Journal Club by Oleg Chalaev

Statistics of Hopping Coulomb Glasses

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Plan

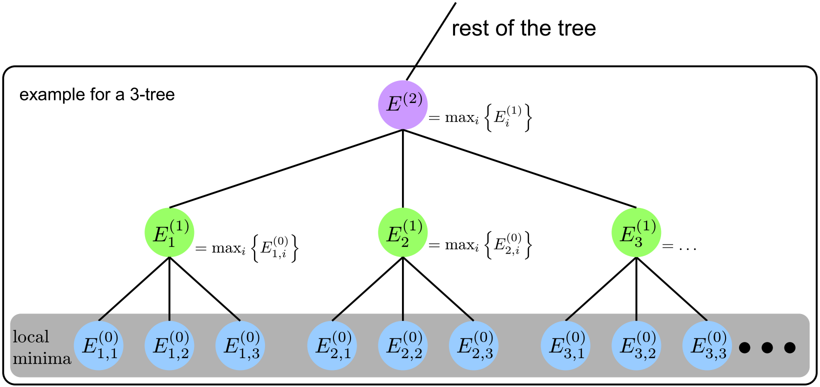
- Introduction – a few remarks on glasses
- ultrametric structure leads to exponential distribution of lowlier energies
- Confirmation: Numerical simulations of the glassy regime $\Longrightarrow$ evidence of ultrametricity + exponential statistics + log energy relaxation

A few remarks on glasses

- Almost degenerate ground state: infinite number of the low-lying states separated by barriers growing infinitely in the thermodynamic limit.
  $\longleftarrow$ results in the ultrametric structure of the configurational space.
- Coulomb gap (Efros & Shklovskii): $\nu_{E_{\mathrm{F}}} = 0$.
- The Hamiltonian:

$$\mathcal{H} = \sum_i \varepsilon_i, \quad \varepsilon_i = U\alpha_i n_i + \frac{e^2}{2} \sum_{j \neq i} \frac{(n_i - \nu)(n_j - \nu)}{r_{ij}},$$

What is ultrametric topology



- reminds Cantor set
- almost degenerate ground state
- energy relaxation is just a random walk over this tree

Calculation 1

$\{X_i\}_{i=1}^n \longleftarrow$ identical random variables $=$ energies within one set of sibling(=relating) states.

Then $M \stackrel{\mathrm{df}}{=} \max_i X_i$ is also a random variable.

Let $P_1(x) \stackrel{\mathrm{df}}{=} P\{X_i < x\}$

$$P_n(x) \stackrel{\mathrm{df}}{=} P\{M \leq x\} = [P_1(x)]^n.$$

Theory of extreme distributions says: Stability postulate:
Many iterations (going to the root the tree) do not change the distribution. $\Longrightarrow$ functional equation

$$P_n(x) = [P_n(a_n x + b_n)]^n \,, a_n > 0, b_n > 0$$

It can be shown that $x \in \mathbb{R} \cup \{-\infty, +\infty\} \Longrightarrow$

$$P_n(x) = \exp[-n \exp(-x)], \quad a_n = 1, \quad b_n = \ln(n),$$

Calculation 2

Thus we have to plug the extreme distribution

$$P_n(E) = \exp[-n\exp(-E)]\,,$$

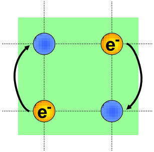
in to the formula for the *global* distribution density

$$p(E) = \int dn\, w(n)\frac{dP_n(E)}{dE},$$

where $w(n)$ is the weight of the n-trees in the configurational space.

Calculation 3

An example of how a glass can hop from one energy minima to another (minimas have almost equal energy)



How many possibilities of the branch with n sibling states are? We unite sites in pairs.

$\Longrightarrow$ this is like a cluster composed of 2 pairs.

(we need that pairs touch each other, otherwise we can move one atom without moving the other)

The number of clusters in the percolation theory

$$w_n \propto n^{-s}, \quad s \geq 2$$

(near the percolation threshold $s = 187/91$)

$$\Longrightarrow p(E) \propto \exp[-(E/E_0)],$$

where E_0 is some characteristic energy (s-dependent).

Some relax with no formulas

Exponential statistic of low-lying energy levels results in creep motion (e.g., of vortices in HTSC or domain walls), which, in its turn, results in the $1/f$-noise.

Are we sure that we really have ultrametricity?

Numerics: Model

Let's do numerical simulations with the Hamiltonian

$$\mathcal{H} = \sum_i \varepsilon_i, \quad \varepsilon_i = U\alpha_i n_i + \frac{e^2}{2} \sum_{j \neq i} \frac{(n_i - \nu)(n_j - \nu)}{|\vec{r}_i - \vec{r}_j|}, \quad \bar{n}_i = \nu.$$

$\alpha_i \in [-1; 1] =$uniformly distributed random site energies.
Choice of parameters:
$U =$Coulomb interaction at the distance of the lattice constant
$\Longrightarrow$ we are well in the glassy regime.

Numerics: local minima

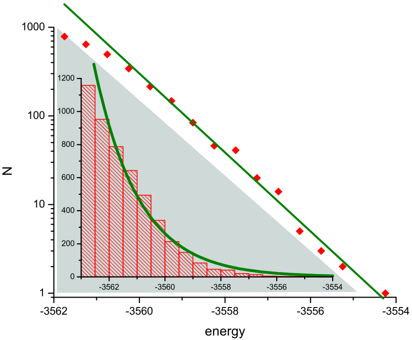


Figure: Energy distribution of about 12000 local minimum states in half-log representation with linear fit. Linear scale with exponential fit (triangular inset).

⟵ in fact, the level distribution is exponential.

Numerics: evidence of the ultrametricity

Are those local minima differ a lot? Let's calculate $\longrightarrow$
Normalized site occupation number difference:

$$\Delta_{\alpha\beta} = N^{-1} \sum_i |n_i^\alpha - n_i^\beta|$$

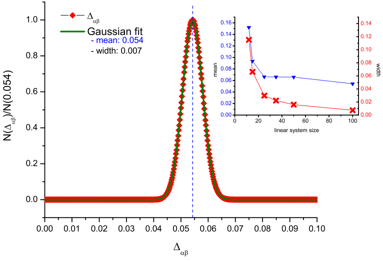
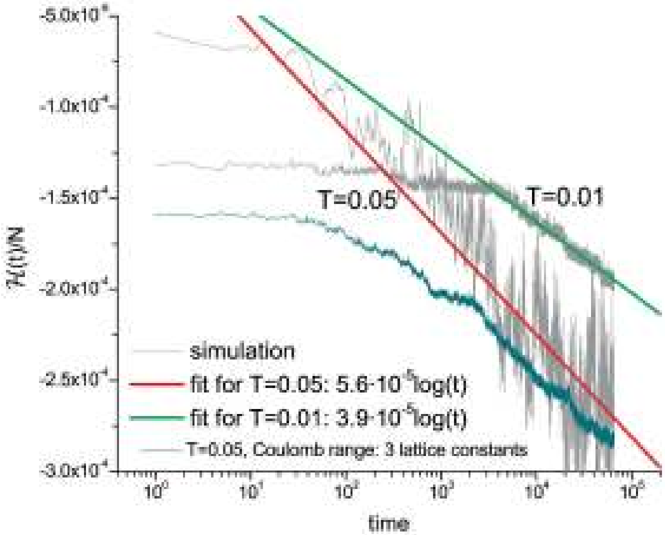


Figure: distribution of $\Delta_{\alpha\beta}$.

Interpretation: we can obtain all our numerous energy minima by moving only 5.4% of electrons to different cites $\Longrightarrow$ we have ultrametricity!

Essential: system size should not be small!

Numerics: Energy relaxation



Conclusions

- Ultraparametricity results exponential distribution of deep levels.
- Glassy Hamiltonian (strong disorder $+$ long-range Coulomb) leads to both ultraparametricity and exponential distribution.
- It also manifests logarithmic ralaxation.
- Size matters!
- Speculation: all disordered strongly correlated systems have creep motion and $1/f$ noise.

added later: literature list

cond-mat/0703149