze the transition from the $3D$ case to $1D$ case as the wire thickness d is reduced. We consider a $3D$ lattice with a period a. This lattice lies inside a circular cylinder with a base diameter d. We assume $d \gg a$. We insert some imaginary membranes to partition the cylinder into sections of height d. Incorporating the Coulomb interaction within each section leads to the formation of a Coulomb gap of width $\Delta_3 = (e^2/\kappa a)(e^2/\kappa a A)^{1/2}$ in the state density.[2,3] At $|\epsilon| \ll \Delta_3$ the state density per unit length of the cylinder is

$$g(\epsilon) = \frac{3d^2\kappa^3}{4e^6} \epsilon^2 . \tag{7}$$

This expression holds at $|\epsilon| \gg e^2/\kappa d$ and thus has a range of applicability only if the condition $d \gg e^2/\kappa\Delta_3$ holds. We now remove the membranes separating the sections. The change in the energy of each site which is caused by the Coulomb interaction of the electrons from different sections is on the order of $e^2/\kappa d$, so that a substantial change in the state density after the removal of the membranes occurs in the energy interval $|\epsilon| \lesssim e^2/\kappa d$. The number of sites with energies in this interval in each of the sections is given in order of magnitude by $d(e^2/\kappa d)g(e^2/\kappa d) \sim 1$, so that we end up with an effective $1D$ model analogous to that discussed above with the parameters $a \sim d$ and $A \sim E_M \sim e^2/\kappa d$. The inequality $E_{M/A} = g_\infty e^2/\kappa \ll 1$ does not hold here, but at low energies, $|\epsilon| \ll e^2/\kappa d$, where the state density is determined by the Coulomb interaction at distances $e^2/\kappa|\epsilon| \gg d$, expression (6) remains valid, so that the state density is

$$g(\epsilon) = \frac{\kappa}{e^2} \left[\ln\left(\frac{e^2}{\kappa d |\epsilon|} \right) \right]^{-1} \tag{8}$$

The general expression for the state density $g(\epsilon)$ at $\epsilon \ll \Delta_3$ is

$$g(\epsilon) = \frac{\kappa}{e^2} f\left(\frac{\kappa d |\epsilon|}{e^2} \right) , \tag{9}$$

where the dimensionless function f is of such a nature that we have $f(x) = 1/\ln(1/|x|)$ at $|x| \ll 1$ and $f(x) = 3x^2/4$ at $|x| \gg 1$. In this case, $e^2/\kappa d \ll \Delta_3$, the state density has a universal form and does not depend on a or A at $|\epsilon| \ll \Delta_3$.

In the case with $d \gg a$ but $e^2/\kappa d \gg \Delta_3$, the Coulomb gap is of a purely $1D$ nature. In this case expression (6) holds with $g_\infty = \pi d^2/8Aa^3$, and E_M should be replaced by $e^2/$

κd. The gap width is $\Delta_1 \approx (e^2/\kappa d)\exp[-8/\pi(e^2/\kappa d\Delta_3)^2]$. In all cases, therefore, $1D$ expression (6) is valid at $|\epsilon| \ll e^2/\kappa d$.

In the experiments carried out by White *et al.*,[1] a wire of thickness $d = 750$ Å lay on a SiO_2 substrate. It is natural to take the dielectric constant κ characterizing the interaction of the charges at distances significantly greater than d to be $(\kappa_{SiO_2} + 1)/2 \approx 2$. Evaluating $e^2/\kappa d$, we find that expression (6) for the state density is applicable at $|\epsilon| \lesssim 10$ meV. The range of voltages V in the experiments of Ref. 1 was from 0.05 mV to 20 mV, but the conductance at low voltages, $0.05 < V < 2.5$ mV, was reported for only a single sample. This logarithmic dependence can be described by expression (6). Unfortunately, data are not available for that sample at high voltages, so that it is difficult to make a detailed comparison with the theory.

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