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Monte-Carlo Simulations of the Dynamical Behavior of the Coulomb Glass

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Abstract

We study the dynamical behavior of disordered many-particle systems with long-range Coulomb interactions by means of damage-spreading simulations. In this type of Monte-Carlo simulations one investigates the time evolution of the damage, i.e. the difference of the occupation numbers of two systems, subjected to the same thermal noise. We analyze the dependence of the damage on temperature and disorder strength. For zero disorder the spreading transition coincides with the equilibrium phase transition, whereas for finite disorder, we find an evidence for a dynamical phase transition well below the transition temperature of the pure system.

1 Introduction

The combined influence of disorder and long-range interactions on the properties of many-particle systems has been a subject of great interest for some time. In electronic systems already disorder or interactions alone can drastically change the physical behavior. Disorder can lead, e.g., to a metal-insulator transition due to Anderson localization. On the other hand, a metal-insulator transition can also be induced by correlations due to electron-electron interactions. If disorder and interactions are both significant then complex physical problems and phenomena arise, many of which are not completely understood.

The behavior of strongly localized correlated electrons in disordered insulators is especially complicated, both experimentally and theoretically. Thus progress has been slow since the first investigations [1, 2]. Many properties of such systems are still poorly understood. In particular there are only few and contradicting results on thermodynamics, phase diagram, phase transitions or critical behavior, and the examination of the dynamical behavior is only at its beginning [3]. Two of the central questions are whether or not the disordered interacting electron system shows glassy behavior and what is the nature of the glassy "state". Two different views can be found in the literature. In the earlier work the formal similarity between disordered localized electrons and spin glasses had lead to speculations about a possible equilibrium phase transition to a spin-glass-like low-temperature phase [4, 5]. More recent investigations show, however, growing experimental and theoretical evidence of the transition being of dynamical nature [6, 7, 8, 9].

In this paper we study the dynamical behavior of disordered localized electrons by means of the damage-spreading method. In this type of Monte-Carlo simulations the microscopic differences of the time evolution between two systems are investigated. In particular, we address the question of a dynamical phase transitions from a dynamically active high-temperature phase to a frozen low-temperature phase upon changing characteristic parameters like disorder or temperature. Our paper is organized as follows. In Sect. 2 we introduce the Coulomb glass model, the prototype model of disordered localized electrons. In Sect. 3 we describe the damage spreading technique, whereas in Sect. 4 we present the results for the dynamical behavior of the model. Section 5 is dedicated to some discussions and conclusions.

2 Model

Our investigations are based on the Coulomb glass model first proposed by Efros and Shklovskii [2] to describe compensated doped semiconductors. Later it has also been applied to simulate granular metals [10] and conducting polymers [11, 12]. The model consists of a square or cubic lattice of linear size L with $N = L^d$ sites (in d dimensions) and lattice constant a. The sites can be occupied by KN ($0 < K < 1$) electrons. These electrons are interacting via an unscreened Coulomb potential. To guarantee charge neutrality every site carries a compensating charge of $+Ke$ ($-e$ is the charge of the electron). The disorder of this system is described by the random potential φ_i. The Hamiltonian of the Coulomb glass is given by

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

where μ is the chemical potential, n_i (with values 0 or 1) is the occupation number of site i and r_{ij} denotes the distance between sites i and j. In the rest of the paper we set the interaction strength between nearest neighbor sites $e^2/a = 1$ which fixes the energy scale. The random potential energies φ_i are independent from each other and chosen according to some probability distribution $W(\varphi)$. We use the box distribution with mean 0 and width W_0. The parameter W_0 measures the strength of the disorder. Specifically, we investigate a half-filled system ($K = 1/2$). Then the Coulomb glass model is particle-hole symmetric and the chemical potential vanishes. (Note that the two quantities K and μ are not independent of each other. We treat K as a free parameter and calculate μ from it.)

For later reference we briefly mention some properties of the Coulomb glass model. One of the central quantities is the single-electron density of states

$$g(\epsilon, T) = \frac{1}{N} \sum_i \langle \delta(\epsilon - \epsilon_i) \rangle \tag{2}$$

at energy ϵ and temperature T, where $\langle \ldots \rangle$ denotes thermal and disorder averages. ϵ_i are the single-electron energies given by

$$\epsilon_i = \varphi_i - \mu + \sum_{j \neq i} U_{ij}(n_j - K). \tag{3}$$

The single-electron density of states of the Coulomb glass shows a pronounced gap, called the Coulomb gap, close to the Fermi energy ϵ_F (see fig. 1). At zero temperature the density of states actually vanishes at the Fermi energy [2], close to the Fermi energy it can be described by a power law

$$g(\epsilon) \propto |\epsilon - \epsilon_F|^\alpha \tag{4}$$

where α is approximately 1.2 for two-dimensional (2D) and 2.5 for 3D systems [13]. At finite temperatures the Coulomb gap is filled gradually (for recent simulation results see, e.g., Ref. [14]).

The Coulomb glass model (1) describes a system without internal dynamics. In reality the electrons, though localized, are coupled to additional (vibrational) degrees of freedom, which lead to transitions between the many-electron states. Phenomenologically this can be simulated by a Monte-Carlo method. In every Monte-Carlo step we change the occupation numbers of one or several sites with a certain probability. Within the Metropolis algorithm this probability is given by

$$P = \begin{cases} 1 & , \Delta H < 0 \\ exp[-\frac{\Delta H}{k_B T}] & , \Delta H > 0 \end{cases} \tag{5}$$

where ΔH is the energy difference between the many-particle states before and after such a change and k_B is the Boltzmann constant. N such Monte-Carlo steps are called a Monte-Carlo sweep which is the natural time scale of our calculations.

To simulate the dynamics one can use different "move classes", which determine how the occupation numbers are changed in every Monte-Carlo step to get the new configuration. The simplest move class consists of exchanging a single electron with a reservoir (i.e. the conduction band in the case of doped semiconductors), other classes include hopping of single electrons between the sites, or correlated hopping of several electrons. In this paper we present results obtained

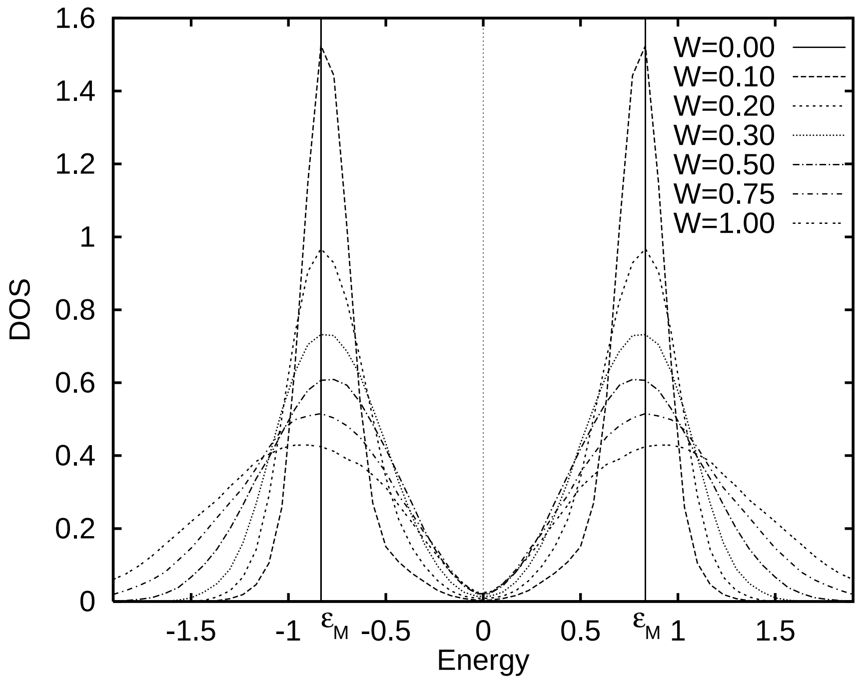

Figure 1: Single-electron density of states of the Coulomb glass at $T = 0.008$ for different strengths of disorder.

by using only single-electron exchanges between the system and a reservoir, but we have also checked more complicated move classes. As long as we do not include distance-dependent "tunneling terms" into the transition probabilities (5) applying different move classes yields data which do not show a qualitatively different behavior. We attribute this result to the fact that single and multiple electron hops can be combined from the moves in our implementation of single electron exchanges with an external reservoir. Thus all many-electron states with KN electrons are available in our simulation. A more detailed investigation of this question including the effects of distance-dependent transition probabilities on the damage-spreading simulations is in progress.

3 Damage Spreading

The damage-spreading technique [15] is a modification of the usual Monte-Carlo method. The idea is to look not at the time evolution of a single system but to compare the time evolutions of *two* systems which are subjected to the same thermal noise (i.e., the same random numbers are used within the Metropolis algorithm). Usually, at the beginning of the simulation the occupation numbers of both systems differ only at a single site (or at a few sites, e.g. a single column in a 2D lattice system).

Since both systems are thermodynamically identical, averages of equilibrium quantities will be the same for both systems. Microscopically, however, the two systems may evolve differently from each other. The central observable in damage-spreading simulations is the Hamming distance $D(t)$, which is the portion of sites for which the occupation numbers differ between the two systems. $D(t)$, which measures the "damage", is given by

$$D(t) = \frac{1}{N} \sum_i |n_i^o(t) - n_i^c(t)| \tag{6}$$

where $n_i^o(t)$and $n_i^c(t)$ are the occupation numbers of site i of the original system and the copy at (Monte-Carlo) time t. For $D(t) = 0$ the two systems are identical, $D(t) = 1/2$ describes completely uncorrelated configurations, and for $D(t) = 1$ the two systems are totally anticorrelated. In the course of the time evolution the two systems evolve towards a steady state, in which $D(t)$ fluctuates around an asymptotic average value

$$D = \lim_{\tau\to\infty} \lim_{t\to\infty} \frac{1}{\tau} \int_t^{t+\tau} dt' D(t') \tag{7}$$

Depending on the values of the external parameters temperature and disorder strength different regimes can be observed in principle if the initial damage $D(0)$ is small: The damage may heal out during the time evolution ($D = 0$), the systems may stay partially correlated for infinite time ($D < 1/2$), or the systems may become completely uncorrelated so that $D = 1/2$. In contrast to the thermodynamics the detailed behavior of $D(t)$ depends on the choice of the dynamical algorithm. Whereas Metropolis, Glauber and heat-bath dynamics give the same results for equilibrium quantities of a single system, the damage spreading results differ. For the Metropolis dynamics which we use (as well as for the Glauber dynamics) the damage tends to heal at low temperatures and tends to spread at high temperatures [15]. In contrast, the heat-bath dynamics yields healing at high temperatures and frozen configurations at low temperatures [16]. (Note that since D is *not* a thermodynamic quantity but measures the microscopic differences between two systems, there is no reason to expect that different dynamical algorithms give the same results.)

We apply the damage-spreading technique to the 2D Coulomb-glass model at half filling $K = 1/2$ and linear system sizes $L = 20, ..., 80$. The simulation proceeds as follows: (i) We create the initial system by choosing random potential values according to the probability distribution $W(\varphi)$ and occupy the sites at random with KN electrons. (ii) We equilibrate this system at temperature T by performing several (at least 300) Monte-Carlo sweeps according to the Metropolis algorithm. (iii) A copy of the system is created and modified at a single site (or several sites). This difference in the occupation numbers constitutes the initial damage. (iv) We study the time evolution of the original and the copy using the same random numbers in the Metropolis algorithm for both systems. The damage $D(t)$ is recorded and its asymptotic value D is determined.

Note that there is a modification of the damage-spreading method that can be used to determine *equilibrium* quantities instead of purely dynamic ones [19, 20]. In that kind of simulations the occupation number of a single site in one of the systems is fixed whereas it is allowed to fluctuate in the other system. Consequently, the two systems are thermodynamically *different* and the damage can be related to equilibrium correlation functions. Since in this paper we are interested in the properties of the dynamics rather than in equilibrium quantities, our data is gained by means of the original damage-spreading method, where the occupation numbers of the systems are allowed to fluctuate.

4 Results

4.1 Time evolution

In this subsection we present data on the time evolution of the damage $D(t)$ starting with an initial damage consisting of a single site. In analogy to the well studied 2D Ising model [15, 17, 18] we find that for temperatures below a certain temperature T_S, called the spreading temperature, the damage $D(t)$ remains small and eventually heals, giving an asymptotic value of $D = 0$. For temperatures larger than T_S the damage increases with time until a steady state is reached where $D(t)$ fluctuates around a finite value. Consequently, the asymptotic damage D is finite in this regime. In Fig. 2 the time evolution of $D(t)$ is shown for the Coulomb glass with zero disorder $W_0 = 0$. The three curves presented correspond to the three regimes discussed in the last section. At $T = 0.5$ the damage increases quickly and then fluctuates around $D = 1/2$. This means the two systems become completely uncorrelated very fast. Consequently we are above the spreading temperature T_S. At $T = 0.1$ the evolution of $D(t)$ is much slower and the asymptotic damage is smaller than $1/2$. This behavior occurs, because the system is in the vicinity of the spreading transition at T_S. It corresponds to the critical slowing down in ordinary critical phenomena. At $T = 0.06$ the damage remains small and eventually heals, thus the system is below the spreading temperature T_S. In the case of finite disorder W_0 the time evolution of the damage is similar (see Fig. 3). The asymptotic damage D is, however, different from 0 or $1/2$ even far away from the spreading transition. The dependence of the damage on the external parameters temperature and disorder is investigated in more detail in Subsect. 4.3.

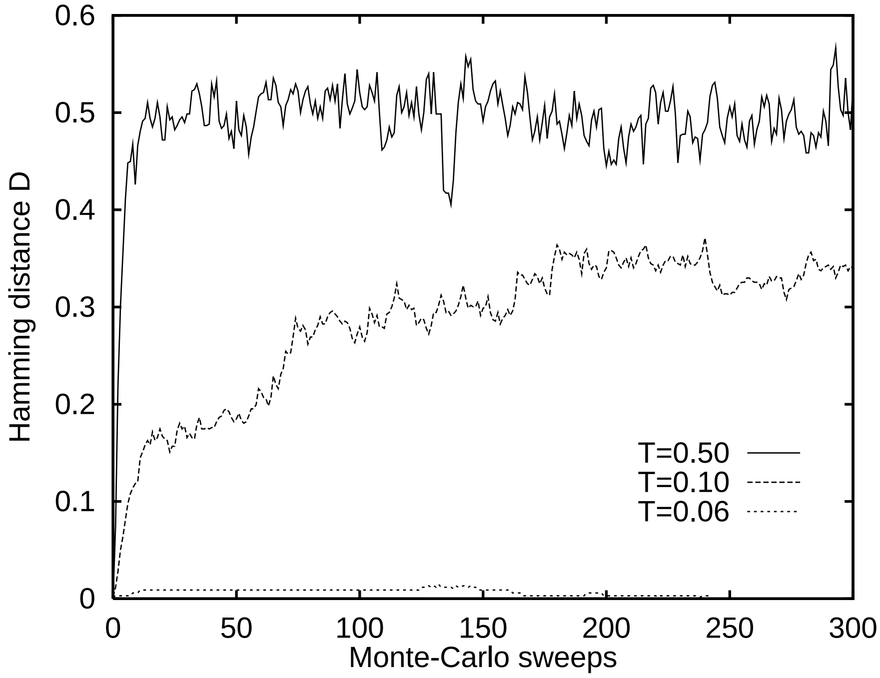

Figure 2: Time dependence of the Hamming distance of the 2D Coulomb glass for different temperatures and $W_0 = 0$.

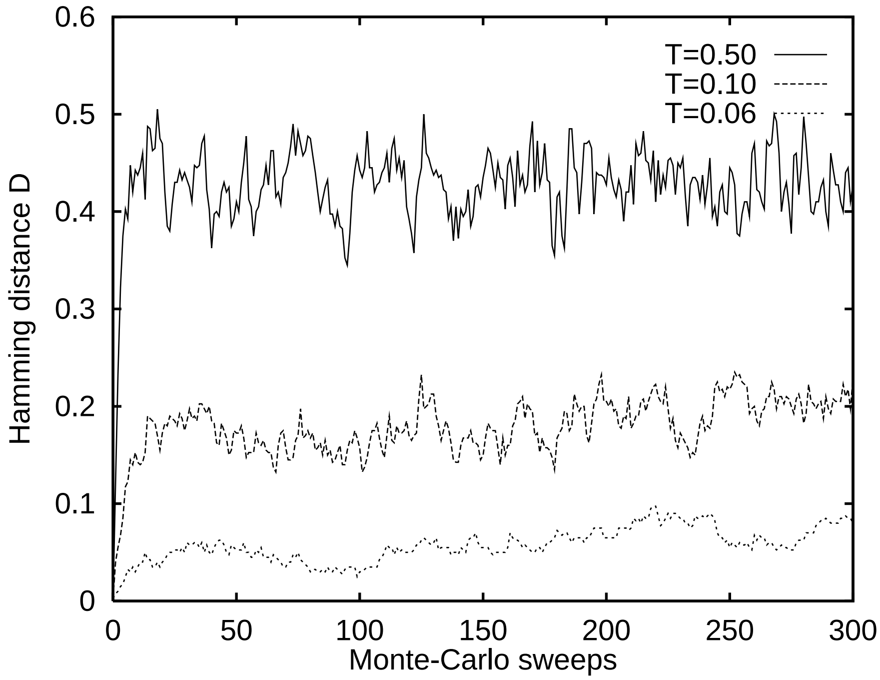

Figure 3: Time dependence of the Hamming distance of the 2D Coulomb glass for different temperatures and $W_0 = 0.5$.

4.2 Influence of the long-range interaction

The character of the interaction has a large influence on the time evolution of the damage. In systems with nearest-neighbor interactions, e.g. the Ising model, the damage can only spread within a single Monte-Carlo step from one site of the system to its neighbor. Therefore the clouds of damaged sites can only grow slowly in space and tend to be more compact (but not necessarily connected). In contrast, in systems with long-range interactions the occupation number of any site effects *all* other sites. The damage can spread from one site of the system to any other site within a single Monte-Carlo step. Therefore the damage spreads much faster as in systems with short-range interactions and the damage clouds are usually not compact. A comparison of the two cases is presented in Fig. 4.

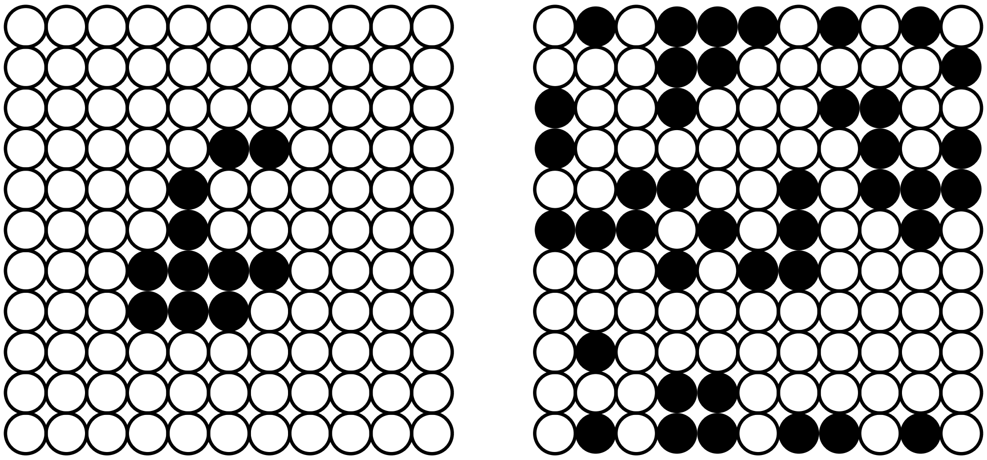

Figure 4: Snapshot of the damage for 2D systems with short-range interactions (*left*) and long-range interactions (*right*) for $T = 0.5$ and $W_0 = 0.5$ at a time of 5 Monte-Carlo sweeps after the introduction of a single damaged site. A filled circle indicates a damaged site where the occupation numbers of the two systems differ, an empty circle indicates that the occupation numbers of that site are identical in both systems.

Note, that since the damage can spread from one site to any other site in the case of long-range interactions, some of the methods developed to analyze the damage-spreading simulations [15, 17] cannot be used for systems with long-range interactions. This applies to all methods that measure the spatial extension of the damage, and its evolution, because the spatial extents of the damage cloud is not a well defined quantity for systems with long-range interactions.

4.3 Temperature and disorder dependence of the asymptotic damage

We now turn to the main results of this paper. Figure 5 shows an overview of the temperature and disorder dependence of the asymptotic Hamming distance D. For disorder strength $W_0 = 0$ there is a pronounced transition at a spreading

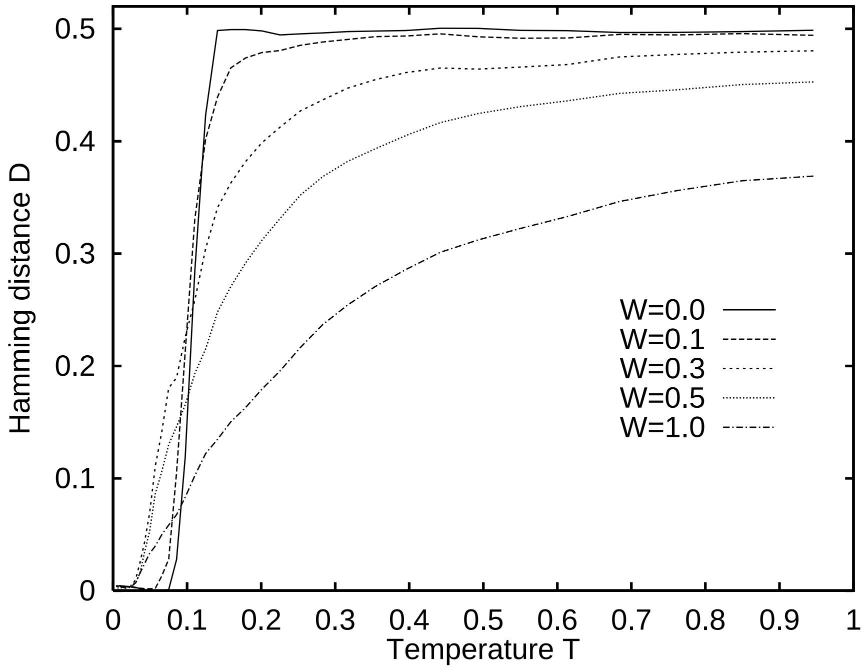

Figure 5: Overview of the temperature dependence of the Hamming distance for various strengths of disorder of a 2D system with $N = 20^2$ sites.

temperature of approximately $T_S = 0.1$ between a low-temperature regime with $D = 0$ and a high-temperature regime with $D = 1/2$. Within our numerical accuracy the spreading temperature T_S coincides with the equilibrium critical point T_c of the model without disorder which we determined from the peak in the specific heat C_v of the Coulomb glass model as a function of temperature (see Fig. 6). For very high temperatures $T \to \infty$ the spreading of the damage is drastically slowed down due to the fact that the probability P in the Metropolis algorithm, Eq. 5, becomes independent of the actual configurations of the two systems (original and copy) and reaches $P = 1$. This means that in both systems nearly every exchange of electrons is performed and differences in the occupation numbers occur only rarely. Our investigations of the spreading behavior for very high temperatures show that the Hamming distance D still reaches a plateau if plotted versus time as in Figs. 2 and 3, but the relaxation time diverges as is predicted in a recent mean-field theory [21]. The damage-spreading transition in the Coulomb glass model without disorder occurs thus in complete analogy to

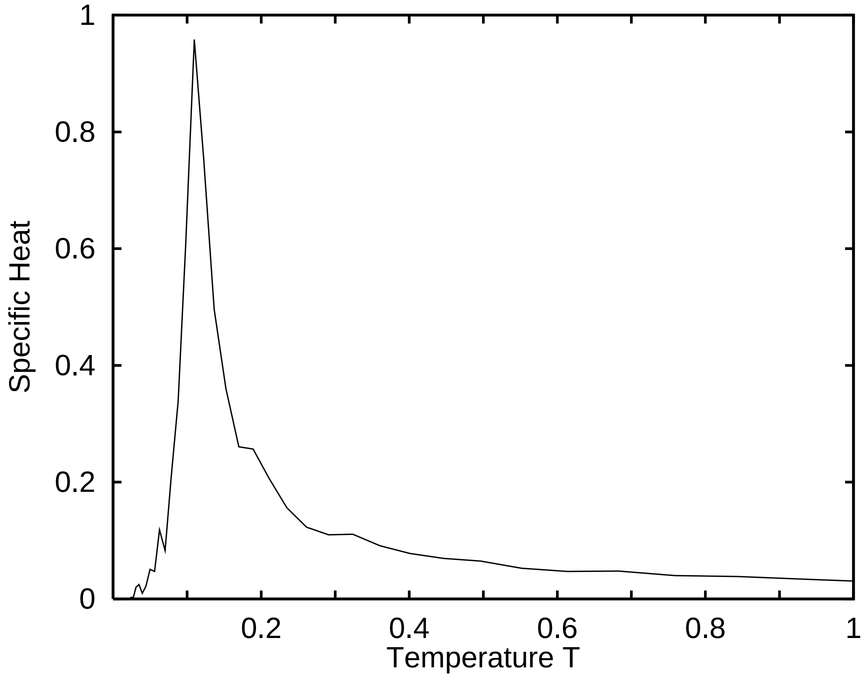

Figure 6: Specific heat of the 2D Coulomb glass at $W_0 = 0$ calculated via the derivation of the internal energy of the system.

that in the Ising model [15].

For finite disorder strength W_0, however, this behavior changes in several aspects. First, the values of the asymptotic Hamming distance in the high-temperature regime are smaller than $D = 1/2$. This means, the two systems remain partially correlated even for high temperatures. The reason for that is easy to understand: In the presence of a random potential the electrons are trapped (repulsed) at sites with small (high) potential values φ_i. These sites are identical in the original system and its copy. Therefore the presence of a random potential tends to reduce the damage. With increasing strength of disorder this trapping effect becomes larger, so that the maximum value of the damage is more and more reduced. On the other hand, increasing temperature makes it easier to overcome the potential differences so that the described reduction of the damage becomes less effective.

The second effect of the disorder concerns the behavior of D at low temperatures and close to the spreading point. This region is shown in more detail in Fig. 7. In the case of finite disorder the asymptotic damage remains finite even at temperatures below the spreading temperature of the model without disorder. This somewhat counterintuitive result, viz. an acceleration of the dynamics by disorder, can be understood by looking at the single-electron density of states of the Coulomb glass model (see Fig. 1). For $W_0 = 0$ the single-electron density of states at low temperatures has a hard gap around the Fermi energy $\epsilon_F = 0$ and

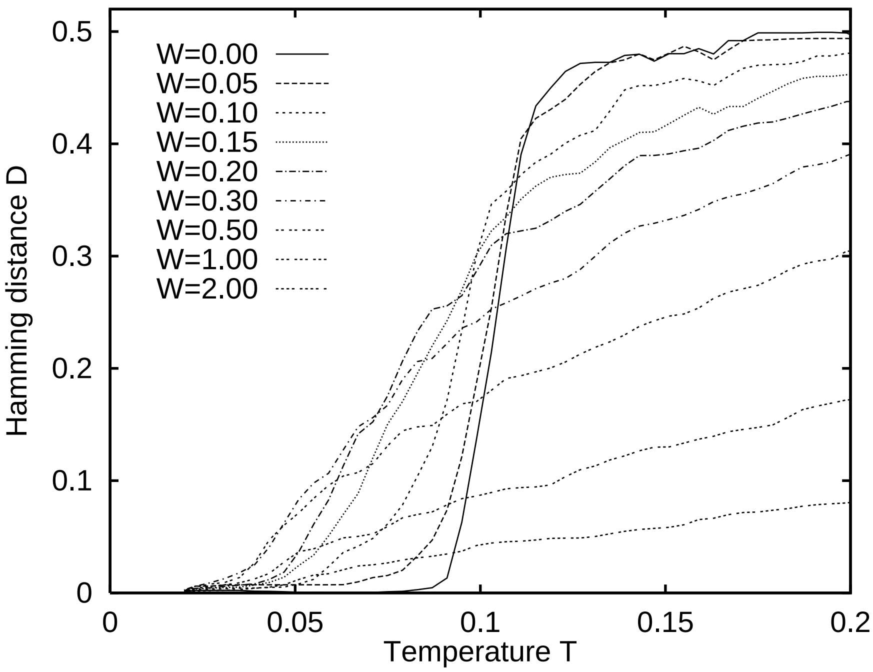

Figure 7: Hamming distance versus temperature for various strengths of disorder of a 2D system with $N = 20^2$ sites.

two peaks at the Madelung energies $\pm\epsilon_M$. Therefore there are only exponentially few sites that can be excited at low temperatures and thus the Hamming distance vanishes. In contrast, for finite disorder W_0, the gap in the density of states is not exponential but the power-law Coulomb gap (4). Therefore more sites can be excited at low temperatures and the dynamics does not freeze completely, i.e., the Hamming distance remains finite.

As can be seen in Fig. 7, even for finite disorder strength W_0 there is, however, a spreading temperature $T_S(W_0)$, below which the asymptotic damage vanishes. $T_S(W_0)$ decreases with increasing W_0, but seems to tend to a finite limiting value for large W_0 which we approximately determined to $T_S(\infty) \approx 0.03$. Note, that the existence of a spreading transition in the case of finite disorder is a purely dynamic phenomenon, since the system does not undergo an equilibrium phase transition.

In order to determine more detailed properties of the spreading transition a careful analysis of finite size effects is necessary. In Fig. 8 we show the dependence of the Hamming distance D on the system size. As expected from the analogy with usual critical phenomena the spreading transition becomes sharper with increasing system size. Figure 8 also shows that a system size of $L = 20$ already gives reasonable results for the location of the spreading temperature of the Coulomb glass model, provided the disorder strength is comparatively small.

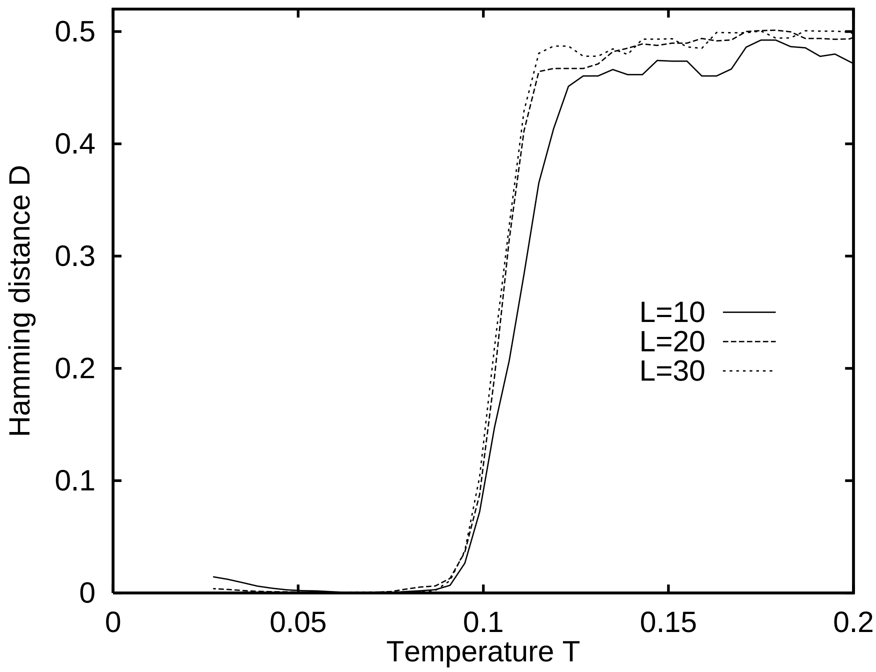

Figure 8: Hamming distance versus temperature for various system sizes at $W_0 = 0$.

5 Conclusions and Outlook

We have used the damage-spreading technique to examine the low-temperature dynamics of disordered electronic systems with localized states based on the Coulomb glass model. We have found that the dynamics of the system freezes below a spreading temperature T_S. For zero disorder this damage spreading transition coincides with the equilibrium phase transition within our accuracy. At finite disorder strength, when there is no equilibrium phase transition, the spreading point T_S is shifted to lower temperatures. However, T_S remains finite even for larger disorder strengths. Consequently, there is a low temperature "phase" of the Coulomb glass with frozen dynamics and a high temperature phase where the damage spreads through the system. In the case of finite disorder W_0 the spreading transition is a purely dynamic transition which does not possess an equilibrium counterpart. A more detailed investigation of this transition is in progress. It is, however, hampered by finite-size effects since the long-range interaction severely restricts the possible system sizes in our simulations. These limited system sizes are also the reason why the spreading point T_S for high values of disorder could not yet be determined exactly. For small disorder strengths the spreading point T_S is still close to the (second-order) equilibrium phase transition temperature T_c of the system without disorder. Since physical quantities in the vicinity of a critical point can usually be described by scaling laws we expect the

Hamming distance D to obey the homogeneity relation

$$D(W_0, T) = t^{\beta} f\left(\frac{W_0}{t^{\varphi}}\right), \qquad t = |T - T_c| \tag{8}$$

with the critical exponents φ and β. The confirmation of this scaling law and the determination of the exponents remain a task for the future.

One might also ask, how the results change if more sophisticated dynamical algorithms are used, that represent the physical processes in disordered insulators better than the simple Metropolis algorithm with single-particle exchange with a reservoir. The question is of particular importance, since the properties of damage spreading depend on the type of dynamics used in the simulation more strongly than the thermodynamic quantities. We have begun to study the Coulomb glass model with distance-dependent tunneling probabilities between the sites. Results of this numerically much more involved investigations will be published elsewhere.

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