Coulomb gap revisited – a renormalisation approach

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Abstract. One of the most prominent features of the Coulomb glass is the soft gap in the single-particle density of states. Previous detailed numerical studies of the gap yielded clear deviations from the analytical result. Because of the long-range interaction, the energy region which could be considered in those simulations was bounded by severe difficulties arising from finite-size effects. To approach this problem, we use a renormalisation-like procedure. It is not based on composing a large sample out of pre-relaxed small pieces but on introducing a cut-off length of the interaction which increases step by step during relaxation.

For one- to three-dimensional samples, we study the influence of the disorder strength. The consideration of samples of up to \(2 \times 10^9\) sites opens new insight: There is a tendency to universal behaviour in all three cases as predicted analytically. Asymptotic power laws with the predicted exponents seem to hold in the two- and three-dimensional cases, but the prefactors are smaller than predicted by about a factor of 2 to 3. However, this behaviour is observed only in the region of very low energies.

1. Introduction

More than three decades have elapsed since the seminal papers by Efros and Shklovskii \cite{1, 2} predicted that, at zero temperature, the single-particle density of states of a disordered system of localised charges vanishes as the chemical potential is approached. Despite a series of numerical studies ranging from \cite{3} to \cite{4}, a basic question is still open: Are the deviations from the predicted universal behaviour, observed in detailed simulations \cite{4, 5}, only an effect of too small sample size, or do they arise from an insufficient treatment of correlations in the analytical studies?

We numerically investigate \(d\)-dimensional simple hypercubic lattices of size \(L^d\), which are half-filled with particles interacting via the Coulomb potential, where background charges -1/2 are attached at each site for neutrality. The Hamiltonian reads

\[H = \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i,j \neq i} f_{ij} (n_i - 1/2) (n_j - 1/2)\]  \hspace{1cm} (1)

with \(f_{ij} = 1/|\mathbf{r}_i - \mathbf{r}_j|\), modified according to periodic boundary conditions and minimum image convention. Here, \(n_i \in \{0, 1\}\) denote the occupation numbers of states localised at the lattice sites \(\mathbf{r}_i\). The values of the random potential \(\varphi_i\) are uniformly distributed between \(-B/2\) and \(B/2\). Elementary charge, lattice spacing, and dielectric constant are taken to be 1. The single-particle energies, depending on the occupation of all sites, are given by

\[E_i = \varphi_i + \sum_{j \neq i} f_{ij} (n_j - 1/2)\.]  \hspace{1cm} (2)
In the following, we focus on the study of the density $g(E)$ of the $E_i$. For pseudoground states, i.e. states which are stable with respect to arbitrary single-particle hops, $g(E)$ vanishes as $E \to 0$, but details of the asymptotic behaviour are masked by several finite-size effects [5]. Here, we present a new algorithm which enables a considerable reduction of these systematic errors.

2. Algorithm

The numerical construction of a pseudoground state starts from a random charge configuration $\{n_i\}$. Then, a relaxation by means of single-particle hops is simulated. Thus, the determination of the set of single-particle energies $\{E_i\}$ for a pseudoground state of a large sample includes three types of tasks which are, per se or due to their multiple recurrence, particularly cpu-time consuming: (a) The calculation of $\{E_i\}$ for a given initial configuration $\{n_i\}$, (b) the repeated search for a total-energy-reducing single-particle hop, that means for a pair of sites $(i, j)$ with $n_i = 1$, $n_j = 0$, and $\Delta H = E_j - E_i - f_{ij} < 0$, and (c) the respective subsequent recalculation of the single-particle energies for all sites, $E_k := E_k - f_{ki} + f_{kj}$.

At first glance, task (b) seems to be most demanding. However, by smart programming, the related effort can be reduced so far that it increases only slightly faster than proportional to $L^d$. Therefore, the relevant pairs of sites are constructed in the following way: One site is selected cyclically sweeping (in a random sequence) through all sites, where the sweep is continued after each single-particle hop. The other site is found considering the neighbouring sites according to increasing distance. Mostly, the search for the second site can be terminated already in an early stage, for a detailed reasoning see [6].

However, for both the tasks (a) and (c), the total number of necessary operations in an exact calculation is in principle proportional to $L^{2d}$. (For (a), the only exception would be starting from an ordered configuration $\{n_i\}$, but this is physically not meaningful [5].) Thus, a strong acceleration of tasks (a) and (c) can only by reached by appropriate approximation schemes for determining the $E_i$ and their modifications. It seems natural, to consider the arising numerical errors of the $E_i$ afterwards as part of the stochastic potential $\phi_i$. If these corrections are small, the related correlations should be negligible.

We turn first to task (a), the determination of the initial $\{E_i\}$. In our algorithm, approximation means reduction of the infinite interaction range to a finite value $L_{\text{ini}}$. However, in order that the numerical errors are small, the initial disordered charge distribution has to be sufficiently homogeneous. In particular, long-range charge density fluctuations must be avoided. Therefore, we randomly assemble the initial $\{n_i\}$ from two alternative types of elementary hypercube occupations, see Fig. 1. In calculating the initial $\{E_i\}$, for all sites of a given elementary hypercube, the same interaction cut-off is used, see Fig. 2.

Consider now task (c), the recalculation of $\{E_i\}$ during the relaxation by means of single-particle hops. Each hop corresponds to the creation of a dipole. In the approximative calculation of the $\{E_i\}$ change, we take the potential of the dipole into account only for the sites within the hypercuboid envelope of both the hypercubes with edge length $2L_{\text{rel}}$, which circumscribe the two affected sites, see Fig. 3. Outside this envelope, we neglect the dipole potential.

Our global procedure follows a strategy which resembles the renormalisation approach to phase transitions. Stepwise increasing the maximal hopping length, that is decreasing the
minimal interaction energy $f_{ij}$, we repeatedly sweep through the sample searching for total-energy-reducing single-particle hops. Recalculating $\{E_i\}$ for the corresponding occupation modifications, we use a cut-off length $L_{\text{rel}}$ which is a fixed multiple of the maximal hopping length. Experience shows, that a large part of the single-particle hops with a certain hopping length is performed already during the first sweep which takes them into account.

Thus, as relaxation proceeds, we focus on a single-particle energy range of stepwise decreasing width, and simultaneously increase the precision of the calculations. However, sites with high single-particle energy, which are currently irrelevant in the search for total-energy-reducing hops, may again become important in a later stage. Note that the proposed procedure is physically reasonable since the real hopping rate decreases exponentially with the hopping length.

After the current maximal hopping length has reached the largest possible hopping length $d^{1/2}L/2$, we perform the final relaxation. In this stage, we extend the set of relaxation processes taken into account by the inclusion of particle exchange with the “surroundings”, that is a particle bath at infinite distance. In this final relaxation, we have to sweep only a few times through the sample to reach a metastable multi-particle state which is stable with respect to arbitrary single-particle hops. The number of sites, the occupation of which is changed in this final relaxation, is by orders of magnitude smaller than the total number of sites.

Furthermore, in obtaining a series of pseudoground states, we accelerated our computations as follows: We do not always start from a random $\{n_i\}$, but mostly, after random modification of $\varphi_i$ for only a few lattice sites, from the previous pseudoground state. Nevertheless, the low-energy parts of the spectrum of the $E_i$ of successive pseudoground states were found to be not correlated for appropriate parameter choices. For related details, see [6].

3. Results and conclusions
We performed a series of tests of the proposed renormalisation-like algorithm. Already for rather small $L_{\text{rel}}$, we observed perfect agreement between the density of single-particle states data, $g(|E|)$, which were obtained exactly calculating $\{E_i\}$ and, alternatively, by the renormalisation approach. Also the partial modification of the samples, explained in the last paragraph of the previous chapter, proved to be very helpful, in particular for large disorder. In total, the simulations could be accelerated by more than a factor of 1000 compared to the exact approach. Thus the treatable sample size was strongly enlarged. This enabled the extension of the reliable energy region of $g(|E|)$ to considerably lower energies than in the previous studies [4, 5]. The related decrease of the finite-size effects is demonstrated in Fig. 4.

Figures 5 and 6 display our results for one- to three-dimensional systems and various degrees of disorder. The error bars are estimated from averaging of values for a large number of samples in each case. Data are given only for that $|E|$ range where finite-size effects are negligible.
Figure 4. Influence of finite sample size on the density of single-particle states for $d = 2$ and $B = 1$.

Figure 5. Reciprocal single-particle density of states versus logarithm of the energy for $d = 1$ and various $B$ values.

Figure 6. Influence of the disorder strength $B$ on the energy dependence of the single-particle density of states for two- and three-dimensional samples in log-log representation. For comparison, the corresponding analytical predictions from [2] are given.

Inspection of Figs. 5 and 6 lead us to the following conclusions: On the one hand, for $d = 1$, $g(E)$ vanishes as $E \to 0$ in a logarithmic manner, $g(E) = g_0 / \ln(E_c/|E|)$, in agreement with [7, 8]. On the other hand, for $d = 2$ and 3, power law behaviour $g(E) = g_0 |E|^p$, seems to be present at the lowest considered $|E|$. Most important, there is indeed a tendency towards universal behaviour concerning the disorder strength as $|E|$ decreases, but, for $d = 1$, this concerns only the prefactor $g_0$. For $d = 2$ and 3, the exponent $p$ of the asymptotic power law is close to $d - 1$, but the numerical values of $g$ are smaller than the analytical result of [2] by about a factor of 2 to 3. However, for small and large disorder, the universal power law becomes detectable only for very small energies, where, due to the exponentially small rates of the related long-range hops, it probably cannot be observed experimentally.

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