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Coulomb gap at finite temperatures

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The Coulomb glass, a model of interacting localized electrons in a random potential, exhibits a soft gap, the Coulomb gap, in the single-particle density of states (DOS) $g(\varepsilon,T)$ close to the chemical potential μ. In this paper we investigate the Coulomb gap at finite temperatures T by means of a Monte Carlo method. We find that the Coulomb gap fills with increasing temperature. In contrast to previous results the temperature dependence is, however, much stronger than $g(\mu,T)\sim T^{D-1}$ as predicted analytically. It can be described by power laws with the exponents 1.75 ± 0.1 for the two-dimensional model and 2.7 ± 0.1 for the three-dimensional model. Nevertheless, the relation $g(\mu,T)\sim g(\varepsilon,T=0)$ with $|\varepsilon-\mu|=k_BT$ seems to be valid, since energy dependence of the DOS at low temperatures has also been found to follow power laws with these exponents.

The Coulomb glass model of interacting localized electrons in a random potential has been extensively studied within the last 20 years.[1–5] One of the striking properties of this model is the existence of an interaction-induced soft gap, the so-called Coulomb gap, in the single-particle density of states (DOS) at the chemical potential μ. This means that the low-temperature DOS decreases towards μ, but vanishes exactly only at the temperature $T=0$ and the energy $\varepsilon=\mu$. Based on the stability conditions of the ground state against one-particle hops Efros and Shklovskii[2] developed a self-consistent equation (SCE) and predicted that the zero-temperature single-particle DOS $g(\varepsilon,T=0)$ in the Coulomb gap follows a universal power law $g(\varepsilon,0)\sim|\varepsilon-\mu|^{D-1}$, where D is the spatial dimension. The same behavior was recently obtained by means of a Bethe-Peierls-Weiss (BPW) approximation.[6,7] However, in some work an exponential gap has been predicted instead of the power law.[8–11] Several numerical simulations were carried out to determine the DOS and to check the analytical predictions.[12–16] Most of the results agree qualitatively with the power-law suggestions; more recent simulations for larger systems[14–16] yield, however, a slightly stronger decrease of the DOS in the Coulomb gap than $g(\varepsilon,0)\sim|\varepsilon-\mu|^{D-1}$. Consequently, the question whether Efros' prediction is universally valid has not been answered definitely.

Most of the work mentioned above was dedicated to the zero-temperature behavior of the Coulomb gap. In the case of finite temperatures the situation is even less clear. One of the quantities studied is the finite-temperature single-particle DOS $g(\varepsilon,T)$, which determines the transport properties at intermediate temperatures.[17] Besides, if measured directly[18] the DOS can give valuable information on the validity of the model since its interpretation is much simpler than that of transport properties, where additional theoretical assumptions have to be incorporated. According to the analytical theories[7,19] the finite-temperature DOS at the chemical potential is proportional to the zero-temperature DOS at an energy k_BT away from the Fermi energy, i.e., $g(\mu,T)\sim g(\varepsilon,T=0)$ with $|\varepsilon-\mu|=k_BT$. Consequently, the SCE method[2,8] and the BPW approximation[7] predict $g(\mu,T)\sim T^{D-1}$. If one accepts, however, the stronger decrease of the DOS in the zero-temperature Coulomb gap found in the more recent simulations,[14–16] one should expect a stronger dependence of $g(\mu,T)$ on temperature, too. The numerical simulations do not provide any definite answer; several results[16,20] confirm the analytical result $g(\mu,T)\sim T^{D-1}$, even in the case[16] when the zero-temperature DOS shows a stronger energy dependence than $|\varepsilon-\varepsilon_F|^{D-1}$. In a three-dimensional (3D) system with site (i.e., structural) disorder but no energy disorder Grannan and Yu[21] found $g(\mu,T)\sim T$, which is considerably weaker than the analytical prediction. On the other hand, very recently an exponential behavior was suggested in the case of a weak random potential and no site disorder,[22] which constitutes a much stronger decrease than the power laws discussed above. In summary, we are far from having a coherent picture of the temperature dependence of the Coulomb gap. In the present study we therefore want to provide accurate numerical data for the single-particle DOS of the Coulomb glass at finite temperatures which allow us to perform a detailed analysis of its behavior.

Our study is based on the lattice model of the Coulomb glass[2] which consists of $N/2$ strongly localized electrons on the $N=L^D$ sites on a hypercubic lattice. The electrons interact via an unscreened Coulomb potential. Quantum hopping terms (i.e., transfer matrix elements) between the sites are completely neglected, because the electrons are considered to be strongly localized. The disorder is described by a fluctuating potential at the lattice sites. The Hamiltonian of the model is given by

$$H=\sum_i \varphi_i n_i+\frac{1}{2}\sum_{i\neq j}\frac{1}{r_{ij}}(n_i-1/2)(n_j-1/2), \qquad (1)$$

where the variable n_i with the values 0 or 1 describes the occupation of the site i and r_{ij} denotes the distance between sites i and j. The random potentials φ_i are independent ran-

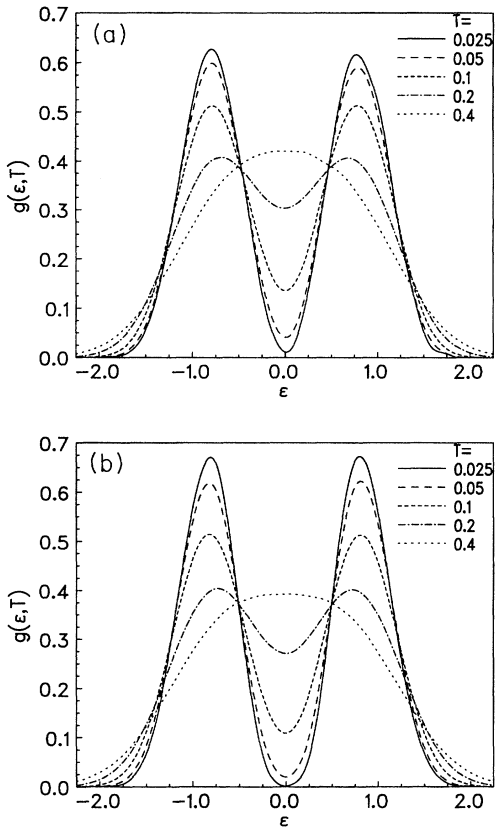

FIG. 1. Temperature-dependent single-particle DOS $g(\varepsilon,T)$ of a 2D system with 36^2 sites (a) and of a 3D system with 14^3 sites (b).

dom variables with the probability distribution $W(\varphi_i)$ which we choose as a box distribution

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

Since this distribution is symmetric with respect to $\varphi_i=0$ and each site has been given the compensating charge 1/2 in the interaction terms in Eq. (1), the model defined by Eqs. (1) and (2) is particle-hole symmetric and the chemical potential is therefore given by $\mu=0$ for all temperatures. In this paper we use $W_0=1/2$ for all calculations as it was done in most of the numerical work before. This means disorder and interaction strength have the same order of magnitude. The single-particle excitation energy ε_i (which corresponds to adding one electron to the system, leaving the occupation of the other sites unchanged) is defined as usual by

$$\varepsilon_i=\varphi_i+\sum_j (n_j-1/2)/r_{ij}. \tag{3}$$

Because of the interaction terms the excitation energy in Eq. (3) depends very sensitively on the occupation of all sites of the system. The DOS for these single-particle excitations

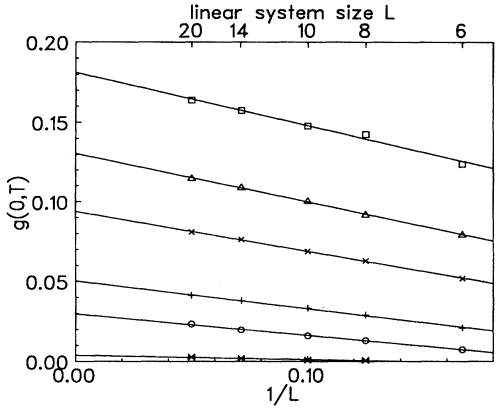

FIG. 2. Extrapolation of the DOS at the chemical potential in the 3D system to infinite system size $L=\infty$ for different temperatures $T=0.125$ (□), 0.1 (△), 0.0833 (×), 0.0625 (+), 0.05 (○) and 0.025 (⋈).

$$g(\varepsilon,T)=\int_{-\infty}^{\infty}d\varphi_i\cdots\int_{-\infty}^{\infty}d\varphi_N\prod_j W(\varphi_j)\frac{1}{N}\sum_i \langle\delta(\varepsilon-\varepsilon_i)\rangle \tag{4}$$

is the quantity under consideration in this paper. $\langle\cdot\rangle$ denotes the thermodynamic average for a given configuration of the random potentials. We note that in this definition the excitation energies are averaged thermally (and with respect to disorder) over configurations of the many-particle system. The DOS is *not* calculated from the thermally averaged occupation numbers as in a mean-field-like approximation.[13] Since the model is particle-hole symmetric, $g(\varepsilon,T)$ is symmetric with respect to the chemical potential $\mu=0$.

Our computation of the DOS is based on the Monte Carlo investigation,[23,24] which has been used to determine the thermodynamic properties and the many-particle states of the Coulomb glass. We have performed the respective Metropolis procedure for 2D and 3D systems at temperatures from 0.025 up to 0.4 in units of the interaction energy between nearest neighbors. To study the system-size dependence we have investigated different lattices with $N=6^3$ to 20^3 sites in 3D and with $N=16^2$ to 50^2 sites in 2D, applying periodic boundary conditions. Each Monte Carlo run starts with an equilibration procedure. Then the single-particle DOS is measured several times (from 5000 for the smallest system to 500 for the largest) by calculating all single-particle energies [Eq. (3)]. The measurements are separated by 80 to 600 Monte Carlo sweeps (i.e., $40N$ to $300N$ Monte Carlo steps), depending on temperature, to keep subsequent configurations uncorrelated. By the Metropolis algorithm we have automatically performed an importance sampling according to the Boltzmann distribution, so that the thermal average of the DOS is simply given by the arithmetic average over all measurements of the Monte Carlo run. To reduce the statistical error we have additionally averaged over the results from seven different configurations of the random potential.

A survey of our results is displayed in Fig. 1(a) for a 2D system with 36^2 sites and in Fig. 1(b) for a 3D system with 14^3 sites. Obviously the Coulomb gap is filled with increasing temperature, it has completely disappeared for $T=0.4$. The temperature dependence of the single-particle DOS shows two remarkable fixed points at energies close to $|\varepsilon|=0.5$, which were found also in the spatially disordered

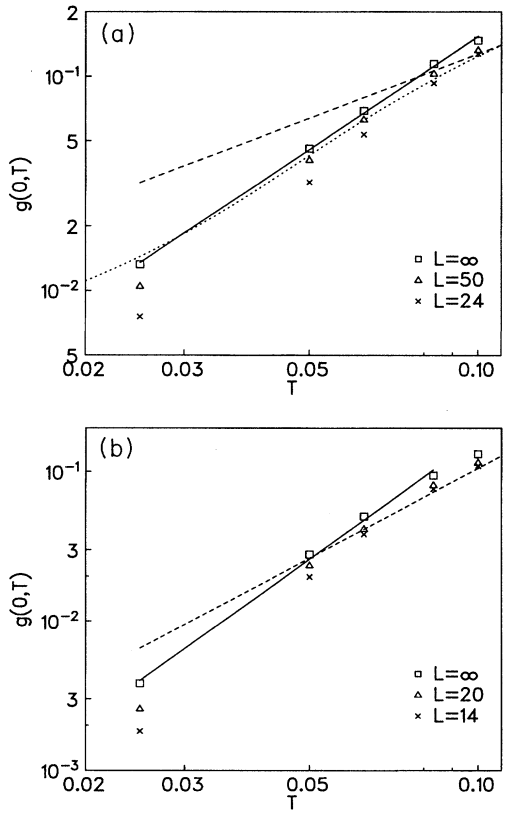

FIG. 3. Log-log plot of the DOS at the chemical potential versus the temperature for the 2D system (a) and for the 3D system (b). The solid lines give the ranges of the power-law regressions of the $L=\infty$ values. The dashed lines show the analytical predictions (Ref. 20). The dotted line in (a) is the result of the crossover theory [Eq. (5)] (Ref. 22).

Coulomb glass,[21,25] but have never been discussed in detail. An investigation of these fixed points will be published elsewhere.

In the following we study the behavior of the single-particle DOS at the chemical potential μ. To reduce the significant finite-size effects we have extrapolated our numerical results to infinite lattices $L=\infty$. The extrapolation scheme is displayed in Fig. 2 for the 3D case where the DOS is plotted against the inverse $1/L$ of the linear system size. We assumed a linear dependence between the DOS and $1/L$ in our parameter range. The results in Fig. 2 demonstrate that the data between $N=216$ and $N=8000$ agree with this assumption for all investigated temperatures. Therefore we believe that the extrapolation will eliminate most of the finite-size effects. Analogously we have extrapolated the results for the 2D model. In Figs. 3(a) and 3(b) we plot the single-particle DOS at the chemical potential μ against the temperature for the 2D and the 3D systems, respectively, and compare it with the analytical predictions.[20] Obviously the temperature dependence is much stronger than the analytical result $g(\mu,T)\sim T^{D-1}$. It cannot be decided from our data whether the DOS follows a simple power law $g(\mu,T)\sim T^{\alpha}$ in the low-temperature region or not. If so, the exponents α are 1.75 ± 0.1 for the 2D system and 2.7 ± 0.1 for the 3D

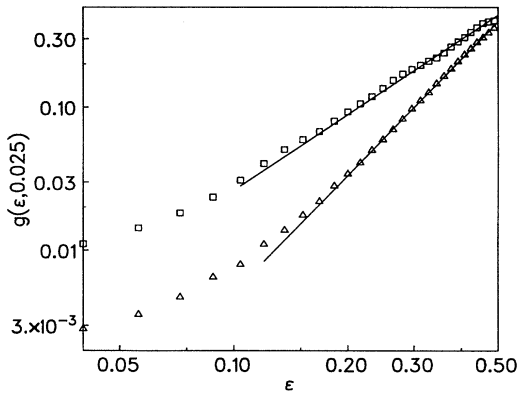

FIG. 4. Log-log plot of the DOS at $T=0.025$ versus energy for a 2D system with 36^2 sites (□) and for a 3D system with 14^3 sites (△). The straight lines show power laws with the exponents $\alpha=1.75$ and $\alpha=2.7$, respectively.

system. To check the hypothesis $g(\mu,T)\sim g(k_BT,T=0)$ we have investigated the energy dependence of the DOS at the lowest temperature studied ($T=0.025$), which should well agree with the zero-temperature DOS except for very small energies deep inside the Coulomb gap. In Fig. 4 we plot the DOS at $T=0.025$ versus the energy. We found a very strong energy dependence that can be described by power laws $g(\varepsilon,0)\sim|\varepsilon-\mu|^{\alpha}$ with the same exponents α as the temperature dependence of $g(\mu,T)$. The deviations at low energies can be attributed to finite-temperature effects. Consequently the relation $g(\mu,T)\sim g(k_BT,T=0)$ seems to be valid, although the DOS does not follow the analytical laws $g(\varepsilon,0)\sim|\varepsilon-\mu|^{D-1}$ and $g(\mu,T)\sim T^{D-1}$. We note here that we recently found a similar strong energy dependence in an extensive simulation for the zero-temperature DOS.[26]

Recently, it was suggested by Pikus and Efros[22] that the behavior of the DOS $g(\mu,T)$ at the chemical potential may be described by a simple crossover from the zero-disorder case to the infinite-disorder case. For 2D systems they predicted the formula

$$g(\mu,T)=g_{\infty}(\mu,T)[1-\exp(-W_0/W_c)]+g_0(\mu,T)\exp(-W_0/W_c), \quad (5)$$

where g_{∞} and g_0 are the DOS at infinite and zero disorder W_0, respectively, and W_c is a constant $W_c=0.5$. The asymptotic functional forms of the DOS, g_{∞} and g_0 are given by

$$g_0(\mu,T)=0.85\ \exp(-0.15/T)$$

and (6)

$$g_{\infty}(\mu,T)=0.86T.$$

In Fig. 3(a) we compared the result of Eq. (5) with our data and found it in reasonable agreement within the temperature region studied. We note, however, that Eq. (5) yields a linear decrease of the DOS for very low temperatures, where the exponential term has already vanished. In our data we did not find any indication of the temperature dependence becoming linear at low temperatures. So, the validity of Eq. (5) has to be checked by more detailed work.

In conclusion, in this paper we have presented the single-particle DOS of the Coulomb glass at finite temperatures calculated by means of a Monte Carlo method. We studied 2D and 3D systems within 216 to 8000 sites for temperatures between 0.025 to 0.4 in units of the nearest-neighbor interaction energy. The width W_0 of the random potential distribution was fixed to 1/2. In particular, we investigated the behavior of the DOS $g(\mu,T)$ at the chemical potential. We found a temperature dependence much stronger than the analytical result $g(\mu,T)\sim T^{D-1}$. It cannot be decided definitely from our data whether $g(\mu,T)$ follows a simple power law $g(\mu,T)\sim T^{\alpha}$ or not. If so, the exponent α is 1.75 ± 0.1 for the 2D system and 2.7 ± 0.1 for the 3D system. This strong temperature dependence corresponds to an analogously strong energy dependence of $g(\varepsilon,T)$ for the lowest temperature studied, $T=0.025$, which can be described by power laws with the same exponents. The relation $g(\mu,T)\sim g(k_BT,T=0)$ that links the DOS at finite temperatures to the zero-temperature DOS is therefore found to be valid, although the analytical laws $g(\varepsilon,0)\sim\varepsilon^{D-1}$ and $g(\mu,T)\sim T^{D-1}$ are not fulfilled. We note that the large deviations of the exponents from the analytical predictions may be the result of a comparatively small disorder strength W_0. Preliminary results[22,26] suggest that the analytical power laws $g(\varepsilon,0)\sim\varepsilon^{D-1}$ and $g(\mu,T)\sim T^{D-1}$ are fulfilled only in the limit of strong disorder. As a first step in this direction we also investigated the validity of the recently suggested crossover formula (5).[22] In our temperature region we found it in reasonable agreement with our data. We found, however, no indication of a linear temperature dependence at low temperatures, as implied by Eq. (5). Thus, more detailed investigations of this problem are in progress.

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[1] M. Pollak, Discuss. Faraday Soc. **50**, 13 (1970).
[2] A. L. Efros and B. I. Shklovskii, J. Phys. C **8**, L49 (1975).
[3] A. L. Efros and B. I. Shklovskii, in *Electron-Electron Interactions in Disordered Systems*, edited by A. L. Efros and M. Pollak (North-Holland, Amsterdam, 1985), p. 409.
[4] M. Pollak and M. Ortuño, in *Electron-Electron Interactions in Disordered Systems* (Ref. 3), p. 287.
[5] M. Pollak, Philos. Mag. B **65**, 657 (1992).
[6] T. Vojta and W. John, J. Phys. Condens. Matter **5**, 57 (1993).
[7] T. Vojta, W. John, and M. Schreiber, J. Phys. Condens. Matter **5**, 4989 (1993).
[8] A. L. Efros, J. Phys. C **9**, 2021 (1976).
[9] J. H. Davies, Philos. Mag. B **52**, 511 (1985).
[10] R. Chicon, M. Ortuno, B. Hadley, and M. Pollak, Philos. Mag. B **58**, 69 (1988).
[11] R. Chicon, M. Ortuno, and M. Pollak, Phys. Rev. B **37**, 10 520 (1988).
[12] S. D. Baranovskii, A. L. Efros, B. L. Gelmont, and B. I. Shklovskii, J. Phys. C **12**, 1023 (1979).
[13] M. Grünewald, B. Pohlmann, L. Schweitzer, and D. Würz, J. Phys. C **15**, L1153 (1982).
[14] J. H. Davies, P. A. Lee, and T. M. Rice, Phys. Rev. Lett. **49**, 758 (1982).
[15] A. Möbius, M. Richter, and B. Drittler, Phys. Rev. B **45**, 11 568 (1992).
[16] Q. Li and P. Phillips, Phys. Rev. B **49**, 10 269 (1994).
[17] A. L. Efros, Phys. Rev. Lett. **68**, 2208 (1992).
[18] Measurements of the DOS in the insulating regime are very difficult, a first attempt has been made by D. Schmeißer, W. Göbel, H. Fuchs, K. Graf, and P. Erk, Phys. Rev. B **48**, 4891 (1993).
[19] A. A. Mogilyanski and M. E. Raikh, Zh. Eksp. Teor. Fiz. **95**, 1870 (1989) [Sov. Phys. JETP **68**, 1081 (1989)].
[20] E. I. Levin, V. L. Nguen, B. I. Shklovskii, and A. L. Efros, Zh. Eksp. Teor. Fiz. **92**, 1499 (1987) [Sov. Phys. JETP **65**, 842 (1987)].
[21] E. R. Grannan and C. C. Yu, Phys. Rev. Lett. **71**, 3335 (1993).
[22] F. G. Pikus and A. L. Efros (unpublished).
[23] K. Tenelsen and M. Schreiber, Philos. Mag. B **65**, 695 (1992).
[24] K. Tenelsen and M. Schreiber, Phys. Rev. B **49**, 12 662 (1994).
[25] P. Sobkowicz, Z. Wilamowski, and J. Kossut, J. Phys. Condens. Matter **5**, 5283 (1993).
[26] T. Vojta and M. Schreiber (unpublished).