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LETTER TO THE EDITOR

The Coulomb glass on a fractal lattice

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Abstract. The single-particle density of states (DOS) is investigated for a system of localized electrons with Coulomb interaction in a random potential situated on a fractal lattice of the Vicsek type with a fractal dimension of two embedded in three-dimensional Euclidean space. To check the universality hypothesis of Efros we calculated the DOS numerically and compared it with the results for the square lattice model. We found that the DOS is determined by the geometric fractal dimension of the lattice instead of the spectral dimension, which usually determines the DOS. In particular, we found that the DOSs of the fractal lattice model and of the square lattice model show the same behaviour within the Coulomb gap provided that the ratio between the strengths of the random potential and the Coulomb interaction is identical for the two models. Thus the universality hypothesis of Efros is found to be valid with respect to different lattice structures.

The behaviour of interacting localized electrons in disordered materials has been investigated for several years (Pollak 1970). The main characteristics of such systems are strongly influenced by the interplay between the long-range unscreened Coulomb interaction and the disorder. After a long controversy, today it is generally accepted (see e.g. Pollak 1992) that the single-particle density of states (DOS) is reduced close to the chemical potential μ. At zero temperature the DOS is expected to vanish at the Fermi energy; it is, however, finite at every energy different from the Fermi energy. Thus, there exists a soft gap in the DOS, which is called the Coulomb gap. Several groups have tried to calculate the single-particle DOS within the Coulomb gap analytically (Efros and Shklovskii 1975, 1985, Efros 1976, Davies 1985, Vojta and John 1993, Vojta *et al* 1993) and numerically (Baranovskii *et al* 1979, Davies *et al* 1982, 1984, Möbius *et al* 1992). While the various results agree qualitatively, the detailed behaviour of the DOS remains a puzzle. Efros (1976) proposed that the DOS follows a universal power law that is independent of both the lattice structure and the disorder strength. While the validity of this universality hypothesis is doubtful with respect to the disorder strength (Davies *et al* 1984, Möbius *et al* 1992), nobody has so far, to the best of our knowledge, systematically investigated the influence of the lattice structure.

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In this paper we study the single-particle DOS of localized and disordered electrons on a fractal lattice with fractal (though integer) dimension of two and compare it with the DOS of the usual two-dimensional system. The investigations are based on the lattice model of the Coulomb glass first proposed by Efros and Shklovskii (1975). It consists of strongly localized electrons on the sites of a lattice, which interact via an unscreened Coulomb potential. Quantum hopping terms (i.e. transfer matrix elements) between the sites are neglected. The disorder is described by a fluctuating potential at the lattice sites. The Hamiltonian of the model is given by

$$H = \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{1}{r_{ij}} \left(n_i - \tfrac{1}{2}\right)\left(n_j - \tfrac{1}{2}\right) \tag{1}$$

where the variable n_i with the values zero or unity 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 identically distributed random variables with the probability distribution $W(\varphi_i)$. As is generally accepted, the properties of the Coulomb gap do not depend on the exact shape of this distribution, provided that it is slowly varying near the chemical potential μ. Without loss of generality we can therefore use the box distribution

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

Since this distribution is symmetric with respect to $\varphi_i = 0$ and each site has been given the compensating charge $\frac{1}{2}$ in the interaction terms in (1), the model defined by (1) and (2) is particle–hole symmetric. In the case of half filling ($N/2$ electrons on N lattice sites) the chemical potential is therefore given by $\mu = 0$ for all temperatures.

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

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

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

$$g(\epsilon) = \int \mathrm{d}\varphi_1 \ldots \int \mathrm{d}\varphi_N \prod_j W(\varphi_j) \frac{1}{N} \sum_i \langle \delta(\epsilon - \epsilon_i) \rangle \tag{4}$$

is the quantity under consideration in this paper. $\langle \cdot \rangle$ denotes the thermodynamic average for a given configuration of the random potentials. Since the model is particle–hole symmetric, $g(\epsilon)$ is symmetric with respect to the chemical potential $\mu = 0$.

The zero-temperature single-particle DOS of the lattice model (1) on a regular square or cubic lattice has been analytically calculated by the self-consistent equation method of Efros (1976) and, more recently, by a Bethe–Peierls–Weiss approximation (Vojta *et al* 1993). A detailed analysis of the analytical theories shows that the DOS is determined only by the functional behaviour of $N(r)$, which gives the number of sites within a hypersphere of radius r around a particular lattice site. If $N(r)$ scales as r^α, the DOS is asymptotically close to the Fermi energy ϵ_F given by

$$g(\epsilon) \sim |\epsilon - \epsilon_F|^{\alpha - 1}. \tag{5}$$

This result suggests that the asymptotic behaviour of the DOS within the Coulomb gap is independent of the disorder strength W_0 and the lattice structure. This behaviour is called the universality of the DOS within the Coulomb gap.

In a hypercubic Euclidean lattice $N(r)$ is for $r \to \infty$ asymptotically given by

$$N(r) = V_d[r/a]^d \tag{6}$$

where d is the (Euclidean) dimension of the lattice, V_d is the volume of the d-dimensional unit sphere and a is the lattice constant. In a fractal lattice with a lower cut-off length (i.e. lattice constant) a_f the number $N(r)$ is given by

$$N(r) = C_f[r/a_f]^{d_f} \tag{7}$$

where d_f is the geometric fractal (capacity) dimension (Mandelbrot 1982) of the lattice, and the distance r has to be measured in the embedding Euclidean space. (In a regular Euclidean lattice d and d_f are identical.) The proportionality constant C_f depends on the detailed structure of the fractal.

Since $N(r)$ of the fractal lattice and of the Euclidean lattice have the same functional form, the DOS for Coulomb glasses on these lattices should asymptotically obey the same law. In particular, the DOS for two models on lattices with the same fractal dimension d_f and appropriate lattice constants should show identical asymptotic behaviour. Here it is important to note that, according to the analytical theories, the DOS in our system is determined by the geometric fractal dimension d_f and not the spectral dimension d_s (Alexander and Orbach 1982) as is the case for dynamical processes on fractals (Rammal and Toulouse 1983, Malozemov 1993; for a recent review see the article by Nakayama *et al* (1994)). The reason for this discrepancy is that our system is a purely static one.

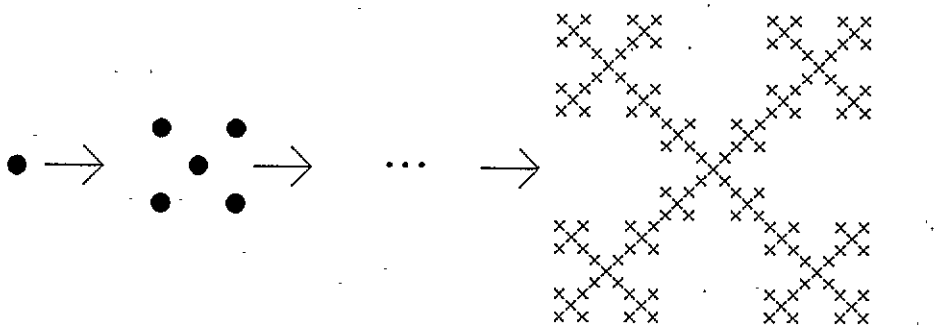

Figure 1. Construction of the Vicsek fractal (demonstrated by means of the analogon embedded in two spatial dimensions with the fractal dimension of $d_f = \ln 5/\ln 3 = 1.465$). For the simulation we used the analogous fractal embedded in three dimensions, where the basis is given by the corners and the centre of a cube. In this case $d_f = \ln 9/\ln 3 = 2$.

In order to check this special version of the universality hypothesis, we have numerically calculated the single-particle DOS of the Coulomb glass (1) on a Vicsek fractal (Vicsek 1992) embedded in three spatial dimensions. This fractal has a fractal dimension of exactly $d_f = 2$, therefore the results can be compared to that of a regular square lattice model. The construction of the Vicsek fractal is demonstrated by means of a lower-dimensional analogon in figure 1. Although the analytical results predict that the DOS in the Coulomb

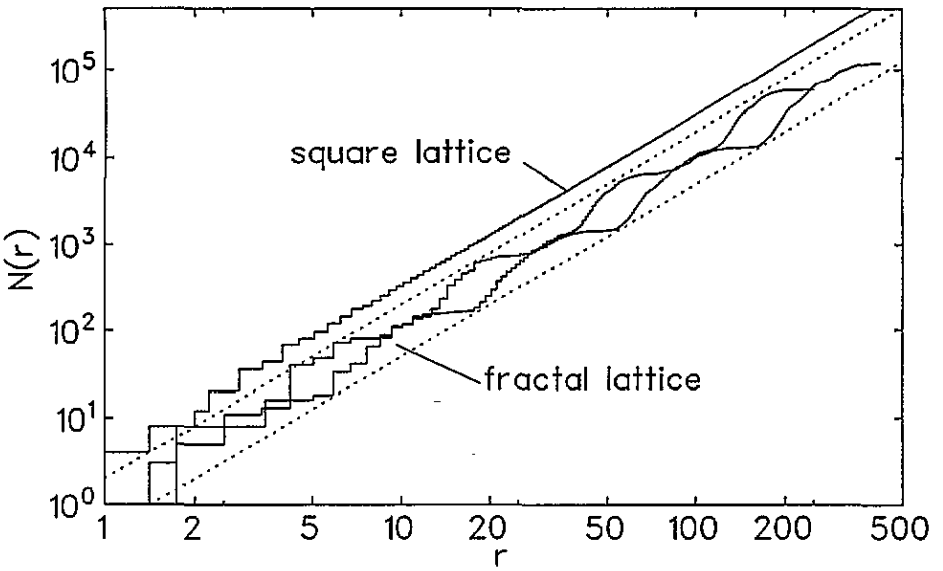

Figure 2. The number $N(r)$ of points within a hypersphere of radius r around a particular site for the square lattice ($V_2 = 4\pi/3$) and for the Vicsek fractal. In the case of the fractal the fluctuations represent the self-similar structure. Since the lattice sites are not equivalent we present the data for two typical cases. The dashed lines show the boundaries $C_f = 0.5$ and $C_f = 2.0$.

gap is independent of the ratio between interaction and disorder strength, there is numerical evidence that this is not exactly the case (Möbius *et al* 1992, Pikus and Efros 1994). Therefore it is necessary to choose the lattice constants a and a_f so that the two models have the same ratio between interaction and disorder strength.

To determine the proportionality constant C_f in (7) we have numerically calculated $N(r)$ for a Vicsek fractal of 59 049 sites (five generations of self-similarity) and lattice constant $a_f = 1$ and compared it with the corresponding $N(r)$ for the square lattice. The result is shown in figure 2. Since the fractal lattice is not a homogeneous system, it has density fluctuations on all length scales. Consequently, $N(r)$ is not a straight line in the log–log plot; it fluctuates around an average power law. (In contrast, for the square lattice $N(r)$ fluctuates only for $r \sim 1$, where the discrete lattice structure plays a role.) Therefore it is difficult to define an exact value of C_f for the Vicsek fractal. However, we determined an upper and a lower boundary, which are given by $0.5 < C_f < 2$.

From (6) and (7) one obtains a condition for the ratio a_f/a so that both lattices have same (average) $N(r)$:

$$a_f/a = \left(C_f/V_2\right)^{1/2}. \tag{8}$$

The boundaries for a_f are therefore given by

$$0.40 \approx a/\sqrt{2\pi} < a_f < a/\sqrt{\pi/2} \approx 0.80. \tag{9}$$

We have calculated the zero-temperature single-particle DOS of the Coulomb glasses on the square and the fractal lattice by means of the zero-temperature Monte Carlo algorithm of Baranovskii *et al* (1979), which was also used by Davies *et al* (1982, 1984) and more

recently by Möbius *et al* (1992). We have taken into account the stability conditions with respect to one-particle hops. The width W_0 of the random potential distribution (2) is set to unity in both models. The calculations are carried out with periodic boundary conditions applying the minimum-image convention. These boundary conditions are, however, appropriately modified for the fractal model by taking into account only those of the neighbouring volumes of the central periodicity volume that are occupied according to the structure of the fractal lattice (see figure 3).

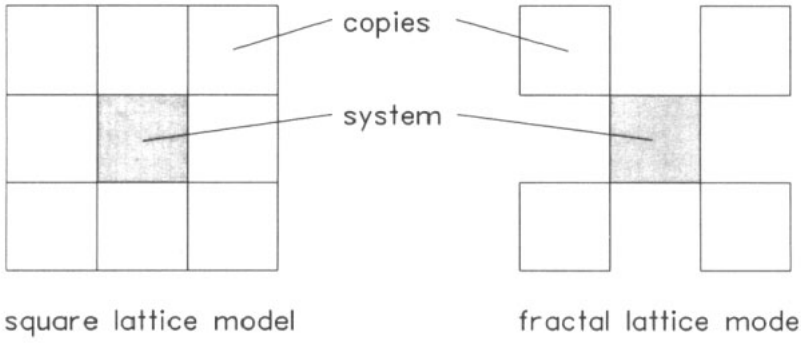

Figure 3. Modification of the periodic boundaries for the simulation of the fractal Coulomb glass (demonstrated by means of the two-dimensional analogon). Copies of the system are placed only on the positions that would be occupied according to the construction rule of the fractal.

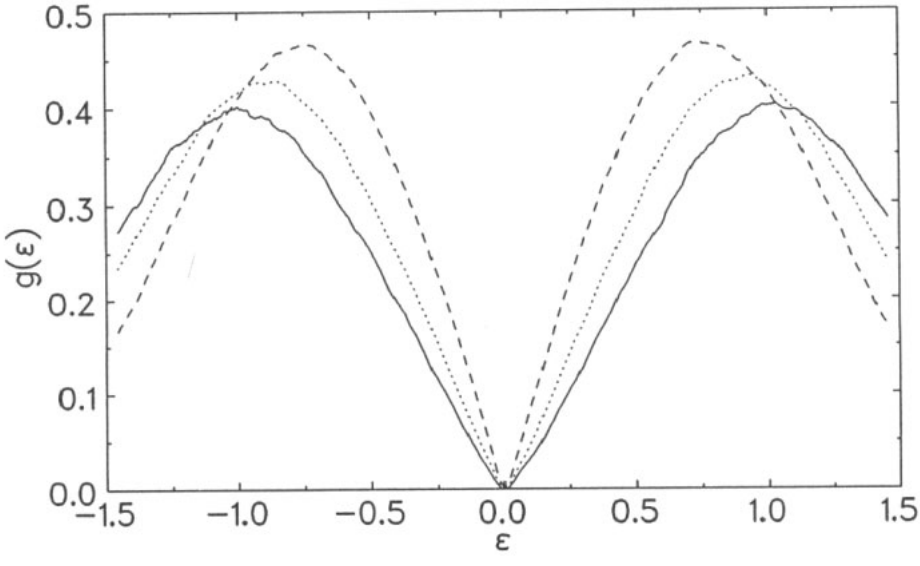

Figure 4. The single-particle DOS for the Coulomb glass on the Vicsek fractal for different values of the lattice constant: $a_f = 1/2.5$ (solid line), $a_f = 1/2$ (dotted line) and $a_f = 1/1.5$ (dashed line).

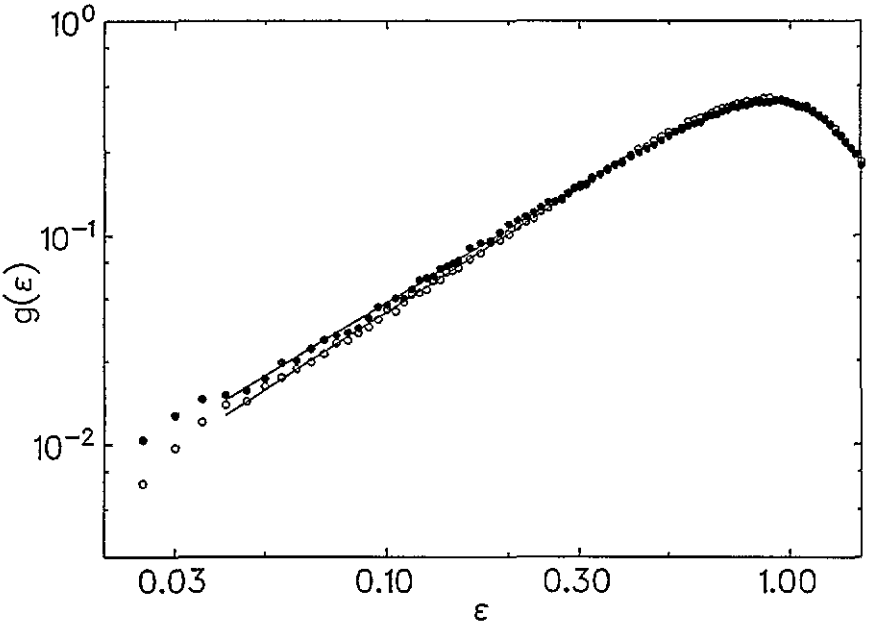

Figure 5. A comparison of the single-particle DOS of the Coulomb glasses on the Vicsek fractal with $a_f = 0.5$ (●) and the square lattice model with $a = 1$ (○). The full lines show the power law regressions in an energy range from 0.04 to 0.4.

The resulting DOS of the fractal Coulomb glass of 6561 sites (four generations of self-similarity) for different values of the lattice constant a_f is presented in figure 4. We have averaged over 500 different realizations of the random potential to minimize the statistical error. Figure 4 shows that a larger a_f corresponds to weaker interactions and thus yields a narrower Coulomb gap. We empirically found that the fractal Coulomb glass with a lattice constant $a_f = 0.5$ yields the same DOS (within the statistical errors) as the square lattice model of 10 000 sites with $a = 1$. Figure 5 shows the DOS of these two models within the Coulomb gap. The asymptotic behaviour of the DOS can be described by power laws with the exponents 1.22 ± 0.05 for the square lattice model and 1.19 ± 0.05 for the fractal model. Below the energy $\epsilon = 0.04$ finite-size effects cause deviations from the pure power law behaviour. The exponents found are in good agreement with recent numerical results of Möbius *et al* (1992); they disagree, however, with the analytical prediction (5) of $d - 1 = 1$ from the self-consistent equation (Efros 1976) and the Bethe–Peierls–Weiss approximation (Vojta *et al* 1993). We note that we can also exclude the possibility of the exponent being given by $d_s - 1$ since d_s is never larger than d_f (Nakayama *et al* 1994) and consequently $d_s - 1 \leqslant 1$.

In order to check the lattice size dependence of the exponents we also calculated the DOS for a fractal model with 59 049 sites (five generations of self-similarity) and a square lattice model with 40 000 sites. Within the statistical errors the resulting curves perfectly agree with that given in figure 5 and the region of the power law behaviour extends to energies down to 0.01. Consequently the exponents of the power laws are unchanged.

In conclusion, we have compared the Coulomb glass model of disordered and interacting electrons on the square lattice and on a Vicsek fractal with a fractal dimension of two in order to check the validity of Efros' universality hypothesis with respect to the lattice

structure. We found that the single-particle DOS of the fractal Coulomb glass is determined by the geometric fractal dimension of the lattice instead of the spectral dimension. For an appropriate choice of the lattice constants the zero-temperature single-particle DOSs of the fractal lattice model and of the square lattice model are identical, although they do not obey the power law $g(\epsilon) \sim \epsilon^{d-1}$ found analytically. Thus the universality hypothesis appears to be valid with respect to the lattice structure. However, further work is necessary to clarify the origin of the value $a_f = 0.5$ for the lattice constant of the fractal and to extend the studies to different lattice structures and different disorder strengths. Nonetheless, our results open up the possibility of investigating the Coulomb gap for any (broken) dimensionality to obtain a deeper understanding of its properties.

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