Comment on “Density of States and Critical Behavior of the Coulomb Glass”

In a recent Letter [1], Surer et al. concluded that their simulation results are consistent with the Efros Shklovskii prediction for the density of states in the three-dimensional Coulomb glass. Here, we show that this statement has no relevance concerning the problem of the asymptotic behavior in the Coulomb gap since it is based on unjustified assumptions. Moreover, for the random-displacement Coulomb glass model, we demonstrate that a part of the density of states data by Surer et al. erroneously exhibit a broad gap. This is related to the staggered occupation being instable contrary to [1].

In detail, Efros and Shklovskii considered systems of localized charges (see the review [2]). They showed that the single-particle density of states \( \rho \) vanishes when the energy \( E \) approaches the chemical potential, which equals 0 here. For stability with respect to arbitrary single-particle hops, they analytically derived that, as \( E \to 0 \), \( \rho(E) = a|E|^\delta \) with \( \delta = 2 \) in the three-dimensional case.

Surer et al. [1] state correctly, that the literature situation concerning quantitative numerical studies of this Coulomb gap is not yet satisfactory. Then they claim that their \( \rho(E) \) data “can be fit very well with a form \( \propto |E|^\delta \) with \( \delta \) close to 2. This is puzzling for their samples are considerably smaller than ours in our work [3], where clear deviations from \( \propto E^2 \) were found.

Inspection of Fig. 1 of [1] uncovers a first problem: The simulation data seem to be approximated by the ansatz \( \rho(E) = a|E|^\delta + b \) instead of by the Efros Shklovskii power law, but this is not mentioned in the text of [1].

For a detailed analysis, we digitized Fig. 1 of [1] by means of WinDig. The data for the disorder strength \( W = 0.4 \) are re-plotted in a log-log representation in Fig. 1(a) here. Their precision is confirmed by a fit to \( \rho(E) = a|E|^\delta + b \) for \( |E| < 0.3 \) and \( L = 14 \) yielding \( \delta = 1.84(3) \), in almost perfect agreement with [1].

Figure 1(a) shows that these \( \rho(E) \) data clearly do not follow a pure power law, so that the quality of the fit could be ensured only by the unphysical constant \( b \).

One might argue, \( b \) emulates the finite-size effects not analyzed in [1], being important due to the long range of the interaction [3]. However, the data of [1] exhibit an unexpected feature contradicting this idea: For sample-edge length \( L = 14 \), \( b \) is clearly larger than for \( L = 8 \), although \( b \) should vanish as \( L \to \infty \) [4]. A second con arises from the \( \rho(E) \) by Surer et al. being far larger than the data from Fig. 3(b) in [3] for small \( |E| \), albeit another random potential was used there (compare [4]).

To clarify these points, we performed own simulations for \( W = 0.4 \) and various \( L \) using periodic boundary conditions and minimum image convention. The results are included in Fig. 1(a). For large \( |E| \), our \( \rho(E) \) obtained by relaxation concerning all single-particle hops nicely agree with \( \rho(E) \) from [1], but for \( |E| < 0.3 \), within the whole fit region of [1], they are considerably steeper and smaller.

According to the original reasoning of the Coulomb gap [3], this difference may arise from the minimum search in [1] not considering all single-particle hops. Figure 1(a) includes two \( \rho(E) \) curves which we obtained by relaxation only via short hops ranging up to third-nearest neighbors (length \( \leq \sqrt{3} \)). These relations support our hypothesis.

The situation is even more inconsistent in case of the random-displacement model: Compared to [1], we found far stronger broadening of the \( \delta \) peaks of a charge-ordered (NaCl) occupation of the lattice. Figure 1(b) shows that already for \( W = 0.2 \), a weak Gaussian random displacement, broadening causes \( \rho(0) \approx 0.11 \). Hence, a Coulomb gap is formed by relaxation, in which the perfect charge order claimed in Fig. 2 of [1] for \( T \to 0 \) is disturbed.

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