ulomb gap in disordered systems. Numerical periment in one-dimensional model

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A computer experiment was used to study a one-dimensional disordered system of localized electrons with long-range interaction. It is shown that the density of states has a "soft" gap in the vicinity of the Fermi level. The self-consistent equation agrees well with the experimental curve.

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It was shown in[1,2] that owing to electron—electron interaction in a disordered system with localized states the density of states (DS) of charged excitations vanishes when the energy tends to the Fermi energy. This leads, for example, to a change in the temperature dependence of the conductivity at low temperatures. In the present study the behavior of the DS near the Fermi level was investigated with the aid of a computer experiment.

A relatively simple model of a disordered system was proposed in[2]. In this model the electrons can occupy only the sites of a simple periodic lattice. To maintain neutrality, the charge of a site is assumed to be equal to 1/2 if the site is vacant and to $-1/2$ if it is occupied by an electron, the total number of electrons being half the number of sites. The energy of the electron at each site consists of a random quantity ϕ_i and of the potential produced at this sites by all the other sites

$$\epsilon_i = \phi_i + \sum_j e_{ij} n_j . \tag{1}$$

The values of ϕ_i are uniformly distributed in the interval from $-A$ to A, and e_{ij} is the electron interation energy, while the occupation number is $n_i = 1/2$ for an occupied site and $n_i = -1/2$ for an empty one. The total energy of the system is

$$H = \sum_i \phi_i \left(n_i + \frac{1}{2}\right) + \frac{1}{2} \sum_{i,j} e_{ij} n_i n_j . \tag{2}$$

The problem is to find the set $\{n_i\}$ that minimizes the total energy at a given realization $\{\phi_i\}$ and under the condition that $\Sigma_i n_i = 0$, as well as to find the DS $g(\epsilon)$ corresponding to this set. From the symmetry of the problem it follows that $g(\epsilon) = g(-\epsilon)$ and that the Fermi level is equal to zero, i.e., all the sites with $\epsilon_i < 0$ are filled in the ground state, and those with with $\epsilon_i > 0$ are empty.

In this article we present the results of a numerical experiment on a one-dimensional model, when the interaction potential is given by $e_{ij} = |i-j|^{-1/2}$, where i and j are the coordinates of the sites. (The interaction $e_{ij} = r_{ij}^{-1}$ does not lead to a gap in the one-dimensional model.[2]) It is difficult to minimize directly with a computer the total energy (2) with specified ϕ_i for a strand of a sufficiently large number of sites. We have therefore used the explicit form

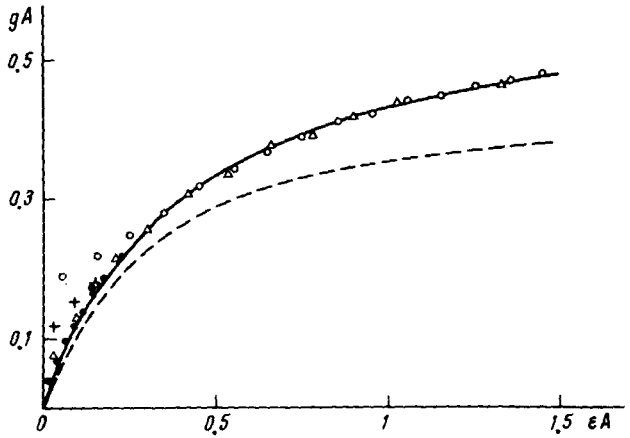

FIG. 1. Results of computer experiment for $A=3$ and $N=100$ (circles), $N=400$ (crosses), $N=2\times10^3$ (triangles), and $N=2\times10^4$ (dots). Solid curve—numerical solution of (4) with account taken of the discreteness of the lattice, dashed—solution (4) in the continual approximation (replacement of the sum by an integral).

obtained in[2] [formula (12)] for the distribution function $\rho(\epsilon_1\cdots\epsilon_N)$ of all the energies of a strand of N sites. This function is equal to $(2A)^{-N}$ if the energy satisfies all the possible inequalities that call for a positive increment of the energy following permutation of any number of electrons. Regions where at least one of the inequalities is not satisfied are forbidden, and $\rho=0$ in these regions. In particular, the inequality corresponding to the transfer of one electron

$$\epsilon_j-\epsilon_i-e_{ij}>0. \tag{3}$$

must be satisfied for all $\epsilon_j>0$ and $\epsilon_i<0$. Our experiment consisted of constructing realizations of the indicated distribution function, taking into account the inequalities connected with all possible permutations of one electron (OE approximation) and two electrons (TE approximation). We present by way of example the OE approximation program. At the first site of a strand of N sites, a random-number generator with uniform distributions from $-A$ to A generated the number ϵ_1. This number and the coordinate were fixed in the computer memory. Then, a number ϵ_2 was generated on the second site, and was memorized only when ϵ_2 and ϵ_1 satisfied (3). In the opposite case ϵ_2 vanished and went over to the next site. The number obtained at site i was verified for

TABLE I.

A	3	3	3	3	6
N	$6\cdot10^3$	10^4	$1{,}5\cdot10^4$	$2\cdot10^4$	$6\cdot10^4$
$g(0)\sqrt{N}$	1.0	1.0	1.0	1.1	1.0

tisfaction of (3) with all the numbers ϵ_j previously generated and fixed in the emory. ϵ_i was fixed when the result was positive and discarded when the sult was negative. After running through all N sites, the computer memory as left with a set of energies satisfying the necessary requirements. This as followed by calculation of the number of levels that fall in each of the escribed intervals, and a histogram of the state density $g(\epsilon)$ was obtained. he number N ranged from 100 to 6×10^4. For each N, the procedure was epeated so many times, that the total number of sites taking part in the veraging was of the order of several million. The number A ranged from 1 to . The TE program was constructed in similar fashion. We verified that the esult does not depend on the order in which the sites were taken. To this end ve used a program in which the sites were traversed not consecutively from eft to right, but in random sequence. Finally, we used a program that constructed, after generating the set $\{\epsilon_i\}$, a set $\{\phi_i\}$ in accordance with formula (1), with allowance for the fact that $n_i = 1/2$ if $\epsilon_i < 0$ and $n_i = -1/2$ if $\epsilon_i > 0$. The distribution of $\{\phi_i\}$ did indeed turn out to be uniform. The results of the experiment consisted in the following:

1. The results of the OE and TE approximations did not differ within the limits of the calculation accuracy (10%). This corresponds to the estimate given in[2] and gives grounds for hoping that the OE approximation is good enough.

2. The state density $g(\epsilon)$ has at small ϵA a gap that agrees exactly with the predictions of[2] (see Fig. 1). We have solved numerically the self-consistent equation for the SD,[2] which takes the following form when account is taken of the discreteness of the strand:

$$\ln[2Ag(\epsilon)] = -\sum_{i<1/\epsilon^2} \int_0^{\frac{1}{\sqrt{i}}-\epsilon} g(\epsilon')\,d\epsilon. \qquad (4)$$

It turned out that at those energies at which the finite dimension of the strand does not affect the state density, the result of our experiment does not differ from the solution (4). So good an agreement is indirect proof of the validity of Eq. (4), since we cannot show that it is exact.

3. Since the strand is finite, the state density does not vanish as $\epsilon \to 0$, but has a finite value $g(0)$. As seen from Fig. 1, the finite character of the strand comes into play only at small ϵ, i.e., the correlation radius R_ϵ increases as $\epsilon \to 0$. According to the theory,[2] as $\epsilon \to 0$ we have $g(\epsilon) = \epsilon$, $R_\epsilon \sim \epsilon^{-2}$ in an infinite strand. It follows therefore that in the finite strand $g(0) \sim 1/\sqrt{N}$. It follows also from the theory that at small ϵ the state density has a universal form determined only by the interaction and the number of dimensions of the space, and independent of A, i.e., that $g(0)$ does not depend on A. As seen from Table I, these conclusions are confirmed within the limits of the experimental accuracy.

[1]A. L. Efros and B. Shklovskii, J. Phys. C 8, 49 (1975).
[2]A. L. Efros, J. Phys. C 9, 2021 (1976).