Statistics of Deep Energy States in Coulomb Glasses

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We study the statistics of local energy minima in the configuration space and the energy relaxation due to activated hopping in a system of interacting electrons in a random environment. The distribution of the local minima is exponential, which is in agreement with extreme value statistics considerations. The relaxation of the system energy shows logarithmic time dependence reflecting the ultrametric structure of the system.

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Possible phases and the corresponding dynamic behaviors of strongly correlated disordered systems remain one of the central unresolved issues. Doped semiconductors in the insulating state are an exemplary system endowed with strong long-range Coulomb interactions and strong disorder. It was hypothesized that the combined action of both inflict a glassy phase, resulting in the term electron- or Coulomb glass [1]. Ever since, the Coulomb glass has been subject of intense research, see [2]; however, despite impressive developments, a consistent picture of its nature is still not available and the consensus on the interrelation between its inherent glassy ingredients like Coulomb gap, slow dynamics and aging, the nature of the low-lying metastable states, and the mechanisms of hopping transport is not yet achieved. A classic qualitative derivation [3] of the Coulomb gap induced in the single-particle density of states due to pair correlations remains the top result in the field.

One of the main characteristics of the glassy state is the existence of an infinite number of low-lying states (valleys in the rugged free energy relief) separated by barriers growing infinitely in the thermodynamic limit. This picture emerged from the study of the infinite range interaction model for spin glasses (Sherrington-Kirkpatrick spin glass) [4] and was later shown to imply an ultrametric structure of the configurational space [5].

There was important recent progress in relating the appearance of the Coulomb gap in electron systems to the generic glassy behavior [6], where a lattice model of spinless interacting electrons in the presence of randomness was considered and a nonlinear screening theory was formulated to tackle Coulomb gap formation and its relation to glassy freezing. The formation of the glass phase with a large number of metastable states was identified via the emergence of a replica symmetry breaking instability. In [7], the connection between the glass phase characteristics and a Coulomb gap was argued, noticing that within the locator-approximation the correlated electron system maps to the Sherrington-Kirkpatrick spin glass. Remarkably, recent experimental studies of low-frequency resistance noise in silicon inversion layers indicated glassy freezing and the presence of long-range correlations, consistent with the hierarchical picture of glassy dynamics [8]. This gives strong support to a hierarchical structure of experimentally observed Coulomb glasses and calls for further comprehensive study of hierarchical glassy systems.

In this Letter we demonstrate that the distribution of low-lying energy states in systems with an ultrametric configurational space obeys extreme value statistics giving rise to an exponential distribution for the extremely low energies, \( p \propto \exp(-E/E_0) \), where \( E_0 \) is a characteristic energy. The exponential tail is verified numerically for the lattice model of a disordered Coulomb system. We find that the system energy relaxes with time following a logr, as indeed expected for ultrametric hierarchical structures [9]. This offers strong evidence that electronic systems with long-range Coulomb interactions form a Coulomb glass with exponential distribution of the lowest energy states.

Exponential distribution.—We start with the derivation of the exponential statistics for the low-lying energy states of systems with ultrametric topology of the configurational space. This space can be represented graphically as a hierarchical tree which is the union (or sum) of hierarchical trees; see Fig. 1. The crown of the tree (leaves) corresponds to a set of nearly equal energies that form an almost degenerate ground state of the system. We consider now the subset of

FIG. 1 (color online). Illustration of a 3-tree, an element of the hierarchical tree representing the configurational space with ultrametric topology.
the configurational space characterized by an \( n \) tree and find the distribution function of the corresponding lowest energy states. It is convenient to introduce positive variables \( \{ E \} \) measuring the depths of the potential wells. Starting with the lowest hierarchical level (crown) we consider one of the sibling states sets, \( \{ E^{(0)}_i \}; i \in \mathbb{N} \leq n \}, \) where the superscript \((0)\) marks the lowest hierarchy level, define \( E^{(1)}_i = \max_{1 \leq i \leq n} \{ E^{(0)}_i \} \), and assign it to the branching point level \((1)\) generating the considered \( 0 \)th set of siblings. Now we have a collection of level-\((1)\) sibling \( n \) sets. Repeating the procedure, we obtain the next generation of low-lying energies \( \{ E^{(2)}_i \} \) that constitute the assortment of the second level sibling \( n \) sets. The described iteration should converge to a limiting distribution for the probability \( P_n(E^{(j)}) \) for the lowest states at the \( j \) level of the hierarchy, as \( j \to \infty \). This distribution must be stable under the max operation. In other words if \( E = \max \{ E_i \} \) then the probability distribution of the extrema \( E \) is the same as that of each member \( E_i \) of the set. The distribution we seek belongs to the class of so-called extreme statistics [10].

To briefly summarize the theory of extreme distributions, we consider a set of identically distributed independent random variables \( X_i \), with \( 1 \leq i \leq n \) (in the present problem these are all the low-lying energies within one set of sibling states). Let \( M_n = \max_{1 \leq i \leq n} \{ X_i \} \) and let \( P_1(x) \) be the probability that any of the random variables \( X_i \) is less than \( x \). The probability that the largest value, \( M_n \), of the set \( \{ X_i; i \in \mathbb{N} \leq n \} \) is less than \( x \) is simply the probability that all of the \( X_i \)'s fall short of \( x \). Since the variables are independent, this is given by

\[
P(\max \{ X_i \} \leq x) = P_n(x) = [P_1(x)]^n. \tag{1}
\]

The central concept of the theory of extreme statistics is the stability postulate [10], stating that after many iterations the distribution describing \( M_n \) for a sufficiently large set \( \{ X_i \} \) is the same as the distribution for each variable \( X_i \). This requires that the probability \( P_n(x) \) satisfies the functional equation \( P_n(x) = [P_1(a_n x + b_n)]^n \), where \( a_n \) and \( b_n \) are positive constants. It can be shown that, under rather nonrestrictive assumptions about the initial distribution of random variables \( \{ X_i \} \) there are only three classes of distribution functions depending on its support. In particular, if \( x \in \mathbb{R} \),

\[
P_n(x) = \exp[-n \exp(-x)], \quad a_n = 1, \quad b_n = \ln(n), \tag{2}
\]

and, therefore, the limiting form for a distribution of the lowest energy states corresponding to an \( n \)-tree subset of the configurational space is \( P_n(E) = \exp[-n \exp(-E)] \), where \( E \) is measured in dimensionless energy units.

As mentioned before, the configurational space of our system endows with an ultrametric structure which can be represented as an union of all possible \( n \) trees. Therefore the global distribution density can be found as

\[
p(E) = \int dw(n) \frac{dP_n(E)}{dE}, \tag{3}
\]

where \( w(n) \) is the weight of the \( n \) trees in the configurational space. The weight \( w(n) \) is determined by the physical properties of the system in question. In our case one observes that the elemental process of generating two nearly degenerate energy states is the pair electron exchange within a specially arranged compact four-sites aggregate [11]. Analogously, compact aggregates allowing the exchange of \( n \) pairs, generate the same number of sibling states of the corresponding hierarchical trees. Thus \( w(n) \) is nothing but the percolation cluster size-distribution function: \( w_n \propto n^{-\alpha} \), where \( \alpha \approx 2 \). Plugging this weight into Eq. (3) one arrives at the exponential density distribution for the low-lying energies, \( p(E) \propto \exp(-E/E_0) \), where \( s \) is absorbed into the normalization energy \( E_0 \).

The extreme value distributions for extremely low-energy states were derived [12] for several systems and problems possessing one step replica symmetry breaking solutions, such as the random energy model and decaying Burgers turbulence. It was found that extremely low-energy states of elastic manifolds in random environment (modeling a rich variety of physical systems including vortices in superconductors, charge density waves, Wigner crystals, domain walls, and many others) also obey exponential statistics resulting in creep motion which is specific for glassy states [13]. Our results taken together with those of [12,13] allow us to arrive at the conclusion that the exponential distribution of the extremely low-lying energy states, the resulting creep response, and the related \( 1/f \) noise [14] are generic properties of all strongly correlated disordered systems possessing a fractal structure of configurational space.

Model.—Now we turn to numerical studies of the energy configurational space. The lattice Coulomb model was studied numerically in the past [15–17], the typical system size was about \( 10 \times 10 \). Optimized numerical procedures enabled us to consider 100 times larger systems and analyze about \( 10^5 \) different energy minima. The Hamiltonian of a 2D Coulomb lattice with disorder is

\[
\mathcal{H} = \sum_i \varepsilon_i n_i + \varepsilon^2 \sum_{j \neq i} (n_i - \nu)(n_j - \nu) / r_{ij}, \tag{4}
\]

where \( i \) and \( j \) label the lattice sites, \( r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \), \( U \alpha_i \) with \( \alpha_i \in [-1; 1] \) define the quenched uniformly distributed random site energies, and \( n_i \) are the occupation numbers (values 0 or 1) with average \( \nu \).

The simulations were performed on the lattices with typically \( N = 100 \times 100 \) sites with periodic boundary conditions and the filling factor \( \nu = 0.5 \). We took the disorder spread, \( U \), be equal to the Coulomb interaction at the distance of the lattice constant. Consequently, \( U \), the lattice constant, and \( e \) were set to unity; vectors \( \mathbf{r} \) label square lattice sites. The behavior of the system is governed by the interplay between disorder and Coulomb interactions. At very weak disorder the system is crystal-like; an increase in \( U \) leads to glassy behavior.
Local minima.—To track down local minima of the system free energy, we choose an arbitrary initial distribution of electrons and perform sequential transfer of electrons between adjacent sites (of course such an elemental hop can be realized only if the target neighboring site is vacant). At each step the total Coulomb energy of the system is calculated using Eq. (4). If all possible nearest site hops gives rise to an increase of the total energy, as compared to its value at a previous step, the state and the corresponding energy is marked as energy minimum. In subsequent iterations one finds electron transfers that decrease the total energy, thus the system diffuses into more and more deep energy valleys. Note that this algorithm lists all the possible low-lying states. To ensure evolving the system into true low-lying minima we were starting collection statistics after reaching the states where at least $10^5$ random hops were needed to go from one local minimum to another. The obtained distribution of energies corresponding to local minima is shown in Fig. 2; one sees that the distribution tail obeys the exponential law, $N_{\text{min}}(E) \sim e^{-E/E_0}$.

For all the computed minima we define the normalized site occupation number difference $\Delta_{\alpha\beta} = N^{-1} \sum_i (n^\alpha_i - n^\beta_i)$ corresponding to all pairs of minima $\{\alpha, \beta\}$. The distribution of $\Delta_{\alpha\beta}$, i.e., the fraction of the system which has different occupation numbers for two different minima is shown in Fig. 3. To drive our system (with filling factor 0.5) from one minimum to another, about 5.4% of the electrons has to be transferred to different lattice sites. This shows that the (pseudo-)ground state of our system is indeed highly degenerate: it is enough to move around only a few electrons in order to get into another energetically close local minimum. This well illustrates the ultrametric structure of the configurational space.

The $\Delta_{\alpha\beta}$ distribution is also calculated for smaller systems with the same filling factor. For system sizes above $25 \times 25$ the fraction of the electrons different between minima and the width of the distribution stay essentially the same. Both increase upon lowering the system size; see inset in Fig. 3. For very small systems (below $15 \times 15$) the distribution is not Gaussian anymore since there is only a small number of possible local minima. This indicates that small systems do not have an ultrametric structure and therefore do not represent physical systems.

Energy relaxation.—Next we analyze the relaxation of the system at finite temperatures. Because of the ultrametric structure of the system the relaxation can be described as diffusion or random walk on the tree representing the structure [9] (Fig. 1). Starting from a local minimum, nearest neighbor hopping with Boltzmann factors $e^{-\Delta E_{ij}/T}$ is applied to all particles in the system—random permutations are used to address the lattice positions in one time step. The typical energy difference $\Delta E_{ij}$ of two adjacent lattice sites $i$ and $j$ is of order one in the used dimensionless units.

In Fig. 4 the time evolution of the system energy is shown for two different low temperatures. Since the relaxation is very slow and the fluctuations are significant (even after averaging over several time series) and furthermore increase with temperature, a conclusive discrimination of the behavior is not possible. However, it can be well fitted by a logarithmic law in agreement with the result of [9]. This lends an additional support to the hypothesis of the glassy nature of long-range interacting, disordered Coulomb systems. Previously the time evolution in the Coulomb lattice model was studied via Monte Carlo methods, see, e.g. [18–20]. In [20] the energy relaxation observed via evolution of the system after adding a few electrons showed $1/t$ behavior.

Finally, we investigated the relation between the relaxation of the system and electron correlations by reducing artificially the screening length of the Coulomb interaction (in all other simulations the range is of order of the system size). In this case the relaxation deviates from the $\log t$ law

FIG. 2 (color online). Energy distribution of about 12 000 local minimum states in half-log representation with linear fit. Linear scale with exponential fit (triangular inset).

FIG. 3 (color online). Distribution of the difference of the local minima $\Delta_{\alpha\beta}$ (0 for identical states, 1 for complementary ones). The distribution is fitted by a Gaussian curve, with mean at 0.054 and width 0.007. The calculation includes $10^7$ overlap integrals. The inset shows the dependence of the mean (crosses) and width (triangles) of the distribution on system size.
systems with profound long-range electron-electron interactions. Of course the specific manifestation of the energy statistics in the observable quantities requires concrete consideration of the peculiarities of the physical system involved and goes beyond the scope of this work. In particular, one of the most intriguing questions concerning the behavior and the nature of the noise in various disordered electronic systems will be the subject of a forthcoming publication.

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(see lower curve in Fig. 4) indicating the crucial role of long-range interactions in forming a Coulomb glass.

Discussion and conclusions.—In conclusion, we have derived that in a system endowed with an ultrametric configurational space the local energy minima follow extreme value statistics resulting in an exponential distribution of the low-lying energy states. Since in the most strongly correlated disordered systems the energy landscape is expected to be characterized by only one energy parameter, one can assume that barriers separating the low-lying states also obey the same statistics. This suggests that the nonlinear creep dynamic response and the related $1/f$ noise are generic properties of all strongly correlated disordered systems.

Our numerical results for a disordered system with long-range Coulomb interaction—including the exponential distribution of the low-lying energy states and the logarithmic time relaxation of the system towards its ground state—offer strong evidence towards the existence of a Coulomb or electronic glass and relates the formation of the glassiness with long-range correlations in Coulomb systems. This further explains why pronounced glassy properties like aging and memory effects as well as apparently unbounded $1/f$ noise are observed in electronic systems with profound long-range electron-electron interactions.