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Bethe–Peierls–Weiss approximation for the two- and three-dimensional Coulomb glass: zero-temperature and finite-temperature results

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Abstract. The Bethe–Peierls–Weiss approximation is applied to the Coulomb glass Hamiltonian in two and three dimensions. The single-particle density of states (DOS) at zero temperature is calculated analytically; it has a soft Coulomb gap at the Fermi energy. We rederive the self-consistent equation of Efros, but not the altered version given by Baranovskii, Efros, Gelmont and Shklovskii. The DOS is independent of the mean occupation number of the sites. These results are compared with recent numerical simulations of the model. The influence of finite temperatures on the DOS is discussed qualitatively. The Coulomb gap fills with increasing temperature T. For kT smaller than the gap width the DOS at the Fermi energy is proportional to kT^{D-1}.

1. Introduction

Disordered systems with interacting localized electronic states are complicated for theoretical investigations, and new results have been obtained only slowly since the first work on this problem (Pollak 1970, Srinivasan 1971). The long-range unscreened Coulomb interaction plays an essential role in such systems and the interplay between Coulomb repulsion and disorder gives rise to new and interesting properties. For example, the single-particle density of states (DOS) is drastically reduced near the chemical potential μ. At zero temperature it is expected that the DOS vanishes at the Fermi energy; it is, however, finite at every energy different from the Fermi energy. This soft gap is called the Coulomb gap.

Almost all theoretical investigations of disordered systems with localized states, in which the Coulomb interaction plays an important role, have been based on the so-called Coulomb glass model, which was first proposed by Efros and Shklovskii (1975) (for reviews, see also Efros and Shklovskii (1985), Pollak and Ortuno (1985) and Pollak (1992)). It consists of localized electrons at the sites of a regular lattice which interact via an unscreened Coulomb potential. Hopping between the sites is neglected. The disorder is described by a fluctuating potential at the lattice sites. The Coulomb glass is equivalent to an Ising model with long-range antiferromagnetic interactions in a fluctuating magnetic field (Davies *et al* 1982, 1984). Although all eigenstates of the system are known in principle, the search for the ground state and the calculation of thermodynamic properties are complicated many-body problems. Efros (1976) used the stability condition of the ground state against single-particle hops to derive a self-consistent equation (SCE) for the DOS at zero temperature (strictly speaking, an

equation for an upper bound of the DOS). Close to the Fermi energy ϵ_F this equation can be solved analytically. The resulting DOS $g(\epsilon)$ is asymptotically given by

$$g(\epsilon) = (D/2\pi)(|\epsilon - \epsilon_F|^{D-1}/U_0^D) \qquad (\epsilon \to 0) \tag{1}$$

for the D-dimensional system ($D = 2, 3$). Here U_0 denotes the characteristic interaction energy between the electrons. Later, Baranovskii *et al* (1979) altered the result by a factor of 2, yielding

$$g(\epsilon) = (D/\pi)(|\epsilon - \epsilon_F|^{D-1}/U_0^D) \qquad (\epsilon \to 0). \tag{2}$$

Raikh and Efros (1987) applied the SCE method to the one-dimensional Coulomb glass and obtained a logarithmic energy dependence of the DOS. Recently, Mogilyanskii and Raikh (1989) and Hunt (1990) derived SCE-type equations for the Coulomb glass at finite temperatures. Their results show that the Coulomb gap fills with increasing temperature. Vojta and John (1993) applied the Bethe–Peierls–Weiss (BPW) approximation to the one-dimensional Coulomb glass and calculated an upper and a lower bound for the DOS at zero temperature. Besides these analytic approaches there are several numerical simulations of the Coulomb glass. They are either based on the Monte Carlo type of algorithm (Baranovskii *et al* 1979, Davies *et al* 1982, 1984, Efros and Shklovskii 1987, Möbius and Richter 1987a, b, Tenelsen and Schreiber 1992, Möbius *et al* 1992, Schreiber and Tenelsen 1993) or based on the solution of local mean-field equations (Grünewald *et al* 1982, 1983). While the simulation results confirm the idea of a Coulomb gap in the DOS, the exact behaviour of the DOS in the Coulomb gap regime remains a puzzle.

In this paper we generalize the BPW approach of the previous paper (Vojta and John 1993) with regard to three aspects. First we consider higher spatial dimensions, second we extend the calculations to mean occupation numbers different from $\frac{1}{2}$ (i.e. we consider non-half-filled bands), and third we discuss the influence of finite temperatures on the DOS. The paper is organized as follows. In section 2 we introduce the Coulomb glass model and generalize the main ideas of the BPW approach to the Coulomb glass to filling factors different from $\frac{1}{2}$. The results for the single-particle DOS at zero temperature are given in section 3. In section 4 the finite-temperature results are presented.

2. The Coulomb glass model

We consider a simple square or cubic lattice with a lattice constant a and $N = L^D$ lattice sites ($D = 2, 3$). The sites are occupied by NK ($0 < K < 1$) electrons with the charge $-e$. To preserve charge neutrality each site has a compensating charge Ke. The Hamiltonian of the Coulomb glass in the grand canonical ensemble is given by

$$H = \sum_i (\varphi_i - \mu) n_i + \tfrac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij} \qquad U_{ij} = e^2/r_{ij} \tag{3}$$

where the variable n_i (which may have the values 0 or 1) describes the occupation of the site i and r_{ij} denotes the distance between sites i and j. The parameter K and the chemical potential μ cannot be chosen independently. In the following we shall use K as the free parameter which fixes the mean occupation number; μ has to be calculated from K. In the case $K = \frac{1}{2}$ the model is particle–hole symmetric so that $\mu = 0$. The random potentials φ_i are independent of each other; they fluctuate according to a probability distribution $W(\varphi_i)$.

The properties of the Coulomb gap do not depend on the exact form of this distribution, provided that it is slowly varying near the chemical potential μ. Without loss of generality we can therefore use the probability distribution

$$W(\varphi_i) = \begin{cases} 1/2W_0 & |\varphi_i| < W_0 \\ 0 & |\varphi_i| > W_0. \end{cases} \tag{4}$$

The width W_0 of this box distribution is assumed to be large compared with the interaction energy $U_0 = e^2/a$ between nearest neighbours. The single-particle excitation energy ϵ_i (which corresponds to adding or removing an electron from the system, leaving the occupation of the other sites unchanged) is defined by

$$\epsilon_i = \varphi_i - \mu + \sum_j (n_j - K)U_{ij}. \tag{5}$$

Because of the interaction terms in equation (5) the excitation energy depends very sensitively on the occupation of all sites of the system. The DOS for the single-particle excitations given by

$$g(\epsilon) = \int \mathrm{d}\varphi_1 \ldots \int \mathrm{d}\varphi_N \prod_j W(\varphi_j) \frac{1}{N} \sum_i \langle \delta(\epsilon - \epsilon_i) \rangle \tag{6}$$

is the quantity under consideration in this paper. $\langle \cdot \rangle$ denotes the thermodynamic average for a given configuration of the random potentials. $g(\epsilon)$ is symmetric with respect to the Fermi energy $\epsilon_F = 0$ for $K = \frac{1}{2}$.

We now generalize the BPW approach to the Coulomb glass system given by Vojta and John (1993) to filling factors different from $\frac{1}{2}$. The BPW approximation (Bethe 1935, Peierls 1936) is an improvement of the simple mean-field approximation. The main idea is to treat the interactions between one 'central' site and all other sites (boundary sites) exactly, but to include the interactions between these boundary sites by means of effective fields. An additional self-consistency procedure for the effective fields has to ensure that all sites are physically equivalent. The BPW Hamiltonian of the Coulomb glass is given by

$$H_{\mathrm{BPW}} = (\varphi_0 - \mu)n_0 + \sum_{i \neq 0} (n_0 - K)(n_i - K)U_{0i} + \sum_{i \neq 0} (n_i - K)\xi_i \tag{7}$$

with the effective fields

$$\xi_i = \varphi_i - \mu + \sum_{j \neq 0, i} \langle n_j - K \rangle_i U_{ij}. \tag{8}$$

Here $\langle \cdot \rangle_i$ denotes the conditional thermodynamic average for a fixed occupation of site i. The corresponding partition function Z may be calculated by means of the stochastic map method (Rujan 1978, Bruinsma and Aeppli 1983). Within this method the summations over the boundary sites are carried out and the arising terms can be rewritten as exponentials:

$$Z = \sum_{n_0 = 0,1} \exp\left\{ -\beta \left[\left(\varphi_0 - \mu + \sum_{i \neq 0} A(\xi_i, U_{0i}) \right)(n_0 - K) + \sum_{i \neq 0} B(\xi_i, U_{0i}) \right] \right\}. \tag{9}$$

The functions $A(\xi, U)$ and $B(\xi, U)$ are given by

$$\beta A(\xi, U) = \ln\{\exp[\beta K(\xi - KU)] + \exp[\beta(K-1)(\xi - KU)]\} - \ln[\![\exp\{\beta K[\xi - (K-1)U]\} + \exp\{\beta(K-1)[\xi - (K-1)U]\}]\!]$$

$$\beta B(\xi, U) = (K-1)\ln\{\exp[\beta K(\xi - KU)] + \exp[\beta(K-1)(\xi - KU)]\} - K\ln[\![\exp\{\beta K[\xi - (K-1)U]\} + \exp\{\beta(K-1)[\xi - (K-1)U]\}]\!]. \quad (10)$$

The function $A(\xi, U)$ describes the contribution of the boundary sites to the thermodynamic local field h_0 of the central site. The local field h_0 is defined by $\langle n_0\rangle = 1/[1 + \exp(\beta h_0)]$. Comparing this with the partition function Z from (9) one obtains

$$h_0 = \varphi_0 - \mu + \sum_{i\neq 0} A(\xi_i, U_{0i}). \quad (11)$$

The values of $A(\xi, U)$ are of the order of U_0 and the Coulomb correlations limit the contribution of all $A(\xi, U)$ to a value of the order of the Madelung energy of the lattice. In the case $U_0 \ll W_0$ the thermodynamic local field is essentially determined by the random potential φ_0. We now consider different realizations of the random potential for all lattice sites and study the distribution $g_{\rm th}$ of the thermodynamic field h_0. Since φ_0 and $A(\xi_i, U_{0i})$ are statistically independent, the distribution $g_{\rm th}(h_0)$ is simply a slightly modified box distribution. To calculate the single-particle energy ϵ_0 we also need the conditional averages of the occupation numbers of the boundary sites for a fixed value of n_0 which are given by

$$\langle n_i\rangle_0 = 1/[\![1 + \exp\{\beta[\xi_i + (n_0 - K)U_{0i}]\}]\!]. \quad (12)$$

To complete the BPW approach we have to define a self-consistency condition for the effective fields which ensures that all sites of the model are physically equivalent. Since we deal with a random system the self-consistency condition has to be formulated for the distribution of the effective fields instead for the effective fields themselves. Within the BPW approach a unique way to define the self-consistency condition does not exist. However, there are two reasonable choices. On the one hand, one can identify $\xi_i + A(\varphi_0 + \sum_j A(\xi_j, U_{0j}), U_{0i})$ with the thermodynamic field of the site i. In this case the distribution $P(\xi)$ of the effective fields should be similar to $g_{\rm th}$. On the other hand, one can identify $\xi_i + (n_0 - K)U_{0i}$ with the single-particle energy of site i. In this case the distribution $P(\xi)$ of the effective fields is given by

$$P(\xi_i) = g(\xi_i + (n_0 - K)U_{0i}). \quad (13)$$

The consequences of the particular choice of a self-consistency condition for the results are discussed in the following section.

3. Single-particle density of states

In this section we discuss the zero-temperature DOS. To do this we first express the single-particle energy ϵ_0 in terms of the thermodynamic field h_0:

$$\epsilon_0 = h_0 + \sum_{i\neq 0} C(\xi_i, U_{0i}, n_0) \quad (14)$$

where the function C is given by

$$C(\xi_i, U_{0i}, n_0) = (n_i - K)U_{0i} - A(\xi_i, U_{0i}). \tag{15}$$

We now study the behaviour of the function $A(\xi_i, U_{0i})$ and the occupation number n_i for zero temperature and obtain (see also figure 1)

$$A(\xi, U) = \begin{cases} -KU & \xi > KU \\ -\xi & KU > \xi > (K-1)U \\ -(K-1)U & (K-1)U > \xi \end{cases}$$
$$(n-K)U = \begin{cases} -KU & \xi > (K-n_0)U \\ -(K-1)U & (K-n_0)U > \xi. \end{cases} \tag{16}$$

Inserting these results into equation (15) we get the zero-temperature behaviour (see also figure 2)

$$\left.\begin{aligned} C(\xi, U, 1) &= \xi - KU \\ C(\xi, U, 0) &= \xi - (K-1)U \end{aligned}\right\} \qquad KU > \xi > (K-1)U$$
$$C(\xi, U, n_0) = 0 \qquad \text{otherwise.} \tag{17}$$

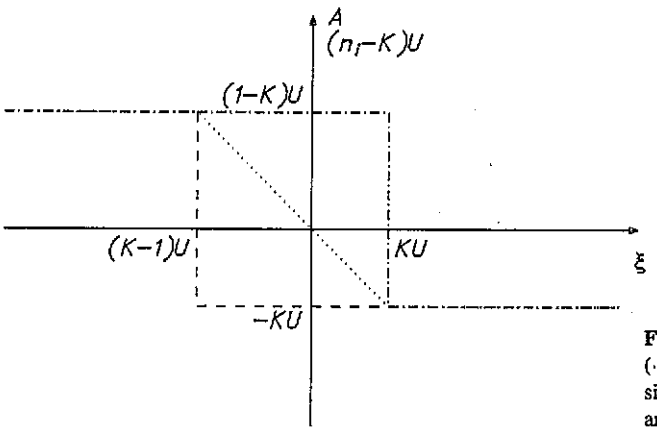

Figure 1. Stochastic map $A(\xi, U)$ (·····) and occupation n_i of a boundary site at zero temperature for $n_0 = 1$ (- - - -) and $n_0 = 0$ (— · —).

In the case of a small interaction energy $U_0 \ll W_0$, correlations between h_0 and ξ_i as well as correlations between different ξ_i are negligible within the calculation of the DOS (6) (for a detailed discussion, see Vojta and John (1993)). For energies $\epsilon \ll U_0$ (within the Coulomb gap) the DOS may be written in the form of a convolution integral:

$$g(\epsilon) = g_{\text{th}}(0) \int_0^{|\epsilon|} \mathrm{d}x \int \mathrm{d}\xi_1 \ldots \int \mathrm{d}\xi_{N-1} \prod_j P(\xi_j)\delta\Big(x \mp \sum_i C(\xi_i, U_{0i}, n_0)\Big) \tag{18}$$

where the upper sign in the δ function corresponds to $n_0 = 0$ and $\epsilon > 0$, whereas the lower sign corresponds to $n_0 = 1$ and $\epsilon < 0$. In the one-dimensional case both of the self-consistency conditions discussed at the end of section 2 can be used to calculate the DOS $g(\epsilon)$. The results constitute in some sense an upper and a lower bound for the DOS.

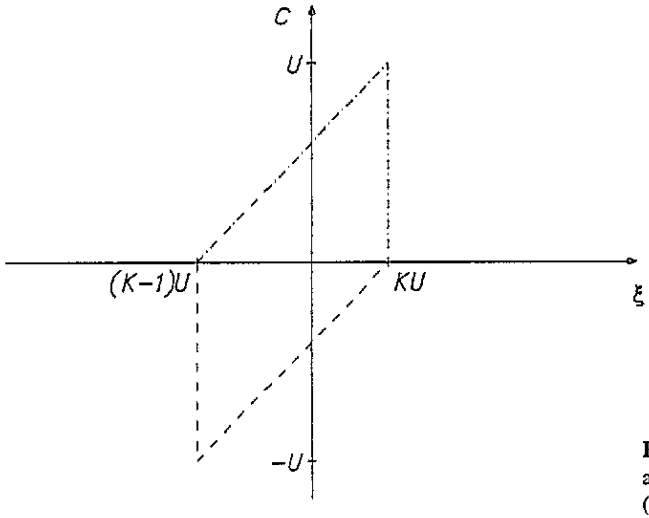

Figure 2. $C(\xi, U, n_0)$ at zero temperature for $n_0 = 1$ (- - - -) and $n_0 = 0$ (— · —).

For the two- and three-dimensional models the condition $P(\xi) \sim g_{\rm th}(\xi)$ yields a gap width which diverges with increasing size N of the system. Consequently, the lower bound of the DOS (which was provided by $P(\xi) \sim g_{\rm th}(\xi)$ in the one-dimensional case) cannot be calculated for the two- and three-dimensional models. In the following we shall use the self-consistency condition (13) which relates the distribution of the effective fields to the DOS.

We first discuss the DOS for $n_0 = 0$ which implies that $h_0 > 0$ and (since the values of $C(\xi, U, 0)$ are positive) $\epsilon_0 > 0$. Owing to the δ function in (18) there is no contribution to $g(\epsilon)$, if $\sum_i C(\xi_i, U_{0i}, 0)$ is larger than ϵ. Taking into account the cases in which already a single $C(\xi, U, 0)$ exceeds ϵ, one obtains an upper bound for the DOS. Using equation (13) to calculate the probability that $C(\xi, U, 0)$ exceeds ϵ we obtain

$$g(\epsilon) = g_{\rm th}(0) \exp\left(-\sum_i \Theta(U_{0i} - \epsilon) \int_{\epsilon - U_0}^{0} {\rm d}\epsilon' \, g(\epsilon') \right) \tag{19}$$

where Θ denotes the Heavyside function. This formula does not contain the mean occupation number K. Consequently, for energies $\epsilon \ll U_0$ the DOS is independent of K and therefore symmetric with respect to the Fermi energy. We now transform the sum over the lattice sites into an integral over the interaction energy U (see appendix 1) and interchange the order of the U and ϵ integrations. The asymptotic behaviour of $g(\epsilon)$ for $\epsilon \ll U_0$ is determined by the integral equation

$$g(\epsilon) = g_{\rm th}(0) \exp\left[-\frac{a_D}{D} \int_0^{U_0} {\rm d}\epsilon' \, g(\epsilon') \left(\frac{U_0}{|\epsilon| + \epsilon'} \right)^D \right] \tag{20}$$

with $a_2 = 2\pi$ and $a_3 = 4\pi$. This is exactly the original version of the SCE of Efros (1976), except for the upper bound of the ϵ' integration. This bound does not influence the asymptotic behaviour of the DOS for $\epsilon \to 0$, which can be obtained from the solution of equation (20) as

$$g(\epsilon) = (D/2\pi)(|\epsilon|^{D-1}/U_0^D) + {\rm O}(\epsilon^D) \qquad (D = 2, 3). \tag{21}$$

So far we have calculated the asymptotic behaviour of an upper limit of the DOS. We now show that the upper bound (21) yields the exact asymptotic behaviour of the DOS within

the BPW approach with the self-consistency condition (13). To do this, we use (13) and (21) to calculate the distribution $P(\xi)$ on the right-hand side of the convolution integral (18). Details of the calculation are presented in appendix 2. The resulting DOS $g(\epsilon)$ on the left-hand side has the correct asymptotic behaviour.

Efros (1976) obtained the SCE using the stability condition of the ground state against one-particle hops. Within that approach, one considers an electron hopping from an occupied site i ($\epsilon_i < 0$) to an unoccupied site j ($\epsilon_j > 0$). If the system is in the ground state, the change Δ_{ij} of the system energy has to be positive for all possible hops, i.e.

$$\Delta_{ij} = \epsilon_j - \epsilon_i - U_0/r_{ij} > 0. \tag{22}$$

This condition prohibits that two sites i and j with a distance r can have energies within an interval U_0/r around the Fermi energy. Summing up the corresponding probabilities leads directly to the SCE (20). Later Baranovskii *et al* (1979) claimed a correction of the exponent in (20) by a factor of $\frac{1}{2}$ because of a supposed error in the original derivation. They argued that the inequality (22) was taken into account twice for every pair i, j in the original derivation. The altered SCE yields a DOS which is twice the original result. However, the reasons for the modification of Baranovskii *et al* (1979) are not quite compelling and possibly it has to be questioned again whether the original or the altered version of the SCE is valid. To compare our calculated DOS with that of the altered SCE and with recent numerical simulation data of Möbius *et al* (1992) we have plotted the DOS for two and three dimensions in figures 3 and 4. Although the simulation was performed for parameters W_0 for which our BPW approximation cannot be expected to be very good, our DOS and the simulation data are in satisfactory agreement. The simulation, however, yields a stronger decrease in the DOS near the Fermi energy. This could be a result of the correlations between the boundary sites which are neglected within the BPW approach. Consequently it cannot be decided from the simulation data which of the self-consistent equations is correct, because neither equation reproduces the asymptotics of the numerical data.

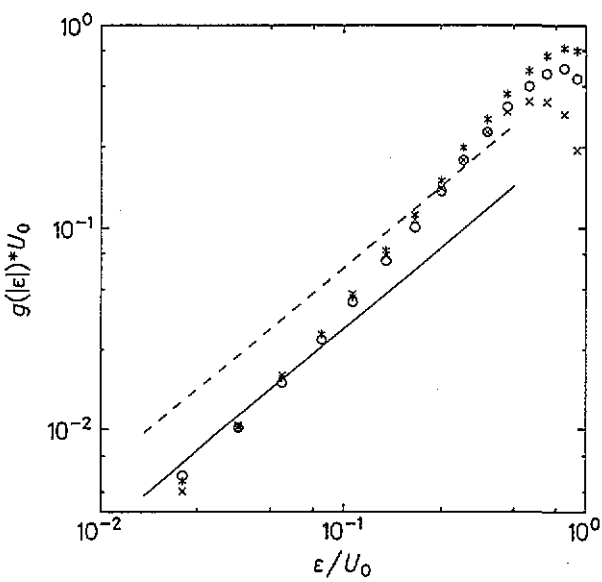

Figure 3. Single-particle DOS for the 2D system from the BPW approximation (21) (——), from the altered SCE (- - - -), and from simulation for $W_0 = 0.5$, $K = 0.5$ (O) and for $W_0 = 0.5$, $K = 0.3$, $\epsilon > 0$ (+) and $\epsilon < 0$ (*).

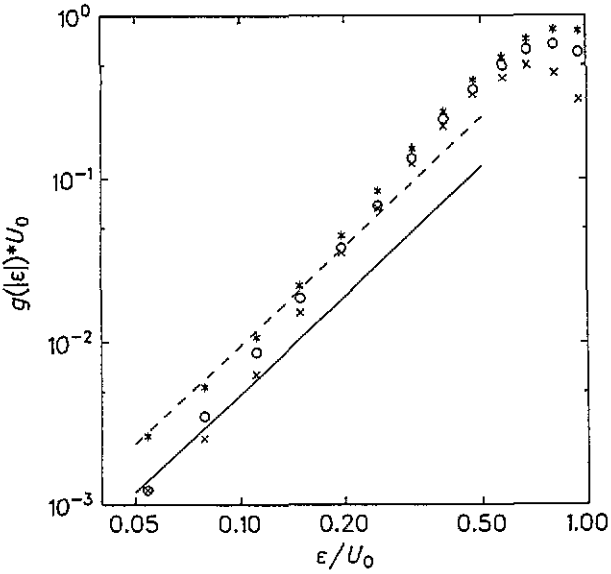

Figure 4. Single-particle DOS for the 3D system from the BPW approximation (21) (——), from the altered SCE (- - - -), and from simulation for $W_0 = 0.5$, $K = 0.5$ (O) and for $W_0 = 0.5$, $K = 0.3$, $\epsilon > 0$ (+) and $\epsilon < 0$ (*).

4. Finite-temperature results

In this section we study the effects of finite temperatures on the DOS. Within the BPW approach we have to distinguish two kinds of excitation. On the one hand, the occupation of the central site may change owing to thermal fluctuations. In this case the occupation of some of the boundary sites, in particular those with small ξ_i, will relax to minimize the energy, taking the new occupation of the central site into account. On the other hand, the occupations of the boundary sites may change owing to thermal fluctuations. In the following we shall qualitatively discuss the influence of these excitations on the DOS. The treatment is restricted to low temperatures $kT \ll U_0$.

To include the influence of thermal fluctuations of the occupation number of the central site, we have to start with a generalized form of the convolution integral (18) for the temperature-dependent DOS:

$$g_1(\epsilon, T) = \sum_{n_0} \int \mathrm{d}h\, g_{\mathrm{th}}(h) \frac{\exp(-\beta h n_0)}{1+\exp(-\beta h)} \times \int \mathrm{d}\xi_1 \ldots \int \mathrm{d}\xi_{N-1} \prod_j P(\xi_j)\delta\Big(\epsilon - h - \sum_i C(\xi_i, U_{0i}, n_0)\Big). \tag{23}$$

After partial integration it may be transformed into a convolution of the zero-temperature DOS and the derivative of the Fermi-distribution function:

$$g_1(\epsilon, T) = -\int \mathrm{d}h\, f'(\epsilon - h) g(h) \tag{24}$$

where

$$f'(x) = (\mathrm{d}/\mathrm{d}x)\{1/[1+\exp(\beta x)]\}. \tag{25}$$

For low temperatures, $-f'(x)$ has a sharp peak with a width of the order of kT at $x = 0$. This means that $g_1(\epsilon, T)$ is approximately given by an average of the zero-temperature DOS over an interval of the width of kT around ϵ.

We shall now discuss how thermal fluctuations of the occupation numbers of the boundary sites influence the DOS. The probability that the occupation number of the boundary site i changes is given by the Fermi function. The total number of sites with a changed occupation number may be estimated from

$$N_C \sim N \int \mathrm{d}\epsilon\, g(\epsilon) \frac{1}{1+\exp(\beta|\epsilon|)} \sim (kT)^D. \tag{26}$$

The contribution of these sites to the single-particle energy of the central site is, of course, a random quantity. To estimate the width of its distribution, one has to take into account the correlations between the boundary sites; otherwise one obtains a diverging width in the thermodynamic limit $N \to \infty$. The correlations limit the contribution of the boundary sites with changed occupation number to the single-particle energy of the central site. The resulting value is of the order of the Madelung energy of these sites which is of the order of kT for all dimensions. Because changes in the occupation numbers of the boundary sites are independent of ϵ_0, the DOS is a convolution of the DOS from equation (24) and a distribution of width kT. In summary we can write

$$g(\epsilon, T) = \int \mathrm{d}\epsilon'\, g(\epsilon - \epsilon') \frac{1}{kT} w\left(\frac{\epsilon'}{kT}\right) \tag{27}$$

where w, which comprises the effects of both kinds of excitation, depends only on the ratio ϵ/kT. For small temperatures, the function $w(\epsilon/kT)$ has a sharp peak with a width of the order of kT at $\epsilon = 0$. Therefore the temperature-dependent DOS $g(\epsilon, T)$ is approximately given by an average of the zero-temperature DOS over an interval with a width of kT around ϵ. Consequently, the DOS remains nearly unchanged for energies $\epsilon \gg kT$. The DOS at the chemical potential, however, increases with increasing temperature according to

$$g(\mu, T) \sim (kT)^{D-1} \tag{28}$$

which is easily obtained if one inserts the asymptotic behaviour (21) into equation (27).

5. Conclusion

In this paper we have calculated the asymptotic behaviour of the single-particle DOS for the Coulomb glass model in two and three dimensions for energies close to the Fermi energy. For zero temperature we have rederived the original version of the SCE of Efros (1976) on the basis of the BPW approximation of the Coulomb glass Hamiltonian. Close to the Fermi energy the SCE may be solved analytically. Since this equation does not contain the mean occupation number K, the resulting DOS is independent of K and symmetric with respect to the Fermi energy. We obtain $g(\epsilon) = D|\epsilon - \epsilon_F|^{D-1}/2\pi U_0^D$ for the D-dimensional system ($D = 2, 3$). Our result differs by a factor of 2 from the altered version of the SCE of Baranovskii *et al* (1979). The modification was based on the argument that the original derivation seemed to consider every stability condition twice and therefore seemed to underestimate the DOS. The origin of this alteration is not quite obvious and we think it should be questioned again in view of the results of the present paper.

We have compared our calculated DOS with recent numerical simulation data of Möbius *et al* (1992). The BPW results are in satisfactory agreement with the simulation data; the simulation, however, yields a stronger decrease in the DOS near the Fermi energy. The

difference between the DOS from the BPW approximation and the simulation data possibly stems from the mean-field character of the BPW scheme which neglects correlations between the boundary sites.

We have qualitatively discussed the influence of finite temperatures on the DOS. For $kT \ll U_0$ the temperature-dependent DOS $g(\epsilon, T)$ may be written as a convolution of the zero-temperature DOS $g(\epsilon)$ and a function $w(\epsilon/kT)/kT$ which describes the influence of the excitations from the ground state. The DOS remains nearly unchanged for $\epsilon \gg kT$. For energies lower than kT, however, the Coulomb gap is filled. The DOS at the chemical potential behaves as $g(\mu, T) \sim (kT)^{D-1}$ where D is the dimensionality of the system.

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Appendix 1. Transformation of the lattice sum into an integral over U

In order to transform the sum over the lattice sites i in equation (19) into an integral over the interaction energy U we consider the number $\mathrm{d}N$ of lattice sites with distances between r and $r + \mathrm{d}r$ from the origin:

$$\mathrm{d}N = a_D r^{D-1}\,\mathrm{d}r \tag{A1.1}$$

where $a_2 = 2\pi$ and $a_3 = 4\pi$. This is used to transform the sum into an integral over r. Since the interaction energy depends only on r, we may transform the r integral into an integral over U. Consequently we obtain

$$\sum_{i\neq 0} \ldots \to a_D \int_a^{\infty} \mathrm{d}r\, r^{D-1} \ldots \to \int_{U_0}^{0} \mathrm{d}U \frac{a_D}{D} \frac{\mathrm{d}(r^D)}{\mathrm{d}U} \ldots . \tag{A1.2}$$

For the Coulomb interaction we have $U = U_0/r$ and the final result is given by

$$\sum_{i} \ldots \to \int_0^{U_0} \mathrm{d}U \frac{a_D U_0^D}{U^{D+1}} \ldots . \tag{A1.3}$$

To be precise, we note that the lower bound of the integration depends on N in a finite system; it tends to zero with N going to infinity. The transformation from the sum over the lattice sites to the integral over U is correct for small U (i.e. for sites far away from the origin). Obviously the transformation is not exact for large U (i.e. if sites close to the origin have to be taken into account). However, the properties of the Coulomb gap are determined by the long-range tail of the Coulomb interaction and the error close to the origin does not affect the gap.

Appendix 2. Asymptotic behaviour of the DOS

In order to show that equation (21) yields the correct asymptotic behaviour of the DOS within the BPW approach to the Coulomb glass, we apply the Laplace transformation to the integral equation (18). It is known from the theory of Laplace transformations that

$$g(\epsilon) = \int_0^{\epsilon} \mathrm{d}\epsilon'\, g'(\epsilon') = \lim_{s\to\infty} \left(\sum_{k=1}^{\infty} \frac{(-1)^k}{k!} f(ks) \exp(ks\epsilon) \right) \tag{A2.1}$$

where $f(s)$ is the Laplace transform of $g'(\epsilon)$:

$$f(s) = \int_0^{\infty} \mathrm{d}\epsilon\, g'(\epsilon) \exp(-s\epsilon) = g_{\mathrm{th}}(0) \prod_i \left(\int \mathrm{d}\xi_i\, P(\xi_i) \exp[-sC(\xi_i, U_{0i}, 0)] \right). \tag{A2.2}$$

Because of the limit $s \to \infty$ in equation (A2.1), $g(\epsilon)$ is determined only by the asymptotic behaviour of $f(s)$. Using the self-consistency condition (13) and the transformation from the sum over the lattice sites to the integral over the interaction energy U, the Laplace transform $f(s)$ may be written as

$$f(s) = g_{\mathrm{th}}(0) \exp\left(a_D U_0^D \int_0^{U_0} \frac{\mathrm{d}U}{U^{D+1}} \int_0^{U} \mathrm{d}\epsilon'\, g(\epsilon') \{\exp[s(\epsilon' - U)] - 1\} \right). \tag{A2.3}$$

If one now inserts the asymptotic behaviour (21) into this expression, the integrals may be directly calculated. The leading term in the asymptotic behaviour of $g(\epsilon')$ determines the general behaviour of $f(s)$ for $s \to \infty$:

$$f(s) = (1/(sU)^{D-1}) \times \text{constant}. \tag{A2.4}$$

Using equation (A2.1) to transform back, we obtain

$$g(\epsilon) = (|\epsilon|^{D-1}/U_0^D) \times \text{constant} \tag{A2.5}$$

where the proportionality factor is determined by the second term in the asymptotic behaviour (21) of $g(\epsilon')$. This correction term has to be chosen in such a way that it provides the correct pre-factor because this pre-factor in turn determines the power of $|\epsilon|$ in the leading term. This interdependence corresponds to the strange 'stabilizing mechanism' that renders the DOS calculated from Efros' SCE independent of the disorder strength W_0.

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