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Properties of the electron glass

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We have carried out numerical calculations on two- and three-dimensional models of highly localized electrons interacting by an unscreened Coulomb potential. A Coulomb gap was found in the density of states for bare single-particle excitations. This "soft" gap was deeper than the power-law gap seen in earlier simulations, but for three-dimensional systems it was fitted well by an exponential form proposed by Efros. The gap fills as the temperature is raised. We also found an unexpected clustering of states with the same occupation and energies close to the chemical potential. The density of states for dressed single-particle excitations ("electronic polarons") showed a Coulomb gap too, but a narrower one than that for the bare excitations. There is a clear analogy between this model of interacting electrons and an Ising spin-glass with $1/r$ antiferromagnetic interactions and a random field on each site. We have exploited this analogy to search for a glass transition in the electronic system by calculating the specific heat, susceptibility, and a modified Edwards-Anderson order parameter.

I. INTRODUCTION

The behavior of noninteracting electrons moving in a random potential and the resulting phenomenon of localization have been studied extensively since Anderson's original paper of 1958,[1] and in the last few years this problem has become reasonably well understood. The effects of electron-electron interaction on such a system have so far received less attention, but interesting results are expected. Altshuler and Aronov[2] have calculated the effect of electron-electron scattering on a dirty three-dimensional (3D) metal, whose wave functions are extended. They find that the scattering of electrons from impurities enhances the Coulomb interaction by reducing the effectiveness of the screening; this causes corrections to the electrical conductivity at low temperatures T proportional to $T^{1/2}$, and corresponding corrections to the density of states (DOS) near the chemical potential μ proportional to $(E-\mu)^{1/2}$. For two-dimensional (2D) systems, the square roots are replaced by logarithms.[3]

For the opposite extreme, a disordered insulator with highly localized electronic states, the effects of electron-electron interaction have been studied longer. The spatial distribution of the electrons is strongly influenced by the long-ranged Coulomb repulsion between them. This leads to a depletion of the single-particle DOS near the chemical potential known as the Coulomb gap.[4–6] It is expected to cause deviations at low temperatures from Mott's $T^{1/4}$ law for electrical conduction by variable-range hopping, for example, since this law was derived[7] assuming a flat DOS and neglecting electron-electron interaction.

An extensive study, both analytical and numerical, of the Coulomb gap has been carried out by Efros, Shklovskii, and co-workers,[6,8–13] reviewed most recently by Shklovskii and Efros.[11] They have studied a classical model of a dilute impurity band,[8] whose Hamiltonian in dimensionless units is

$$H=\sum_i n_i\phi_i+\tfrac{1}{2}\sum_{i,j}{}' \frac{n_in_j}{r_{ij}} . \tag{1}$$

Here n_i is the number operator for site i, taking the values 0 or 1 only; ϕ_i is a random energy on site i; and the final term is the bare Coulomb interaction between the electrons ($r_{ij}=|\vec{r}_i-\vec{r}_j|$). The prime on the summation sign indicates that the term with $i=j$ is to be omitted. Background charges are included to maintain electrical neutrality; this is dealt with more fully later. An excellent practical realization of such a system is the impurity band of a lightly doped, compensated semiconductor, where the disorder arises from the random distribution of impurities over the host's lattice sites. The carriers remaining in the majority band interact strongly by unscreened Coulomb potentials, and are also subject to a large random field from the ionized minority impurities and the unoccupied majority impurities. These forces are all long range, unlike the quantum-mechanical effects which we have neglected, such as tunneling which depends exponentially on the separation between sites. A more detailed justification of the purely classical model has been given by Shklovskii and Efros.[11] Although we shall be considering both two- and three-dimensional lattices, the electrostatic potential always falls off with distance as $1/r$; thus even in the two-dimensional systems we are considering pointlike electrons, rather than interacting lines of charge.

The single-particle energies for this model are defined by

$$E_i=\phi_i+\sum_j{}' \frac{n_j}{r_{ij}} . \tag{2}$$

$E_i-\mu$ is the energy required to add an electron to an empty site i (or minus the energy for adding a hole to an occupied site), holding the rest of the electrons fixed. The distribution of these energies is the single-particle density of states, which is required to have a Coulomb gap. This was shown by Efros and Shklovskii as follows.[6]

If an electron is moved from an occuped site i to an empty one j, the change in energy of the system due to this one-electron hop (or particle-hole excitation) is

$$E_{ji}=E_j-E_i-\frac{1}{r_{ij}} . \tag{3}$$

The last term is the attraction of the electron-hole pair created and its presence causes the Coulomb gap. From the ground state, all excitation energies like (3) must be positive. This implies a minimum separation between pairs of sites whose single-particle energies lie on either side of the chemical potential, and if the states are assumed to be homogeneously distributed through space it leads to a bound on the single-particle DOS $n_1(E)$ of the form

$$n_1(E)\propto |E-\mu|^s \tag{4}$$

with $s\geq D-1$ in D dimensions. By using a "self-consistent" argument, Efros[8] showed that $s=D-1$, within the approximation of considering the stability of the ground state against only single particle-hole transitions, and derived the constant of proportionality. He also obtained a sharper bound for three-dimensional systems by considering many particle-hole excitations in which the surrounding electrons were allowed to relax; this had the form

$$n_1(E)\propto \exp[-|E_0/(E-\mu)|^{1/2}] . \tag{5}$$

This exponential gap arises from the existence of short particle-hole excitations with very low transition energies. Baranovskii, Shklovskii, and Efros[12] showed that the number of such excitations should go to zero logarithmically as the energy goes to zero, and took this into account to obtain another form for the single-particle DOS:

$$n_1(E)\propto \exp\{-\lambda y/[\ln(y)]^{7/4}\},\ \ y=E_0/(E-\mu) .$$

This holds only for very low energies, and so cannot be tested numerically. There is also the possibility that the close pairs with low excitation energies may be removed by quantum-mechanical tunneling in a real material, and that these exponential forms for the Coulomb gap may therefore be unimportant in practice.

The Coulomb gap is a "soft" gap, meaning that $n_1(E)$ vanishes only at $E=\mu$. It is tied to the chemical potential and its form, in the limit of large disorder, should depend only on the strength of the Coulomb interaction, not on the form of the distribution of random energies or on the position of the chemical potential within the band.[8] It is produced by the long-ranged Coulomb forces and is therefore to be distinguished from a Hubbard gap, which is due to short-ranged forces. Only in the case of one electron per site does a Hubbard gap separate a filled and an empty band. It is not present in the model (1) because of the restriction $n_i=0$ or 1 so the chemical potential always lies in the lower Hubbard band.

Although the theory of the Coulomb gap has been derived for the limit of negligible tunneling between sites, it should hold close to the chemical potential in any disordered insulator. This is because the states in a sufficiently small range of energy will be well separated in space and the Coulomb interaction will aways dominate. Thus $n_1(E=\mu)$ vanishes, although the form of $n_1(E)$ discussed above may hold only very close to μ.

Computer simulations of the system defined by the Hamiltonian (1) have previously been carried out,[6,8–13] both for a model with a lattice[9] and for a more realistic model of an impurity band.[10] We have carried out calculations of the model on a lattice by a very similar technique, and find somewhat different results in the region of the Coulomb gap. We have also calculated the distribution of single-particle states in space as a function of energy, the particle-hole density of states, and the DOS for "electron polarons." These may be the dominant single-particle excitations at low temperatures[4,8,14,15]; they include a region of relaxation around the added particle and therefore have a lower energy (measured from μ) than the bare excitations. Efros[8] argued that the polarization cloud should have a finite radius, beyond which the polaron appears simply as a charged quasiparticle, and the density of polaron states $n_p(E)$ should therefore obey (4) [but not (5)]. Mott[14] suggested that there should be no Coulomb gap for polarons. We find that there is a gap, but that it is narrower than that predicted by Efros.

If $n_p(E)$ vanishes at the chemical potential, it is impossible to add an extra particle to the system with an infinitesimal energy increase over the ground state, even if local relaxation is permitted. By contrast, if a total relaxation of the system is allowed, the resulting DOS $dn/d\mu$ for adding an extra electron at the chemical potential is not expected to be zero. This is an indication that the system may be behaving as a glass, with regions of configuration space inaccessible from the ground state at low temperatures. This glassy state arises from competition between the Coulomb energies and the random-site energies. There is a clear analogy here with an Ising spin-glass having random fields on each site. We have explored this analogy, to investigate the possibility of glass transition in the system, and this will be described later in the paper. A short summary of this work has already been published.[16]

II. MODELING THE GROUND STATE ON THE COMPUTER

Following Baranovskii, Efros, Gelmont, and Shklovskii[9] (to be referred to as BEGS), the Hamiltonian

(1) was simplified as far as possible for modeling by computer. The sites were put on a lattice (square or simple cubic) of unit lattice constant. This should not affect states close to the chemical potential as these will be sparsely distributed over the lattice sites and the underlying periodicity should be washed out. The random energies ϕ_i were drawn from a uniform distribution between $\pm\frac{1}{2}B$. There were K electrons per site, with $0<K<1$. Each electron had charge -1 and, to preserve electrical neutrality, each site had a compensating charge of $+K$. The total charge on site i is then $-(n_i-K)$, so the Hamiltonian becomes

$$H=\sum_i n_i\phi_i+\frac{1}{2}\sum_{i,j}{}' \frac{(n_i-K)(n_j-K)}{r_{ij}}$$

$$=\sum_i n_i\phi_i+\frac{1}{2}\sum_{i,j}{}' \frac{n_in_j}{r_{ij}}-K\sum_{i,j}{}' \frac{n_i}{r_{ij}}+\frac{1}{2}K^2\sum_{i,j}{}' \frac{1}{r_{ij}} \ . \quad (6)$$

An important difference between this study and previous work is the treatment of boundary conditions. We used periodic boundary conditions, but took only the shortest distance between two sites in the repeated lattice to calculate the Coulomb energies; thus each site appears to be on one of the middle sites of the finite model. This method has several advantages over the free boundaries used by others.[17–19] There are no problems with surfaces, as each site is equivalent; it is easy to program; it gives good values for the Madelung energies of the crystal (accurate to 1 part in 10^4 for lattices of 20^2 or 10^3 sites); it yields results which are much less sensitive to the size of the sample; and it facilitates the task of finding states which are stable against particle-hole transitions.

Because each site on the lattice is equivalent, the last two terms in the Hamiltonian (6) can be reduced to a constant. Writing $Q_A=\sum_j{}'(1/r_{ij})$ for the sum of all the Coulomb energies to site i in a lattice with A sites, which is clearly independent of i, gives

$$H=\sum_i n_i\phi_i+\frac{1}{2}\sum_{i,j}{}' \frac{n_in_j}{r_{ij}}-\frac{1}{2}K^2AQ_A \ . \quad (7)$$

The single-particle energies (2) take the form

$$E_i=\phi_i+\sum_j{}' \frac{n_j-K}{r_{ij}}=\phi_i+\sum_j{}' \frac{n_j}{r_{ij}}-KQ_A \ . \quad (8)$$

The expression for the energies of excitations, such as (3), are unchanged by the addition of the background charges. For the work described here, a half-filled band was used, $K=\frac{1}{2}$. In this case there is electron-hole symmetry about the chemical potential at $\mu=0$.

The computer program to generate ground states was essentially as described by BEGS. A set of random energies was chosen, the electrons were thrown in at random, and the system was allowed to relax by successive particle-hole transitions, each of which lowered the total energy. In the first stage, called "μ-sub" by BEGS, the single-particle energies were checked to see whether all occupied sites had lower energies than empty ones. If they did not, an electron was moved from the filled site with the highest energy to the empty one with the lowest energy, the single-particle energies were recalculated, and the process was repeated until the ordering was correct. Most of the excess energy was released in this stage.

The next stage of our program, like that of BEGS, checks that the transition energy (3) for a particle-hole excitation is non-negative for every pair of sites. We checked all pairs first and then made the most favorable hop, as we found this to give final states of lower energy. The search for this most favorable hop is speeded greatly by the elimination of unnecessary tests. If a hop was made, the program returned to "μ-sub"; if not, the model state is now stable against all single particle-hole transitions.

It is impracticable to test a model of reasonable size for stability against all multiparticle excitations, but for many samples we carried out a limited check of two-electron hops (double particle-hole transitions). Such a transition is composed of two single-particle transitions but the rise in energy associated with it is less than the sum of the energies of the component hops, although in most cases the difference is small. On a lattice, this reduction in the electrostatic energy of the transition has a maximum value $E_{\max}$ $(=2-\sqrt{2}$ for a square or simple cubic lattice), so one component of a favorable two-electron hop must be a one-electron hop whose energy (necessarily positive) is less than $\frac{1}{2}E_{\max}$. We could therefore construct a table of all one-electron hops whose energy is below this maximum and test all of the two-electron transitions which include these; the stability of this set guarantees stability of the sample against all two-electron transitions. Unfortunately, there were too many one-electron transitions with energies less than $\frac{1}{2}E_{\max}$ and a lower cutoff than this had to be used, leaving the possibility that some very compact two-electron hops of favorable energy change may have been missed.

The final state will not in general be the true ground state of the system. Starting with the same set of random energies but with different initial occupations, a distribution of different "pseudoground" states resulted. If the state of lowest energy occurred frequently in this distribution, we believe (following BEGS) that this is the true ground state. It is possible that the true ground state has peculiar properties which make it difficult to reach by the Monte Carlo procedure outlined above, and that our identification of it is therefore wrong. However, this may mean that the true ground state is difficult to reach for a real system, and that the "selected ground state" which we have calculated may well be the one of physical interest.

It is only possible to test the efficiency of the program in finding ground states when there are no random energies and the crystalline ground state is known. The proportion of "single crystals" among the final states decreases as the size of the samples increases, as would be expected, the most common defects being pairs of grain boundaries. No single crystals were found in 40 attempts to find the ground state of $10\times10\times10$ lattice. For a two-dimensional lattice of 16^2 sites, 11% of the final states were crystalline. BEGS found no true ground states in 30 attempts on a lattice of the same size. We believe that this marked increase in efficiency is due mainly to the boundary conditions. In the presence of random energies with $B=2$, just over half of our simulations led to what we believe to be the true ground state (BEGS found 20% only).

Several checks were made for systematic errors in the modeling procedure. First is the finite size of the lattice used. This affects the Coulomb energies because they are not summed to infinity but, as shown by the accuracy of the Madelung constant, this is a small effect only, despite the long range of the Coulomb force. More important is that there is a longest hop $r_{\max}$ on the lattice, and the main criterion used to determine the ground state is the stability against excitations whose energy change is given by Eq. (3). Therefore states with an energy within about $1/r_{\max}$ of μ might be affected by the finite size of the sample. In fact, most pairs of marginal stability are compact, with $r \ll r_{\max}$, so this effect also is small. This is shown by Figs. 1(a) and 2(a), where $n_1(E)$ is shown for samples of different sizes. This very weak dependence of $n_1(E)$ on the size of the lattice contrasts with results of other workers[9,19] and is, we believe, another benefit of the boundary conditions.

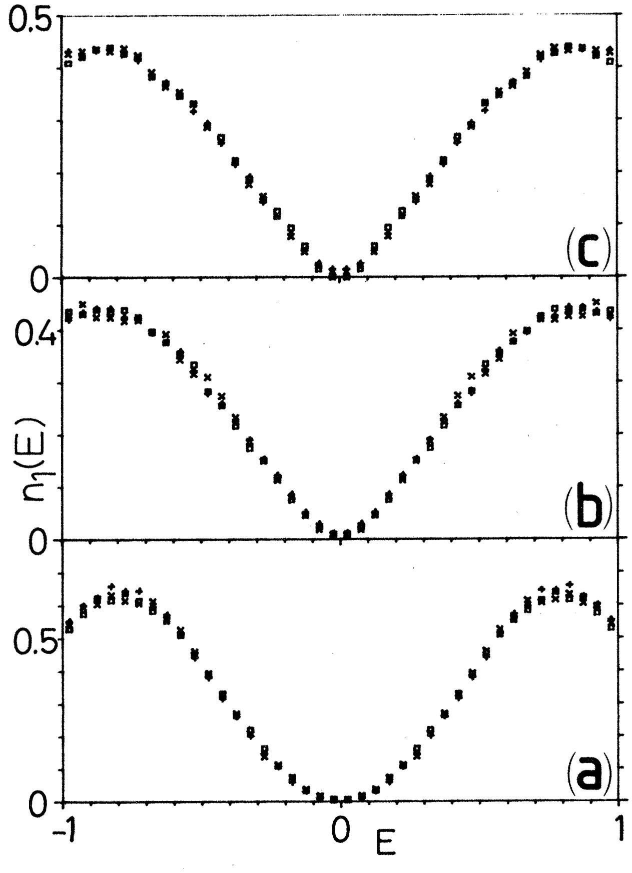

FIG. 1. Single-particle DOS for 2D systems, comparing (a) different sizes of models: with sides of length 10 (pluses), 16 (squares), and 20 (crosses); (b) different qualities of final states: stable against one-electron hops (pluses), stable against one- and two-electron hops (squares), and selected ground states (crosses); (c) different ways of averaging: simple averaging (BEGS) (pluses), μ averaging (BEGS) (squares), and method adopted here (crosses).

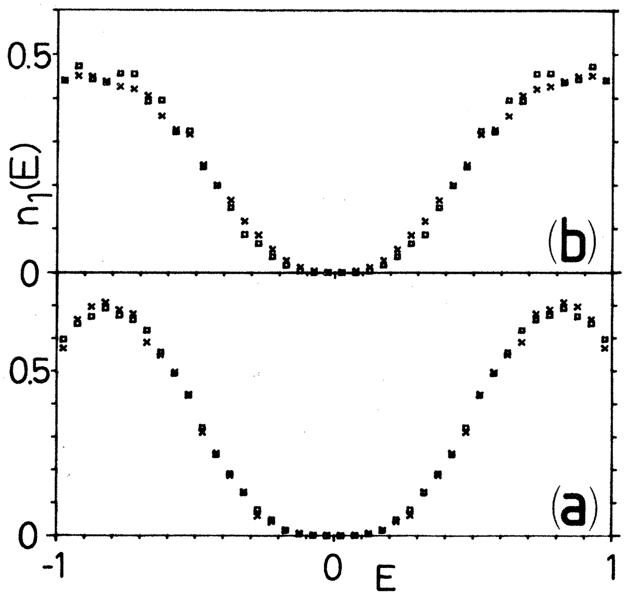

FIG. 2. Single-particle DOS for 3D systems, comparing (a) different sizes of models: with sides of length 6 (crosses) and 10 (squares); (b) different qualities of final states: stable against one- and two-electron hops (crosses) and selected ground states (squares).

A second possible source of error is that the final states may not be true ground states. We compared $n_1(E)$ of models tested for stability against only single particle-hole transitions, of models tested for stability against single and double particle-hole transitions, and of selected ground states. In two-dimensional systems [Fig. 1(b)] there is little discernible difference between these, in agreement with BEGS; but for three-dimensional systems there is evidence of a deeper gap in the DOS of selected ground states [Fig. 2(b)]. As it was found[8] that more complicated excitations put a sharper bound on $n_1(E)$ in 3D systems [Eq. (5)] but not in 2D systems, this greater sensitivity to the quality of ground states in three dimensions is not surprising. Unfortunately, computing selected ground states is very time consuming and most work had to be done with final states tested for stability against only single and (most) double particle-hole transitions.

A third problem arises when combining results from different samples, because the random energies cause the position of the chemical potential μ to fluctuate from sample to sample.[9] This effect washes out the gap in the single-particle DOS if results from different samples are combined directly, as was found by BEGS, although they showed that this was due to the small size of the samples. They proposed instead that μ could be estimated as the mean energy of the highest filled and lowest empty single-particle state. This has two disadvantages: There is a "hard" gap of width $1/r_{\max}$ where there are no states at all in the averaged spectrum and, because the two states used to estimate μ come from a region of low density in energy, the estimated value has a wide distribution about the true value. We exploited the electron-hole symmetry and took μ as the mean of the random energies ϕ_i (the mean of the final single-particle energies E_i had very closely the same value). Data averaged by the three methods are compared in Fig. 1(c) for two-dimensional systems.

Grünewald *et al.*[19] have recently reported a calculation which uses a mean-field approach more akin to that used in spin-glasses. They derived a set of equations for the mean occupation numbers in terms of the mean single-particle energies, which must be solved self-consistently. Fluctuations about the mean occupation numbers are neglected in this method, which is therefore exact only at zero temperature. Also, a self-consistent solution guarantees only that the occupied sites have lower single-particle energies than the empty ones: It does not guarantee stability of the state against particle-hole excitations.

III. CALCULATED PROPERTIES OF THE GROUND STATE

A. Single-particle density of states

The single-particle density of states $n_1(E)$ for models on two-dimensional lattices with 16^2 sites and average occupation $K=\frac{1}{2}$ is shown in Fig. 3(a) for bandwidths B of random energies from $\frac{1}{2}$ to 4. The arrows at $E=\pm 0.81$ indicate the single-particle energies for a perfect crystal, and the curve for $B=\frac{1}{2}$ in particular shows signs of the underlying periodic lattice. The important point is the deep minimum in the DOS near the chemical potential $\mu=0$, separating filled from empty states: This is the Coulomb gap. The DOS appears to go not quite to zero but this is partly an artifact due to the width of the histogram bins, and partly a residual error in the estimate of μ for each sample. For the more disordered systems, the form of the gap seems to be independent of B as expected.[8] It does not, however, have the linear form of Eq. (4) that was seen by BEGS. A comparison of our results and theirs for $B=2$ ($A=1$ in their notation) appears in Fig. 4. There is little difference except at low energies where our results lie consistently below theirs; this is in agreement with their expectation[9] that their results are less accurate for $|E|<0.15$. From a log-log plot, we found that our results for $n_1(E)$ were best fitted by a power law with an index of about $\frac{3}{2}$ near μ.

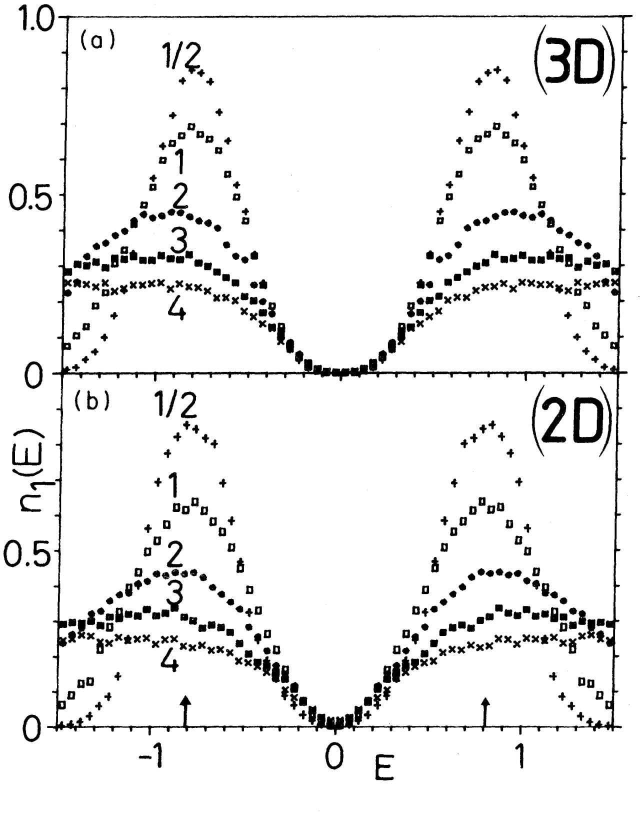

FIG. 3. Single-particle DOS for various bandwidths of random energies for 2D and 3D systems.

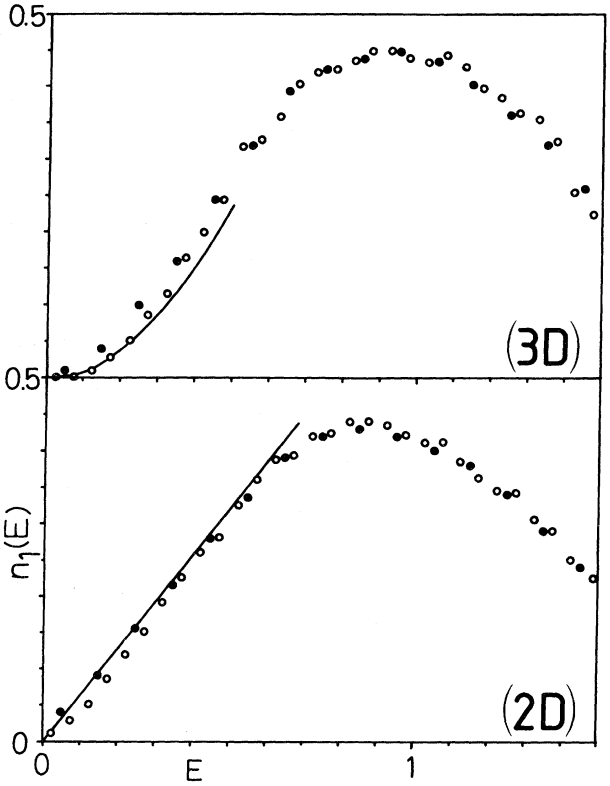

FIG. 4. Comparison of the present results (open circles) with those of BEGS (full circles) for 2D and 3D systems. The curves are from the theory of Efros (Ref. 8).

Corresponding results for 3D systems are shown in Fig. 3(b). The Coulomb gap is evident, and again it is deeper than the parabola seen by BEGS. It is, however, well fitted by the exponential form (5) as displayed in Fig. 5. However, the parameters needed to fit (5) to the data are in poor agreement with those calculated by Efros.[8] The strength of the exponential term decreases as B increases, and a parabola is probably correct in the limit of a very large band width.

The form of the Coulomb gap should be independent of the degree of filling of the band. We verified this for the case of a quarter-filled band. A much wider range of occupation fractions was studied by Efros, Van Lien, and Shklovskii.[10]

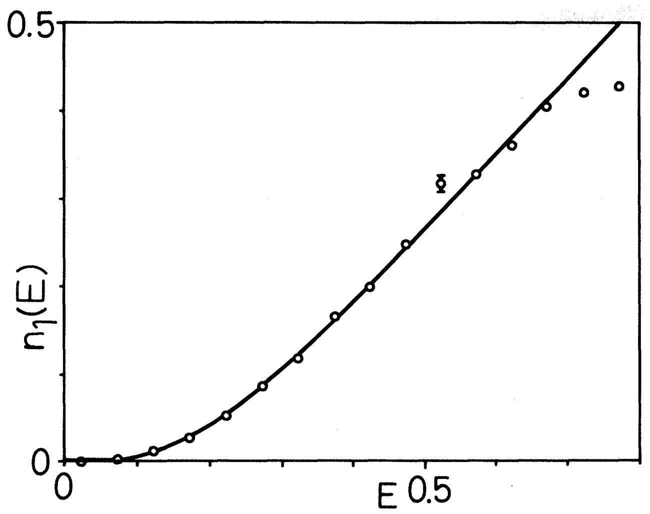

FIG. 5. Single-particle DOS for three-dimensional systems with $B=2$ fitted to the exponential form [Eq. (5)] (Ref. 8).

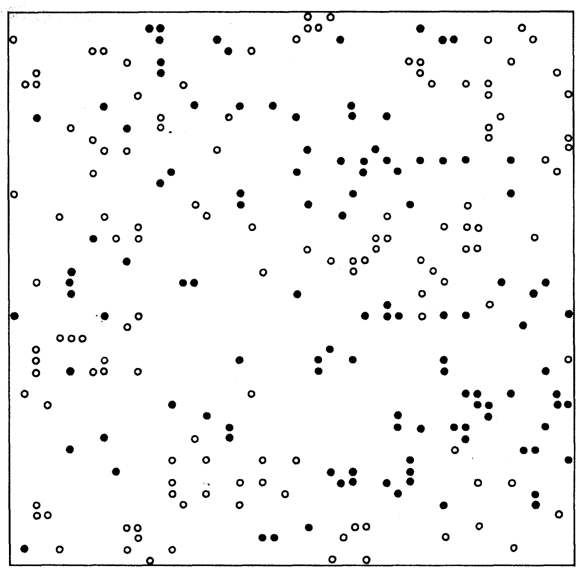

FIG. 6. Map of states whose single-particle energies lie within 0.4 of the chemical potential. The model had 50×50 sites and $B=1$. Filled circles represent filled sites and open circles represent empty sites.

B. Distribution of states in space

In deriving the equations for the Coulomb gap, it was assumed that states are homogeneously distributed in space.[7,8] It is therefore of interest to examine the distribution in space of states with energies close to the chemical potential. Figure 6 shows the positions of sites within an energy 0.4 of μ in a sample with 50^2 sites and $B=1$. It is clear that there is considerable clustering of like states, and that the distance between such clusters is less than the size of the sample; this was confirmed by calculating the spatial correlation function. This makes it unlikely that the clustering is due to a periodic potential permitted by the boundary conditions. The degree of correlation decreases as B increases. The clustering does not lead to local charge imbalances: Between the low-energy empty sites of a cluster are filled sites with energies far below μ. Nor does it contradict the arguments of Efros and Shklovskii,[7] which imply a correlation only between sites of different occupation. However, it does seem surprising that their theory still works so well, considering the failure of a crucial assumption. Perhaps their method should be applied to the clusters rather than to individual states, which could lead to the following picture. Long-ranged fluctuations of potential depress all the single-particle energies in some areas while raising them in others. In a region of lowered energies there are many empty states whose energies are only just above μ, but the filled states lie well below μ in energy, and therefore a cluster of empty states appears in Fig. 6. This nonrandom distribution of states in space will in turn affect the density of particle-hole excitations, which will be considered next.

C. Particle-hole density of states

This density of states $n_2(E,r)$ is that for creating particle-hole excitations of separation r and total rise in energy E. If the positions of sites were uncorrelated with their energies and occupations (as in a noninteracting system), this DOS could easily be calculated from the single-particle DOS by a convolution as follows:

$$\tilde{n}_2(E,r)\propto \int_{\mu}^{\infty} dE_1 \int_{-\infty}^{\mu} dE_2 n_1(E_1)n_1(E_2) \times\delta(E_1-E_2-r^{-1}-E) = g(E+r^{-1}) \tag{9}$$

with

$$g(x)=\int_{\mu}^{\mu+x} d\epsilon\, n_1(\epsilon)n_1(\epsilon-x)\,. \tag{10}$$

At large distances r, any correlation between sites should vanish and $\tilde{n}_2(E,r)$ approaches the true value $n_2(E,r)$. For short transitions or low energies, though, they may be very different.

If the simple arguments used to derive the power-law bound (3) on $n_1(E)$ are repeated for dipole rather than monopole excitations, it is found that $D=3$ is the marginal dimensionality, above which $n_2(E,r)$ is required to vanish at $E=0$. A logarithmic zero is found for $D=3$ by Baranovskii, Efros, and Shklovskii[12] (see below).

Histograms of $n_2(E,r)$ and curves of the function $\tilde{n}_2(E,r)$ calculated from $n_1(E)$ by neglecting correlation are shown in Fig. 7. These are from samples with 10^3 sites and $B=2$. Results from two-dimensional systems are similar. For the largest separation r shown (the longest hop allowed on the lattice before the finite size is felt), the "uncorrelated" function is a good fit to the computed DOS, but it is poor for the shorter hops where it is much too large at low energies. This is what would be expected from the clustering discussed above, but the data are not good enough for $n_2(E,r)/\tilde{n}_2(E,r)$ to be determined accurately. This was studied in more detail by Baranovskii and Efros,[13] who claimed good agreement between their

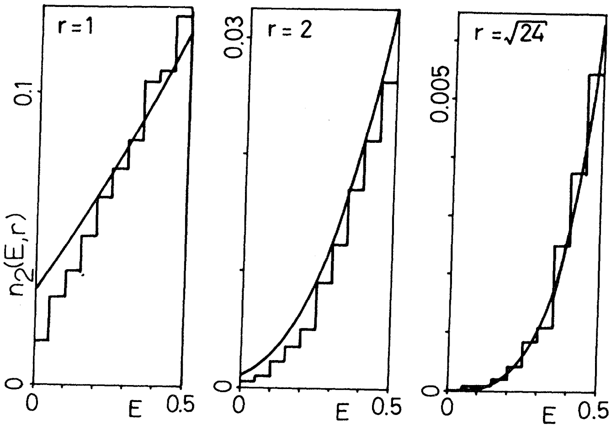

FIG. 7. Particle-hole DOS for 3D models on a $10\times10\times10$ lattice with $B=2$. The histograms are the computed results and the curves are calculated from the single-particle DOS neglecting correlation [Eq. (10)].

computed DOS, and the theory of Baranovskii *et al.*,[12] who predicted that for three-dimensional systems

$$n_2(E,r)\sim\tilde{n}_2(E,r)\exp[-(r/r_0)\phi(E)]\ ,$$

where $r_0=\sqrt{B}$ and $\phi(E)$ has a logarithmic dependence at low energy. No dip is predicted for two-dimensional systems by this theory, but our numerical results appeared to show a depletion of short low-energy excitations there too.

It should be emphasized that the presence of the Coulomb gap in $n_1(E)$ does not imply the absence of *particle-hole* excitations with low energies; the only requirement is that all such excitations should not have negative transition energies. There are in fact many of them, but most involve short hops; only for large separations of the electron and hole is the number of possible excitations with low energy reduced greatly by the Coulomb gap. In a noninteracting system, the particle-hole DOS is linear in energy. The interactions enhance $n_2(E,r)$ because the energies of the electron and hole are no longer restricted to be within E of the chemical potential. This affects, for example, the frequency-dependent conductivity. In a noninteracting system this obeys the Mott[20] ω^2 law at low frequencies,

$$\sigma(\omega)\propto\omega^2\,|\ln\omega\,|^4\ ,$$

but if the Coulomb interaction and a parabolic single-particle density of states for three-dimensional systems are included, the result becomes

$$\sigma(\omega)\propto\omega/\,|\ln\omega\,|\ ,$$

obtained by Efros and Shkovskii[21] and independently by us. Note that a dielectric constant which diverges logarithmically as $\omega\rightarrow0$ is found if this second expression for the conductivity is used in the Kramers-Krönig formula. This rather surprising result, which seems to contradict the initial assumption of an insulator with highly localized electrons, is not yet fully understood. Correcting some of the approximations made in the derivation of this formula would probably remove the divergence; $\tilde{n}_2(E,r)$ rather than $n_2(E,r)$ was used for the density of states, and it was assumed that the pairs of sites contributing to the conduction are distributed at random and act independently.

D. Electronic polarons

The concept of electronic polarons was mentioned in the Introduction. An electron (or hole) is added to a site and the surrounding particles are allowed to relax in order to lower the total energy of the transition. Such excitations may be important for the electrical conductivity at low temperature, but the details of this remain controversial.[22]

It is difficult to define these polarons precisely, and the following method was used to calculate the DOS for polarons, $n_p(E)$. Starting from a selected ground state, an electron is added to a site and held there. If it was possible to move another electron and lower the system's energy, the most favorable transition was made; in practice, the most favorable hops were in the vicinity of the added electron. This was repeated until the system was stable against moving any one electron, and the energy of the final state above the ground state was taken as the energy of the polaron on the selected site.

The DOS for bare and for polaron excitations calculated according to the above definition is shown in Fig. 8. Restrictions of computing time meant that only systems with $B=2$ were studied, with 16^2 or 8^3 sites. The Coulomb gap remains in $n_p(E)$ but it is clearly much narrower than that for the bare excitations. For 2D systems, the linear form suggested by Efros[8] is a fair fit but the coefficient is much larger than he predicted, about 2.1 rather than $2/\pi\cong0.64$. The exponential form (5) and the parabola (4) were fitted numerically to the data for three-dimensional systems, and had roughly equal errors (again the coefficient of the parabola was larger than that predicted for the bare DOS, 4.9 rather than $3/\pi\cong0.95$).

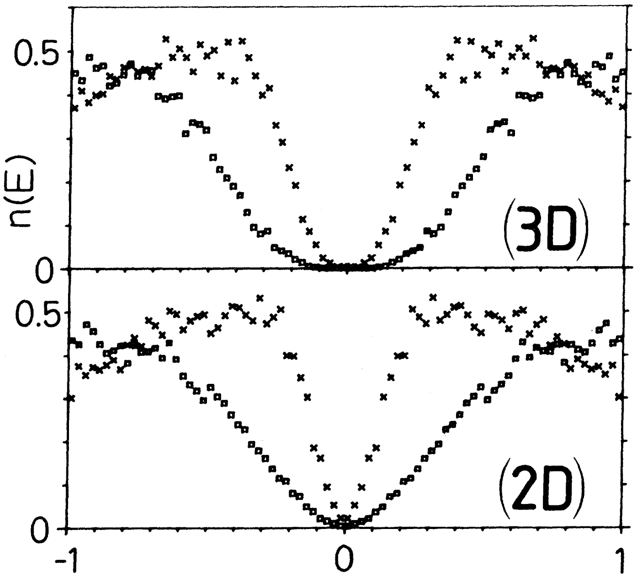

FIG. 8. Bare (squares) and polaron (crosses) DOS for models with $B=2$ for 2D and 3D systems.

The important point about our operational definition is that a polaron is essentially localized around the starting site. In general, the ground state and low-lying excited states of the system with an added electron will have a lower energy than this polaron, and many of these will have the selected site occupied. However, to reach such states it is necessary to rearrange a large number of electrons, and they may therefore not be accessible from the starting state at low temperature. This picture of inaccessible phase space is typical of a glass, a subject to which we will return later.

It is probable that in our simulation the amount of relaxation was limited by the finite size of the samples, as well as the restriction to only single particle-hole transitions; we intend to investigate this more fully in the future. The electrical conductivity is the process in which these polarons are supposed to be important, but it is not yet known how much relaxation is allowed there. For example, Efros[8,23] has suggested that the relaxation around a polaron of energy E_p is limited to a sphere of radius $1/|E_p|$; our calculation is directly applicable to this model. A more precise statement about the relevance of our calculation to polarons in transport cannot be made until more is understood about many-particle excitations in hopping conduction.

IV. EXTENSION OF THE MODELING PROCEDURE TO TEMPERATURES ABOVE 0 K

There are two main motivations for studying these model systems at temperatures above 0 K. The first is that the Coulomb gap is a property of the ground state, and therefore exists strictly only at zero temperature. In a noninteracting system, the occupation of states changes as the temperature rises, but not their energies; in the presence of interaction, a change in the occupation of one state alters the energies of all the others and consequently the form of the density of states, as well as its occupation, is affected. Thus the Coulomb gap is "washed out" by increasing temperature.

The second reason for interest in the properties of these models as their temperature is raised arises from the evidence that the ground state shows behavior typical of a glass; indeed, the Hamiltonian can trivially be rewritten to resemble that of a spin-glass with random magnetic fields on each site and long-ranged $1/r$ antiferromagnetic interactions. Following this analogy, we have calculated the specific heat, susceptibilities, and order parameters to search for a transition from a "paramagnetic" to a "glassy" state at some temperature T_g. Unfortunately, the results are far from conclusive and we are hampered in particular by the lack of a satisfactory order parameter for this problem with random fields rather than random interactions.

The modeling of temperatures above 0 K was carried out using the time-honored algorithm introduced by Metropolis *et al.*,[24] which gives a correctly weighted average of the measured property over phase space by simulating detailed balance. A transition in the model is picked at random, and its energy change E calculated. If $E \leq 0$ the transition is always made, but if $E > 0$ it is made only with probability $\exp(-E/T)$ (Boltzmann's constant is set to unity). For a detailed account of the Monte Carlo method see, for example, Binder in Ref. 25. The total energy and distribution of single-particle energies were monitored to follow the approach to equilibrium. The system was sampled only after several times the number of Monte Carlo steps required for these to settle down to steady values. Subsequent samples were taken sufficiently infrequently to be independent[25]; a few hundred measurements were made at each temperature. Only two-dimensional models with 16^2 sites and a bandwidth of random energies $B=2$ were studied in detail. Most samples were heated up, starting from a selected ground state so that an accurate value of the energy of the ground state was available to calculate the specific heat. Other runs were started with a state where the electrons had been thrown in at random and cooled from there. No significant difference was found between the results from these two procedures.

Figure 9 shows the average distribution of single-particle states at various temperatures. This distribution is that of all single-particle states of all configurations of the system, weighted according to a canonical distribution. At low temperatures there is a deep minimum in the DOS but it fills as the temperature is raised, and for $T > 0.3$ it disappears. This may be of importance for the electrical conductivity. It shows that any attempt to observe the Coulomb gap must be made at temperatures well below 0.3 in these units.

The lower curve on each graph shows the density of occupied states, and from the two curves the occupation function can be found. This is shown in Fig. 10 for $T=0.5$. A Fermi curve for that temperature is a poor fit to the numerical data. This is not surprising, as the Fermi distribution applies to noninteracting systems. However, a Fermi curve assuming $T'=0.42$ is a good fit. Similar results were obtained at other temperatures. We do not be-

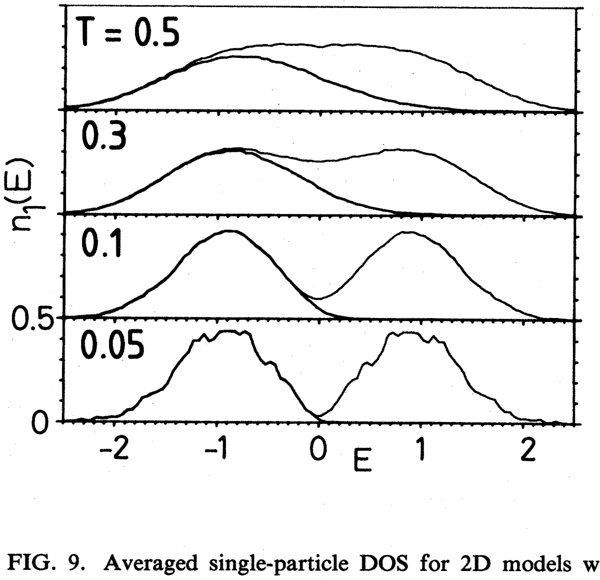

FIG. 9. Averaged single-particle DOS for 2D models with $B=2$ at different temperatures. The lower curves show the filled states at each temperature.

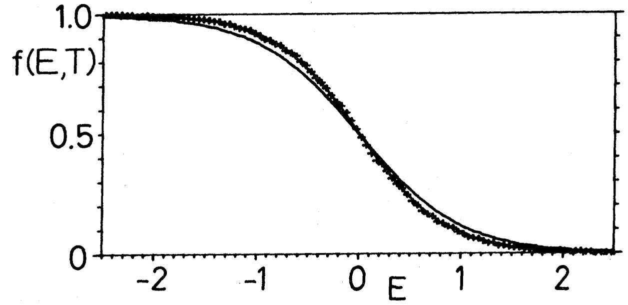

FIG 10. Occupation function at a temperature $T=0.5$. The crosses are the numerical data, the poorly-fitting curve is a Fermi function for $T=0.5$, and the better-fitting curve is a Fermi function for $T'=0.42$.

lieve that this results from a failure of the systems to come into equilibrium, and we verified this by approaching T from above instead of below and obtained identical results. The difference between T and T' may mean that simple mean-field theories, which would give the average occupation numbers as Fermi functions of the average single-particle energies, are seriously in error at all temperatures above 0 K. Grünewald *et al.*[19] used such a mean-field theory and obtained qualitatively different results from us; for example, they did not find a linear term in the specific heat or Edwards-Anderson order parameter (see Sec. V B) at low temperatures. It might be thought that such a mean-field approximation would be quite good, given the long range of the bare Coulomb interaction. However, the interaction is screened if the temperature is raised above 0 K, and the effective range may then become rather short.

V. ANALOGY WITH A SPIN-GLASS

The Hamiltonian (6) for a half-filled band can simply be rewritten to emphasize the analogy with a spin-glass. If s_i is the z component of the spin on site i, taking the values $\pm\frac{1}{2}$, it becomes

$$H=\sum_i s_i\phi_i+\tfrac{1}{2}\sum_{i,j}{}' \frac{s_is_j}{r_{ij}} . \tag{11}$$

This is an Ising model with a random field ϕ_i on each site and with long-ranged antiferromagnetic interactions. It has been shown[26] that a random field is relevant in Ising models with only short-ranged interactions for $D\leq 3$ (D is the number of spatial dimensions), but to our knowledge this model with $1/r$ interactions has not previously been studied. The long range of the interactions is expected to be important at low temperatures, but this may not be the case at high temperatures. After some relaxation time, the system can screen a charge at temperatures above any glass-transition temperature T_g and so the effective range of the interaction may become quite short, as mentioned above. This is generally true of any arrangement of charges which preserves neutrality over small volumes; for example, a neutral grain boundary perturbs the energies of only a few layers of sites.

The density of electrons is the analogous quantity in our models to the magnetization, the chemical potential plays the role of the applied magnetic field, and therefore the magnetic susceptibility is related directly to a density of states. To search for a glass transition, we have calculated the specific heat, various order parameters, and susceptibilities as a function of temperature.

A. Specific heat

The energy per site and the specific heat c_μ as a function of temperature are shown in Fig. 11. The specific heat was calculated from the derivative of the total energy with respect to temperature and from the variance of the fluctuations of energy, with insignificant differences. At low temperatures, $c_\mu=\gamma T$ and it rises to a peak at $T=0.5$. The value of γ is 1.36, which indicates a density of states of 0.83 (per site per unit energy). The total particle-hole density of states extrapolated to zero energy (neglecting the logarithmic zero mentioned earlier) is about 0.19 in these units, so there seems to be a large contribution to c_μ from more complicated excitations. If there were no Coulomb interaction, the specific heat would still be linear at low temperatures with a coefficient $\gamma=\pi^2/3B=1.64$ here, surprisingly close to the computed value for the interacting system.

B. Order parameters

The definition of an order parameter is difficult in an intrinsically disordered system. The parameter which been studied most frequently in spin-glasses is one based on the work of Edwards and Anderson[27]:

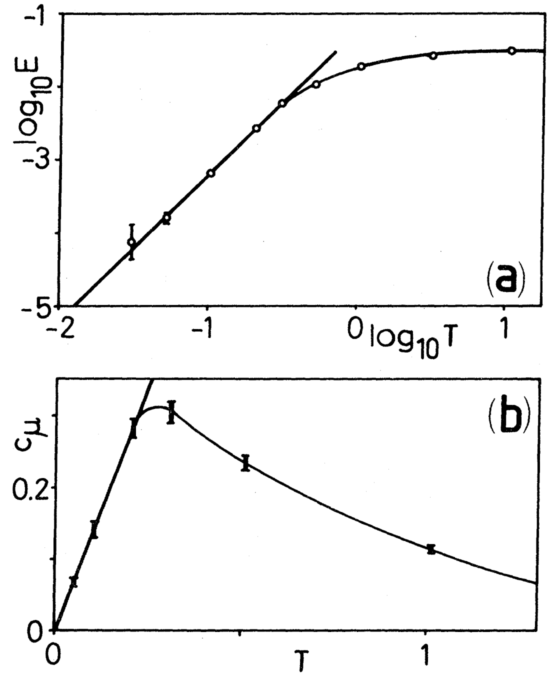

FIG. 11. (a) Excess energy per site above the ground state and (b) specific heat plotted against temperature.

$$q_{\mathrm{EA}}=\langle\langle 2s_i\rangle_T^2\rangle_E \ .$$

The inner average is a thermal average of a single spin, replaced in a numerical simulation by a Monte Carlo time average; the outer average is over all sites and configurations of random energies. The factor of 2 ensures the normalization $0\le q_{\mathrm{EA}}\le 1$. Essentially, q_{EA} measures the tendency of a spin to have some preferential alignment. In a model with no random fields but with random interactions, this should be a measure of glasslike order.

Because it measures the alignment of individual spins, q_{EA} is unsatisfactory for a system with random fields.[28] This is because the random fields by themselves tend to align the spins without any glasslike order being present. For a noninteracting system with a bandwidth B of random energies,

$$q^0_{\mathrm{EA}}(T)=1-x\tanh\frac{1}{x}\quad (x=4T/B)\ . \tag{12}$$

For $B=2$ this fits well the numerical results for the interacting system except at very low temperature, as demonstrated in Fig. 12. Clearly q_{EA} is not useful for describing any glass ordering of these models, but unfortunately we know of no satisfactory order parameter. To demonstrate that the Coulomb fields induce some ordering at low temperature, we introduced[16] a modified parameter

$$q_{\mathrm{mod}}(T)=2\langle[\langle s_i\rangle_T-f(\phi_i)]^2\rangle_E\ , \tag{13}$$

which subtracts from each spin the value $f(\phi_i)$ which would be the Monte Carlo time-average value of s_i if there were no interactions. $q_{\mathrm{mod}}(T)$ vanishes at high temperature or in the absence of interactions; if the Coulomb fields are completely dominant it would go to unity at zero temperature but generally it goes to a value between 0 and 1, which measures the relative importance of the interactions. (Note that q_{mod} here differs from our earlier definition[16] by a factor of 2.) Plots of $q_{\mathrm{mod}}(T)$ for $B=2$ and $\frac{1}{2}$ also appear in Fig. 12. There is some sign, on this log-log plot, that a transition may be taking place at a temperature of around 0.3. However, q_{mod} does not go sharply to 0 at a well-defined transition temperature T_g and it remains a strong function of T down to $T=0$. Expanding (13) gives

$$q_{\mathrm{mod}}(T)=2\langle\langle s_i\rangle_T^2\rangle_E-4\langle\langle s_i\rangle_T f(\phi_i)\rangle_E+2\langle f^2(\phi_i)\rangle_E\ .$$

$4\langle f^2(\phi_i)\rangle$ is identical to $q^0_{\mathrm{EA}}(T)$ and is therefore given by Eq. (12), so it can be seen that q_{mod} will vary linearly with T near $T=0$. The second term has a similar dependence because of the particle-hole and other excitations which exist down to zero energy. The presence of such low-energy excitations means that any *local* definition of the order parameter will have a linear dependence on temperature at low temperatures and will not look like the BCS form, for example. An "antiparamagnetic" order parameter has been suggested[29] as an improvement on q_{mod}, but suffers from the same disadvantages of having no sharp transition and varying linearly at low temperature.

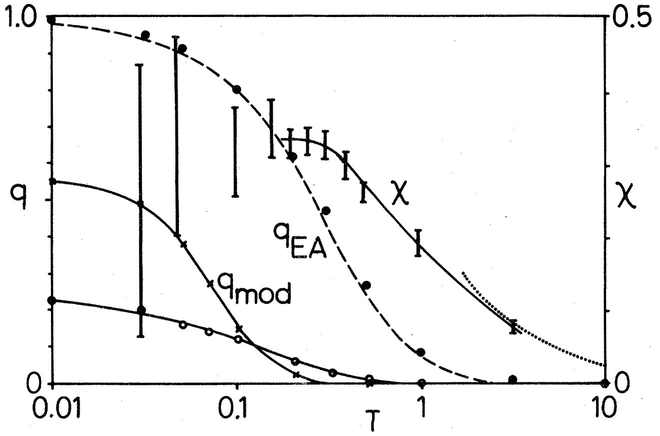

FIG. 12. Calculated Edwards-Anderson order parameter q_{EA} for $B=2$ (filled circles), modified parameter q_{mod} for $B=2$ (open circles) and for $B=\frac{1}{2}$ (crosses), and isothermal susceptibility χ_T for $B=2$ against temperature. The dotted curve for the susceptibility is the Curie law and the broken curve for q_{EA} is the result q^0_{EA} for a noninteracting system.

C. Susceptibility

There are various ways in which a susceptibility can be defined. For example, the usual isothermal susceptibility $\chi_T=\partial M/\partial H$ is measured by holding the sample at a fixed temperature T, applying a small magnetic field, measuring the magnetization, and taking the quotient. Instead, one could measure the "field-cooled" susceptibility χ_μ by applying the field when the sample is very hot, and allowing the sample to cool down to T with the field still applied. Generally, these two procedures would give the same result but in a nonergodic system, such as a glass below its transition temperature, they need not.

The susceptibility per site is given by

$$\chi=\frac{\partial M}{\partial H}=\frac{\partial n}{\partial \mu}=\frac{\mathrm{var}(N)}{AT}\ , \tag{14}$$

where N is the total number of electrons in the system of A sites; $n=N/A$. Since $N=\sum_i n_i$,

$$\mathrm{var}(N)=\sum_{i,j}(\langle n_i n_j\rangle-\langle n_i\rangle\langle n_j\rangle)\ .$$

For systems with only random interactions whose average value is 0, it is often argued that the cross terms in this sum vanish on averaging, so

$$\chi=\frac{1}{AT}\mathrm{var}(N)=\frac{1}{AT}\sum_i \mathrm{var}(n_i)$$
$$=\frac{1}{T}\langle \mathrm{var}(s_i)\rangle=\frac{1}{T}[1-q_{\mathrm{EA}}(T)]$$

but this would not be expected to hold for the models under study here, where the interaction leads to strong correlation between the occupation of nearby sites. Therefore it is vital to allow N, the total number of electrons, to change, so the Monte Carlo procedure must now simulate a grand canonical average rather than just a canonical average. This introduces the serious problem of electrostatic charging energies, arising from the long range and constant sign of the Coulomb interaction. Should an additional background charge be added to compensate for the charge of an added particle and keep the whole system electrically neutral? Consider the field-cooled susceptibility at zero temperature. If $E(N)$ is the energy of the ground state containing N electrons,

$$\begin{aligned}\chi_\mu^{-1} &= \frac{\partial\mu}{\partial n} = A\frac{\partial\mu}{\partial N} \\ &= A[E(N+1)-2E(N)+E(N-1)] \; . \end{aligned} \qquad (15)$$

The difference between the values of $E(N\pm1)$ obtained by maintaining neutrality, spreading the compensating charge uniformly over all sites, and allowing the charge to become unbalanced is $Q_A/2A$, the neutral system being lower in energy, so

$$\frac{\partial\mu(\text{charged})}{\partial n} = \frac{\partial\mu(\text{neutral})}{\partial n} + Q_A \; .$$

The charging energy Q_A is proportional to $A^{1-1/D}$, growing with the size of the system. Provided that neither value of $\partial n/\partial\mu$ is negative, this means that the "charged" value goes to 0 as A goes to infinity, and the susceptibility calculated from the neutral system is the correct one to take. A similar argument can be made for the isothermal susceptibility.

We attempted to calculate this field-cooled susceptibility from Eq. (15) by finding the ground state of $N-1$, N, and $N+1$ electrons in the same set of random energies, using models of 16^2 sites with $B=2$. There were large fluctuations from sample to sample and only in about 20% of them was $E(N)$ the lowest of the three energies. From these, the median value of $dn/d\mu$ was 0.06, but the scatter was large.

The isothermal susceptibility χ_T was calculated from Eq. (14) by using a modification of the Monte Carlo method described earlier. Instead of particle-hole transitions, single-particle transitions (i.e., bringing an extra particle or hole from infinity and adding it to a site) were made according to the algorithm of Metropolis *et al.*[24] Again, the systems were maintained electrically neutral by compensating background charges. Note that this method measures the susceptibility *in a restricted region of configuration space,* unlike the equilibrium value discussed above, and will therefore give different results for temperatures below that of a glass transition. At high temperatures, electrons can be added or removed at will so both susceptibilities tend to a Curie law, $1/4T$. At very low temperature, measuring χ_T involves adding an extra particle to the ground state and χ_T is therefore closely related to the single-particle densities of states $n_1(E)$ and $n_p(E)$. Both of these vanish at $E=\mu$, so presumably $\chi_T(T\to0)\to0$ unlike χ_μ.

The numerical results are shown in Fig. 13. At temperatures above 1.0, χ_T is described well by the Curie law, and its behavior changes below about 0.3. Unfortunately, very large differences between samples arise for temperatures much below this. The trouble is that the behavior is determined mainly by a few single-particle states whose energies lie closest to μ. Their density is low there, hence there are large differences between samples. The problem is exacerbated by the addition of the neutralizing charges, whose effect on the energy is to encourgage the addition of electrons or holes to the ground state. It is not possible to deduce from these results whether or not the isothermal susceptibility vanishes as the temperature is reduced to zero.

Parisi and Toulouse[30] have put forward the hypothesis for spin-glasses that for temperatures below that of the glass transition the entropy is a function only of the temperature and not of the magnetic field: $S(T,H)=S(T)$. Consequently the susceptibility should be independent of temperature in this region; this follows from a Maxwell relation and refers to the "equilibrium" susceptibility χ_μ. For the electronic model this means that $S(T,\mu)=S(T)$: The entropy is not a function of the chemical potential. The entropy at temperature T is given by

$$S(T,\mu)=S(0,\mu)+\int_0^T c_\mu(T',\mu)\,d\ln T' \; ,$$

so, for the hypothesis to hold in this system, it is necessary that both the zero-temperature entropy $S(0,\mu)$ and the specific heat $c_\mu(T,\mu)$ should be independent of μ. It was pointed out earlier that the Coulomb gap is pinned to μ and that its shape (close to μ) is independent of the degree of filling of the band and consequently of the value of μ. Provided that the excitations which give rise to the specific heat involve only single-particle states whose energies lie near the Coulomb gap, the specific heat should therefore not depend on the chemical potential. It is not so clear that this will also be true of the entropy at zero temperature, but numerically this was found to be very small, if not vanishing. Glasses are well known often to have nonvanishing entropies at zero temperature but there seems to be no reason why the value of this entropy should be independent of the chemical potential. It may well be only slowly varying, but it is not clear to what extent the Parisi-Toulose hypothesis will hold in the model system studied here.

VI. CONCLUSIONS

This computer simulation has confirmed that the Coulomb repulsion between the localized electrons causes a soft gap in the single-particle density of states whose form agrees well with theory[8] in three dimensions but is deeper than that predicted in two dimensions.[6,8] There is considerable clustering of sites of the same occupation with energies near the chemical potential. Although the Coulomb gap leads also to a depletion of long particle-hole excitations at low energies, there is a large density of short hops available whose transition energies are very small. The effects of these need more investigation; they may be important for ac conduction but not for dc because a continuous current-carrying path cannot be constructed from them. We have also demonstrated a gap for dressed single-particle excitations ("electronic polarons"), albeit a narrower one than that for the bare excitations. This may mean that they do not give rise to $T^{1/4}$ conductivity as had been suggested before[14] but there is as yet no satisfactory theory for electrical conduction by the hopping of interacting particles.

By extending the modeling to temperatures above 0 K, using the algorithm of Metropolis *et al.*,[24] we have found that the Coulomb gap fills in at a temperature of about 0.3 K. As an example, in silicon doped with donors at about 1% of the concentration at the metal-insulator transition, a typical Coulomb energy between nearby impurities is a few meV, so the Coulomb gap should be important at temperatures below about 10 K.

We have also used the close analogy between this model of interacting electrons and a spin-glass to examine the possibility of a "glass transition" among the electrons. There is some evidence that such a transition has occurred but it is not conclusive. What is needed is a divergence in a relaxation time or a susceptibility to provide an accurate signal of the glass-transition temperature. There is a scope for much future work here, both in theory and an experimental verification of the glassy state, possibly by cooling a sample in an electric field to drive it into a region of phase space from which it cannot return to thermal equilibrium when the field is removed. Theoretically there is also the puzzle of why, in a strongly interacting system, the specific heat and Edwards-Anderson order parameter resemble so closely those calculated for a noninteracting system whose densities of states are very different.

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*Present address.

[1] P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[2] B. L. Altshuler and A. G. Aronov, Solid State Commun. 30, 115 (1979).

[3] B. L. Altshuler, A. G. Aronov, and P. A. Lee, Phys. Rev. Lett. 44, 1288 (1980).

[4] M. Pollak, Discuss. Faraday Soc. 50, 13 (1970).

[5] G. Srinivasan, Phys. Rev. B 4, 2581 (1971).

[6] A. L. Efros and B. I. Shklovskii, J. Phys. C 8, L49 (1975).

[7] N. F. Mott, J. Non-Cryst. Solids 1, 1 (1968).

[8] A. L. Efros, J. Phys. C 9, 2021 (1976).

[9] S. D. Baranovskii, A. L. Efros, B. I. Gelmont, and B. I. Shklovskii, J. Phys. C 12, 1023 (1979).

[10] A. L. Efros, N. Van Lien, and B. I. Shklovskii, J. Phys. C 12, 1869 (1979).

[11] B. I. Shklovskii and A. L. Efros, Fiz. Tekh. Poluprovodn. 14, 825 (1980) [Sov. Phys.—Semicond. 14, 487 (1980)].

[12] S. D. Baranovskii, B. I. Shklovskii, and A. L. Efros, Zh. Eksp. Teor. Fiz. 78, 395 (1980) [Sov. Phys.-JETP 51, 199 (1980)].

[13] S. D. Baranovskii and A. L. Efros, Fiz. Tekh, Poluprovodn. 14, 2233 (1980) [Sov. Phys. Semicond. 14, 1323 (1980)].

[14] N. F. Mott, J. Phys. C 8, L239 (1975).

[15] M. Pollak, Proc. R. Soc. London, Ser. A325, 383 (1971).

[16] J. H. Davies, P. A. Lee, and T. M. Rice, Phys. Rev. Lett. 49, 758 (1982).

[17] A. L. Efros (private communication).

[18] C. J. Hearn, J. A. McInnes, and P. N. Butcher, J. Phys. C 15, 5013 (1982).

[19] M. Grünewald, B. Pohlmann, L. Schweitzer, and D. Würtz, J. Phys. C 15, L1153 (1982).

[20] N. F. Mott, Philos. Mag. 22, 2 (1970).

[21] B. I. Shklovskii and A. L. Efros, Zh. Eksp. Teor. Fiz. xx, xxx (19xx) [Sov. Phys.-JETP, 54, 218 (1981)].

[22] M. Pollak, Philos. Mag. B 42, 781 (1980).

[23] A. L. Efros (private communication).

[24] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).

[25] *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979).

[26] E. Pytte, Y. Imry, and D. Mukamel, Phys. Rev. Lett. 46, 1173 (1981).

[27] S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).

[28] I. Morgenstern, K. Binder, and R. M. Hornreich, Phys. Rev. B 23, 287 (1981).

[29] M. Grünewald, B. Pohlmann, L. Schweitzer, and D. Würtz (unpublished).

[30] G. Parisi and G. Toulouse, J. Phys. (Paris) Lett. 41, L261 (1980).