Coulomb glass simulations: Creation of a set of low-energy many-particle states, non-ergodic effects in the specific heat

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Abstract

We have implemented a new numerical method to obtain the low-energy many-particle states of the Coulomb glass. First, this method creates an initial set of low-energy states by a hybrid of local search and simulated annealing approaches. Then, systematically investigating the surroundings of the states found, this set is completed. The transition rates between these states are calculated. The connectivity of the corresponding graph is analysed in dependence on temperature and duration of measurement. We study how the formation of clusters is reflected in the specific heat as non-ergodic effects.

65.40.+g, 71.10.-w, 71.55.Jv
Disordered systems of interacting localized particles have been extensively studied for over two decades \[1,2\]. A characteristic feature of these systems is a complex many valley structure of the energy landscape of the state space. In semiconductor physics, the Coulomb glass is a prominent example. It plays an important role as a semiclassical model for a disordered system of localized states with negligible quantum tunneling between them.

We consider a half-filled impurity band in the strongly localized regime represented by the standard tight-binding Coulomb glass Hamiltonian \[1,2\]:

\[
H = \sum_i \epsilon_i n_i + \sum_{i<j} \frac{(n_i - 1/2)(n_j - 1/2)}{r_{ij}},
\]

where \( n_i \in \{0, 1\} \) denotes the occupation number of site \( i \). The values of the random potential \( \epsilon \) are uniformly distributed between \(-W/2\) and \( W/2\). \( r_{ij} \) is the distance between sites \( i \) and \( j \) according to periodic boundary conditions. The sites are arranged at random with a minimum separation between them, which we choose to be \( 0.5 \, r \), where \( r = \left(\frac{4\pi \rho}{3}\right)^{-1/3} \), and \( \rho \) is the concentration of sites. We take \( r \) as unit of distance, and the Coulomb interaction over a distance 1 as unit of energy.

It is a complicated task to obtain the low-energy many-particle states \[3–7\]. We have implemented a new numerical method which comprises sophisticated local search \[5,6\], thermal cycling \[8\], and a renormalization approach to combinatorial optimization \[9\]. First, we quench states chosen at random by means of a local search procedure, ensuring stability with respect to excitations on one up to four sites. Thus an initial set of metastable states is created. It is improved by cyclically heating (performing a fixed number of successful Metropolis steps), and quenching \[8\]. In the course of this process, the temperature is decreased stepwise. Finally, we complete the set of low-energy states by systematically investigating the surroundings of the states found \[5,6\].

The set of low-energy states obtained is the basis for the study of different low-temperature properties. As a check, we verified that our results for the equilibrium specific heat agree with \[5,10\]. However, our main aim is to study the influence of the duration of measurement, \( \tau_m \), on the specific heat values, \( c \). For that, we have to analyse the rates of the transitions between the states.

The corresponding transition time (inverse of the transition rate in equilibrium) between two many-particle states \( I \) and \( J \) is a product of an energy factor and a spatial factor \[1\],

\[
\tau_{IJ} = \tau_0 \exp \left(\frac{E_{IJ}}{kT}\right) \exp \left(2 \sum r_{ij}/a\right),
\]

where \( k \) is the Boltzmann constant, taken as 1, and \( T \) the temperature. \( E_{IJ} = \max(E_I, E_J) \), where the ground state energy is assumed to be 0. The sum concerns only the sites, which change their occupation in the transition; it is the minimized sum of the related hopping lengths. \( a \) denotes the localization radius, and \( \tau_0 \) is a constant of the order of the inverse phonon frequency, \( \tau_0 \sim 10^{-13} \, \text{s} \).

We consider the graph of the transitions between the many-particle states: Connections indicate that \( \tau_{IJ} < \tau_m \). Thus the states are grouped into clusters. Assuming that thermalisation has happened inside the clusters, we measure the specific heat of a cluster \( \alpha \),

\[
c_\alpha = \frac{1}{T^2 \rho} \sum_{I \in \alpha} \left( \langle E_I^2 \rangle_\alpha - \langle E_I \rangle_\alpha^2 \right)
\]
where the sum is performed over all states in $\alpha$, and $\langle ... \rangle_\alpha$ means thermal average in this cluster.

We obtain the total specific heat, $c(T, \tau_m)$, as weighted average of the $c_\alpha$. The weight $P_\alpha$ depends on the experimental situation simulated. We consider two situations:

A) The ‘sample’ is at equilibrium. Thus $P_\alpha = Z_\alpha/Z$ where $Z$ denotes the partition function. Fig. 1 shows $c(T = 0.012, \tau_m)$ in comparison to the equilibrium value of $c$, where size effect, and reliability region are illustrated. Its main result is that also for durations of 1 s to several hours the specific heat is significantly smaller than the equilibrium value.

B) The ‘sample’ has been quenched from infinite $T$ to the measuring $T$ within a short time interval. To simulate this we quench first to $T = 0$, and heat then immediately to the measuring $T$: We start assigning the same probability to all states, and connecting them if the relaxation time (eq. 2 without energy factor) is lower than the quenching time $\tau_q$. Note that this graph differs from the ‘equilibrium graph’.

Starting with the highest state of the cluster considered, we distribute its weight according to the transition probabilities to the states of lower energy. This process continues iteratively until only the local minima have a finite occupation probability. Finally, we assign to each ‘equilibrium cluster’ the sum of the probabilities of the included ‘non-equilibrium local minima’.

In Fig. 2 we show the comparisons of both ‘sample’ preparation scenarios. Considering ‘samples’ prepared as described in the previous paragraph, we obtain almost the same result as for ‘samples’ being in equilibrium (case A). Thus the question of the choice of the $P_\alpha$ is not an important task for the $\tau_m$ and $\tau_q$ considered.

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FIGURES

FIG. 1. Dependence of the specific heat, $c$, on the duration of the measurement, $\tau_m$, for three sizes: ◦, □, and ○ denote 64, 216, and 512 sites, respectively. The broken line represents the equilibrium value. The localization radius is $a = 0.1 \, r$, $W = 2$, $T = 0.012$, and $\tau_0 \sim 10^{-13} \, s$. Typical error bars are represented for one point of each curve; the ensemble averaging took into account 200 ‘samples’.

FIG. 2. Comparison of two experiments with different initial conditions: ◦ = equilibrated ‘samples’, □ = quenched ‘samples’. Here $a = 0.1 \, r$, $W = 2$, 216 sites, $T = 0.018$, and $\tau_q = 10^{12}$ $\tau_0 = 0.1 \, s$. Typical error bars are represented for one point of each curve; the ensemble averaging took into account 200 ‘samples’.
Fig. 1

\[\lg \left( \frac{\tau_m}{\tau_0} \right) \]

- \( c \) vs. \( \lg (\tau_m/\tau_0) \)

- Data points and error bars are shown for different \( c \) values.

- The graph illustrates the relationship between \( c \) and \( \lg (\tau_m/\tau_0) \).
Fig. 2