Numerical study of relaxation in electron glasses

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Outline

- Relaxation in electron glasses. Experiments.
- Open questions
- Model. Master equation.
- Renormalization process.
- Results.
- Conclusions.

Experiments

InO	Ovadyahu
In_2O_{3-x}	
Granular Al	Grenet
Granular Ni	Frydman
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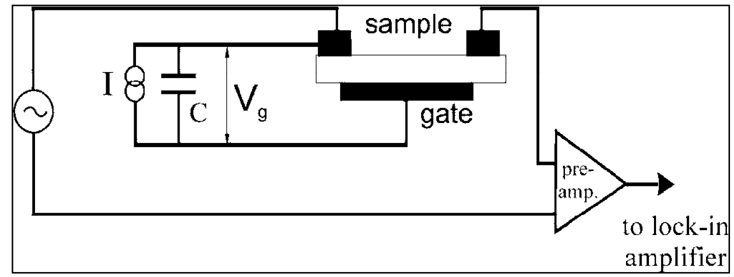
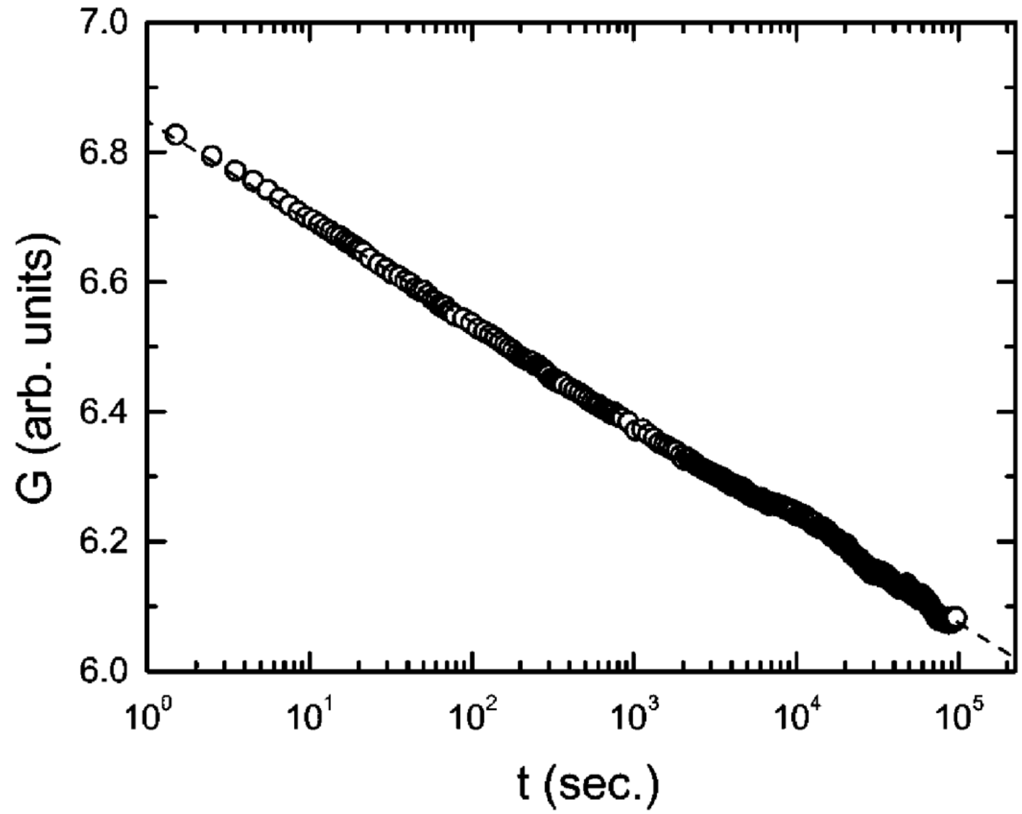
.	.





Model

- Disorder and interactions.

$$H = \sum_i \phi_i n_i + \sum_{i>j} \frac{(n_i - K)(n_j - K)}{r_{i,j}}$$

  - $n_i = \{0, 1\}$ occupation number (very large U).
  - $\phi_i \in [-W/2, W/2]$ random site energy.
  - K compensation.

- Transfer energies considered to lowest possible order

  - 0 for energies, density of states, etc.
  - 1 for conduction, relaxation, etc.
  - No exchange terms. Degenerate with respect to spin.

Model

- Hopping probabilities.
  - 1-electron transition rates

$$\Gamma_{i,j} = \tau_0^{-1} e^{-2r_{i,j}/\xi} \min\{1, e^{-\Delta E_{i,j}/kT}\}$$

  - 2-electrons

$$\Gamma_{\alpha,\beta} = \tau_0^{-1} \Xi_{\alpha,\beta}^2 e^{-2\sum_{i,j} r_{i,j}/\xi} \min\{1, e^{-\Delta E_{\alpha,\beta}/kT}\}$$

    - Shortest possible transition rate.

$$\Xi_{\alpha,\beta} = \frac{1}{r_{1,3}} + \frac{1}{r_{2,4}} - \frac{1}{r_{1,4}} - \frac{1}{r_{2,3}}$$

Open question

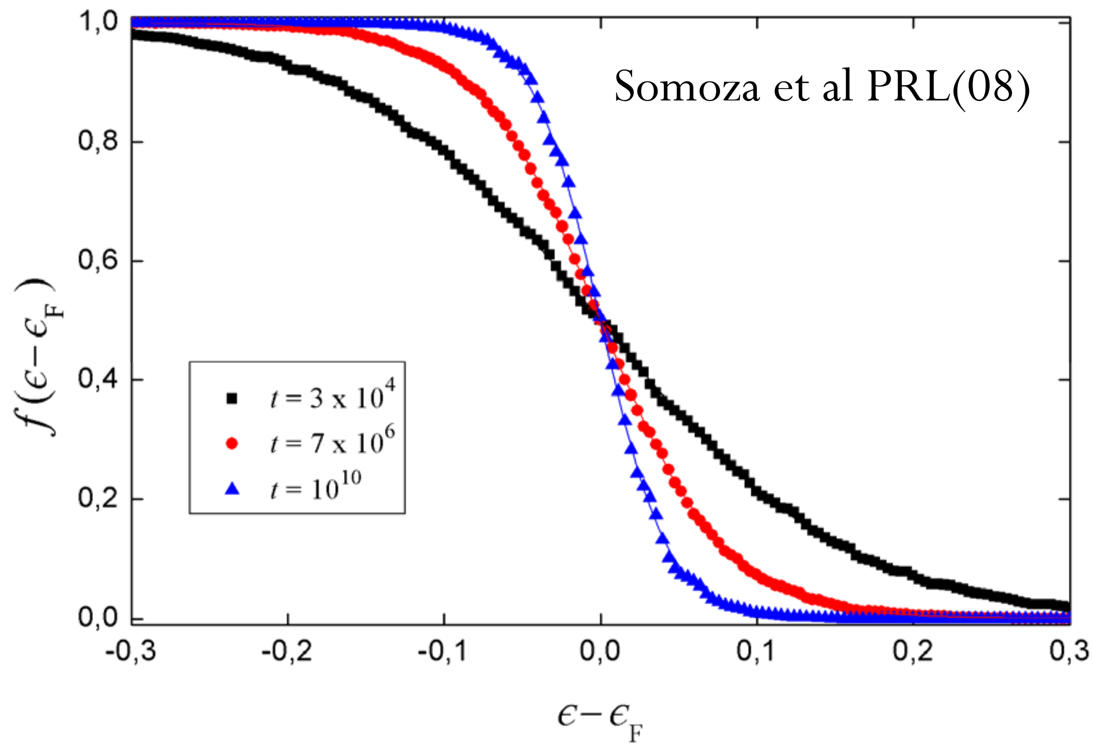
- Are there long relaxation times that affect the conductance?
- Role of many-electrons hopping ?
- Role of quantum effects?
- Mechanism for the establishment of an effective temperature in slow relaxation?

Effective temperature

- Introduced in mean-field models in spin glasses.
  - Cugliando et al (1997)
- Observed in many different systems with slow dynamics.

In Electron Glasses, it affects the occupation near the Fermi level.

$$f(\epsilon_i, t) \approx f_{FD}\left(\frac{\epsilon_i - \mu}{T_{eff}(t)}\right)$$



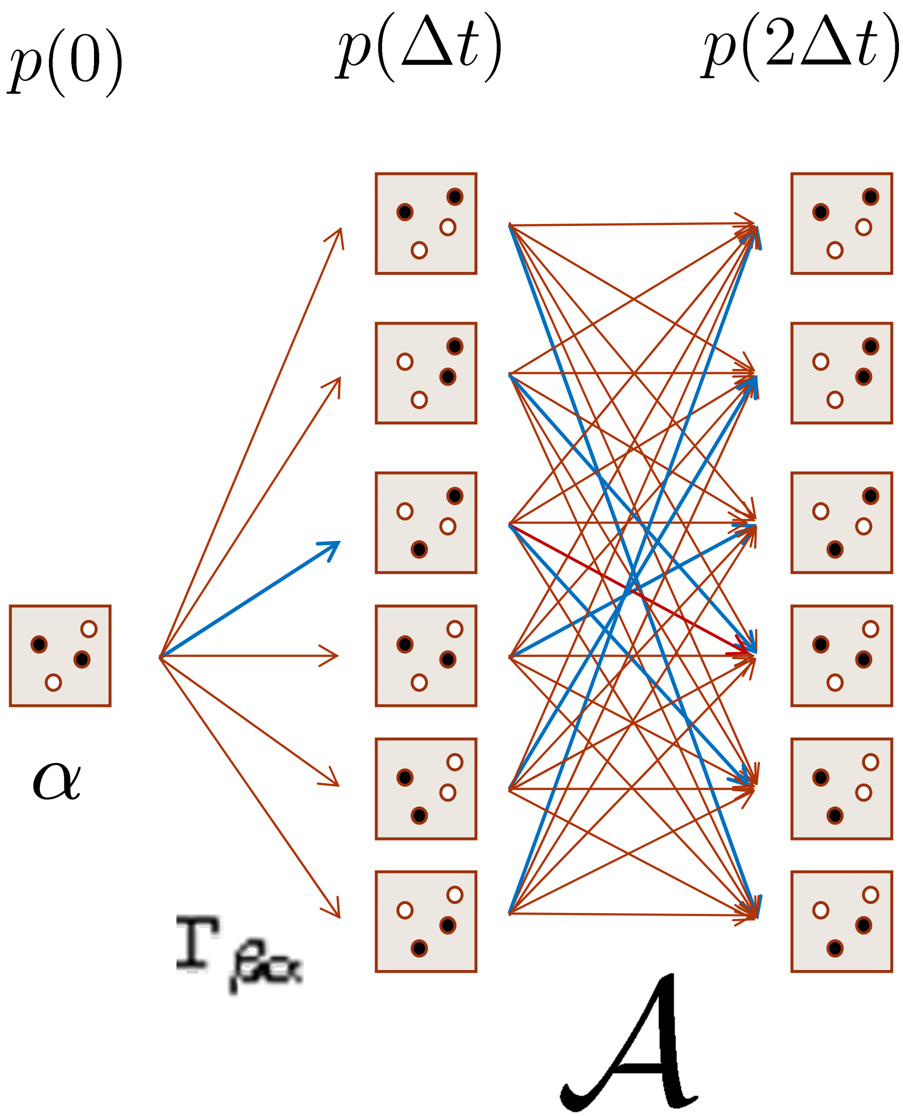
P. W. Anderson
Nobel Lecture, 1977

work both. in the field of magnetism and in that of disordered would like to describe here one development in each held cifically mentioned in that citation. The two theories I will sharply in some ways. The theory of local moments in metals , easy: it was the condensation into a simple mathematical which. were very much in the air at the time, and it had rapid acceptance because of its timeliness and its relative simplicity. ical difficulty it contained has been almost fully- cleared up within the past few years.

Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it. Only now, and through primarily Sir Nevill Mott's efforts, is it beginning to gain general acceptance.

Yet these two finally successful brainchildren have also much in common: first, they flew in the face of the overwhelming ascendancy. at the time of the band theory of solids, in emphasizing *locality* : how a magnetic moment, or an

Master Equation in configuration space



$$\frac{d\vec{p(t)}}{dt} = \mathcal{A} \cdot \vec{p(t)}$$

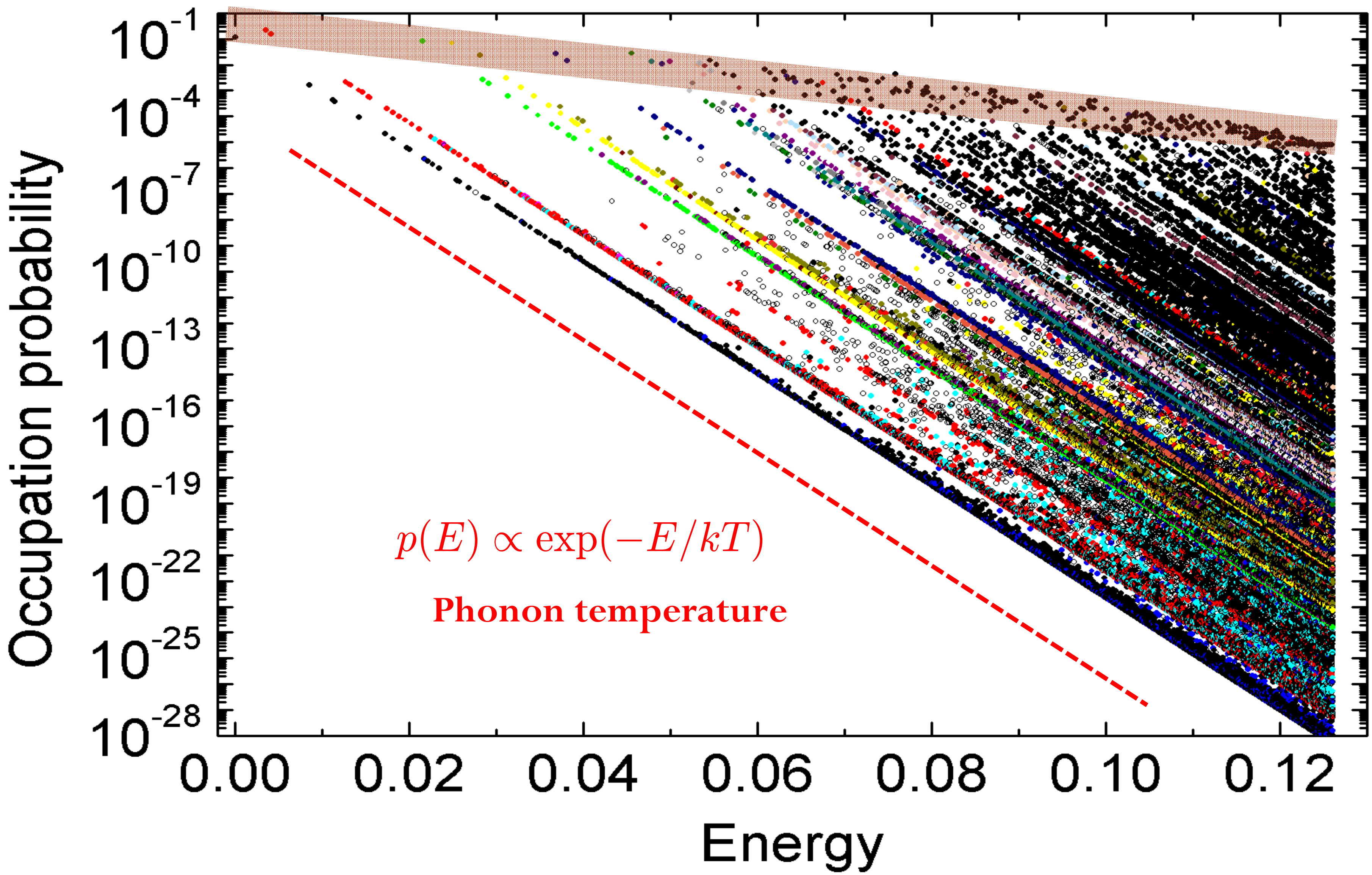
$$\mathcal{A}_{\alpha\beta} = \Gamma_{\alpha\beta}$$

$$\mathcal{A}_{\alpha\alpha} = -\sum_{\beta\neq\alpha} \Gamma_{\beta\alpha}$$

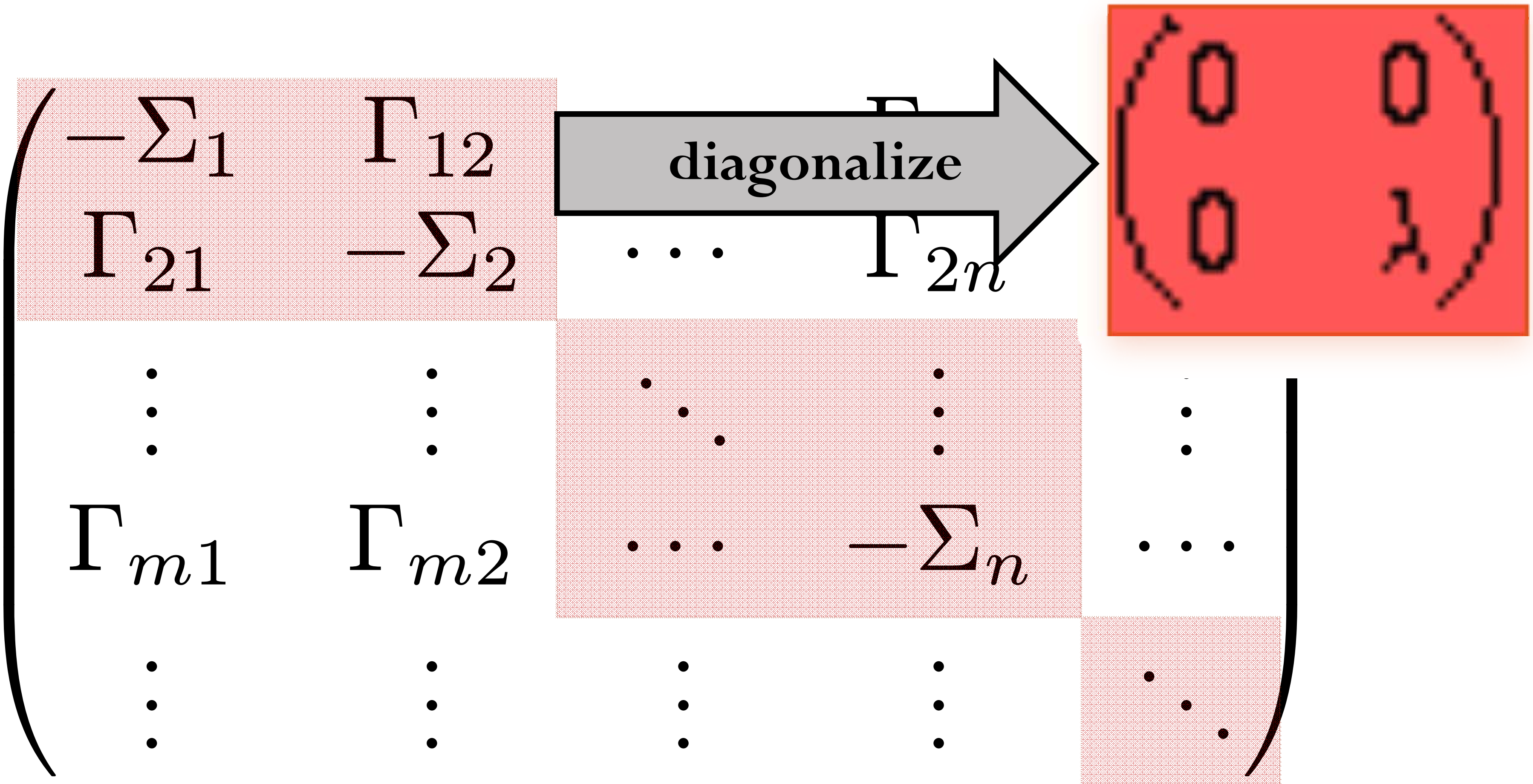
Master Equation

- Store up to 200000 configurations.
- Construct $\mathcal{A}$
  - One electron transitions.
  - Many-electron transitions.
- Integrate numerically the set of differential equations.
- Diagonalize (only for a small number of configurations).

N=1000, M=100000, T=0.002.



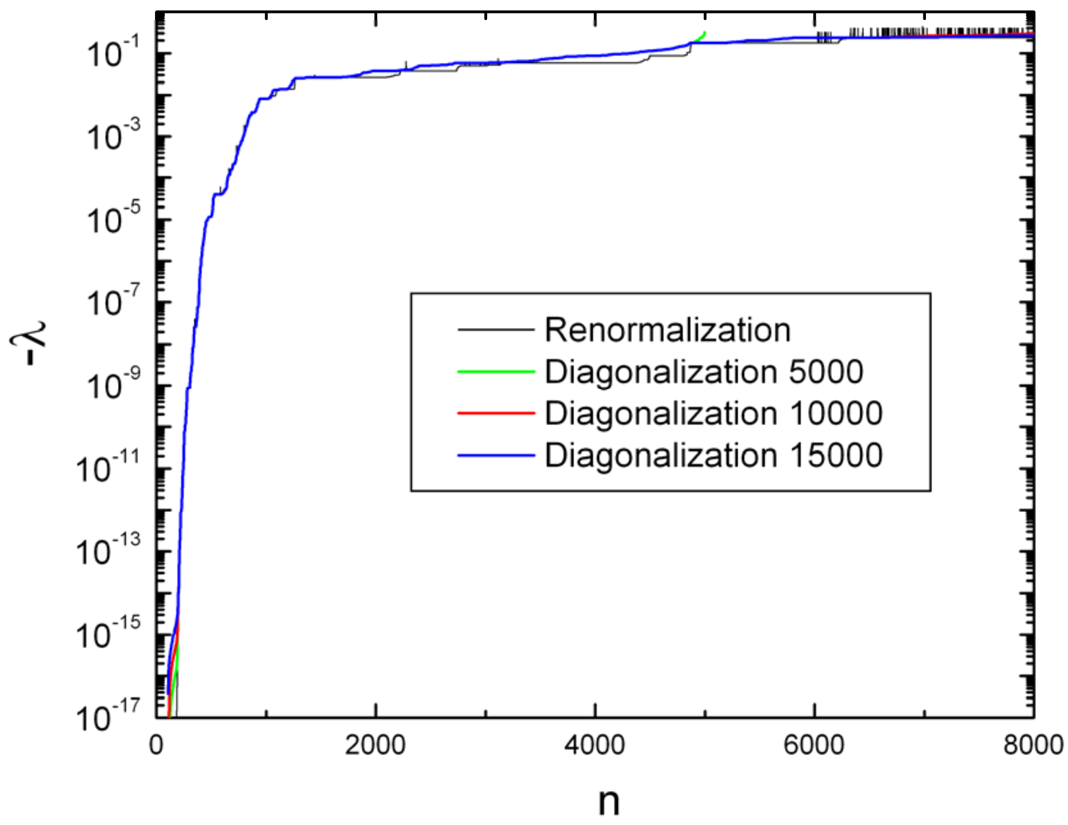
Renormalization procedure



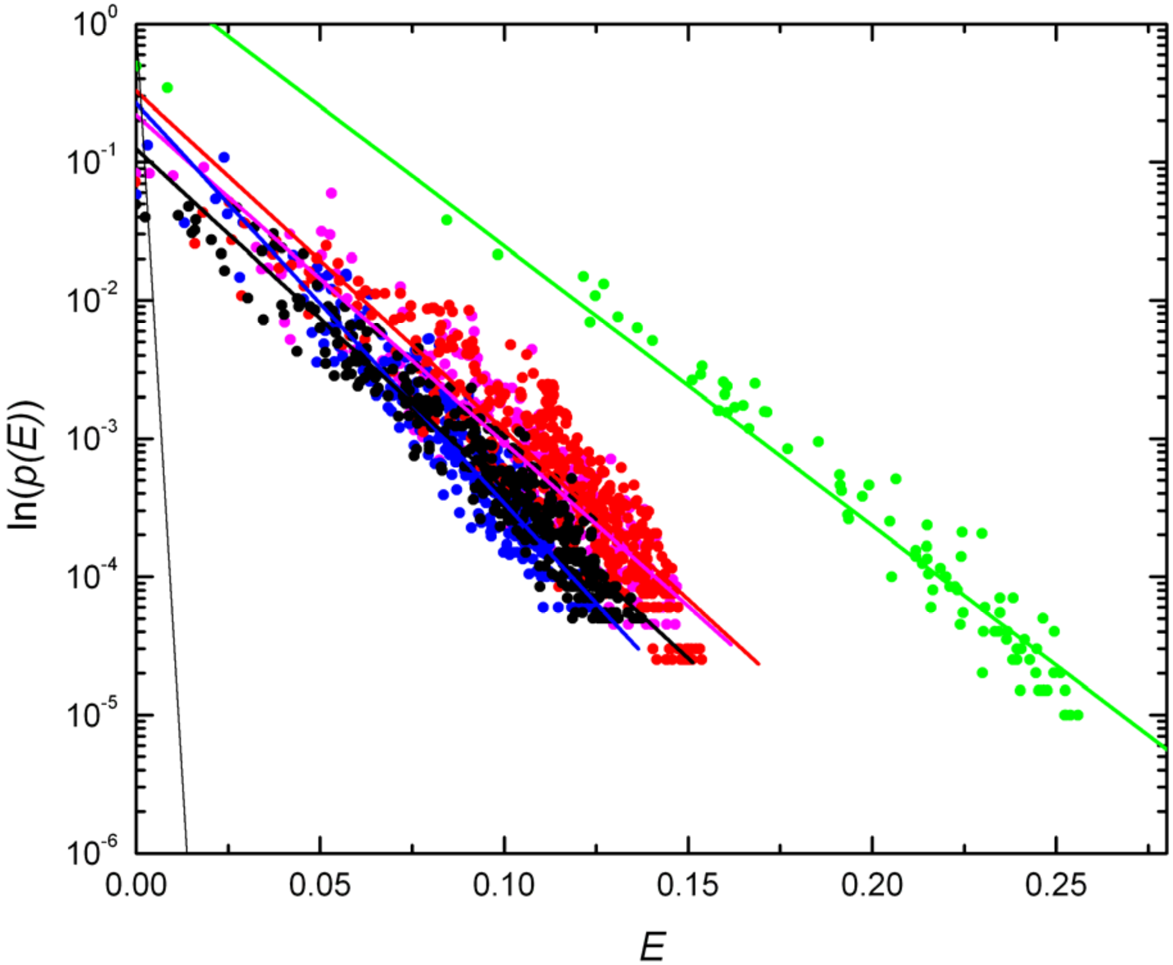
Renormalization procedure

- Search for the largest pair: $\Gamma_{\alpha\beta} + \Gamma_{\beta\alpha}$
- Assume that configurations α and β reach equilibrium, with relaxation time $\tau = 1/(\Gamma_{\alpha\beta} + \Gamma_{\beta\alpha})$.
- Keep only one of them. Renormalize probabilities, matrix elements and partition functions:
  - $\tilde{p}_\alpha = p_\alpha + p_\beta$
  - $\tilde{\Gamma}_{\alpha i} = \Gamma_{\alpha i} + \Gamma_{\beta i}$
  - $\tilde{\Gamma}_{i\alpha} = \frac{Z_\alpha \Gamma_{i\alpha} + Z_\beta \Gamma_{i\beta}}{Z_\alpha + Z_\beta}$
  - $\tilde{Z}_\alpha = Z_\alpha + Z_\beta$

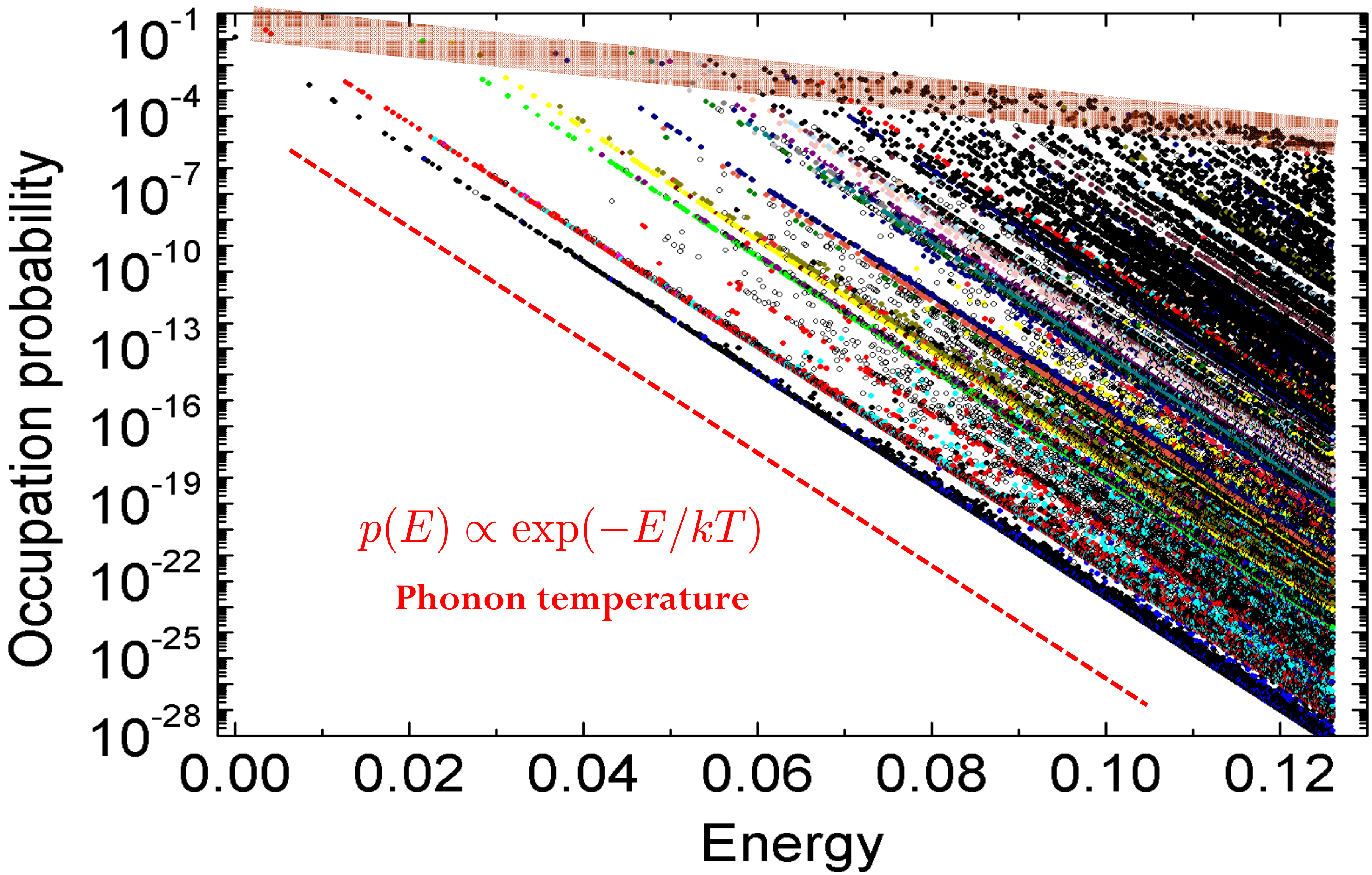
Eigenvalues



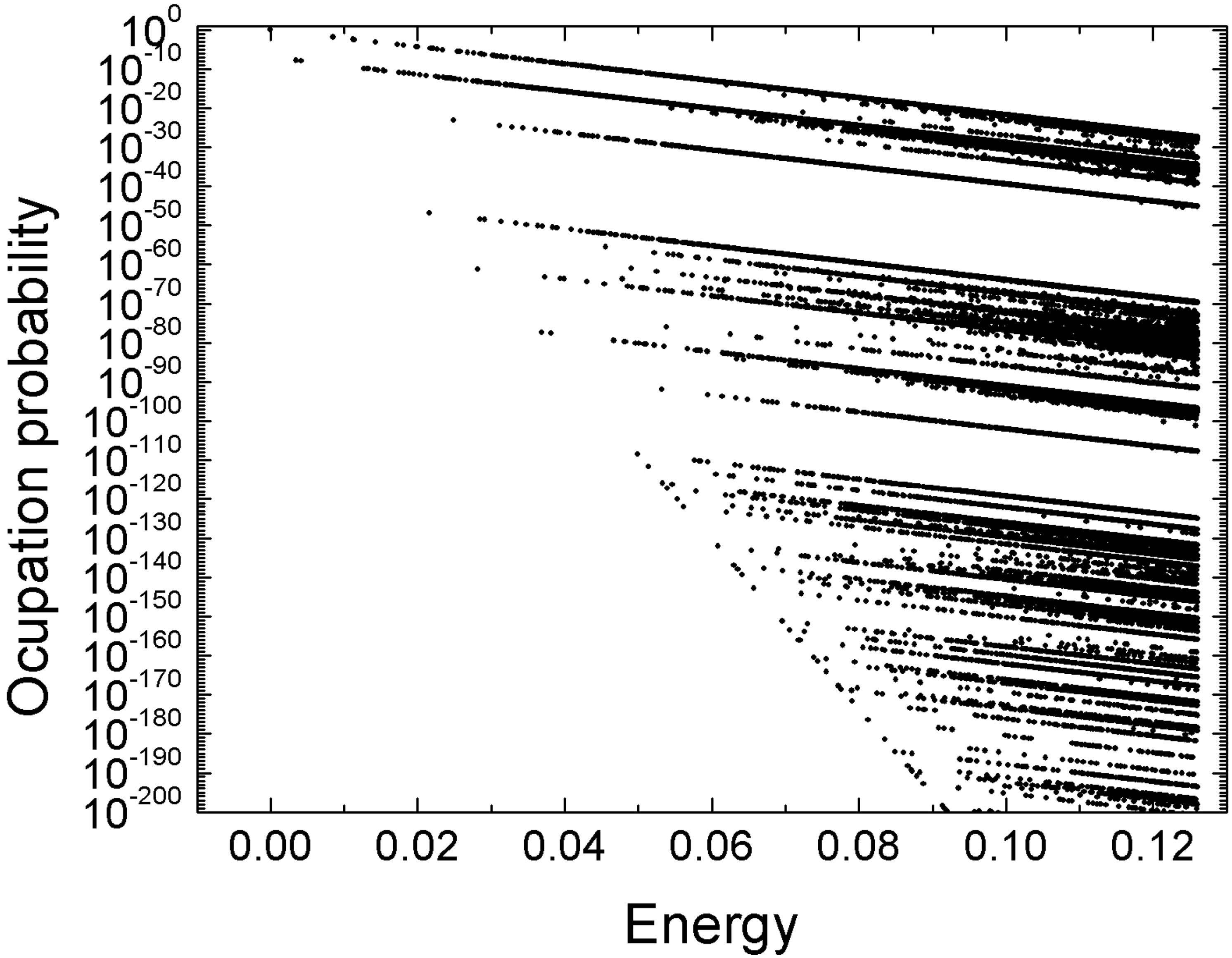
Renormalized system



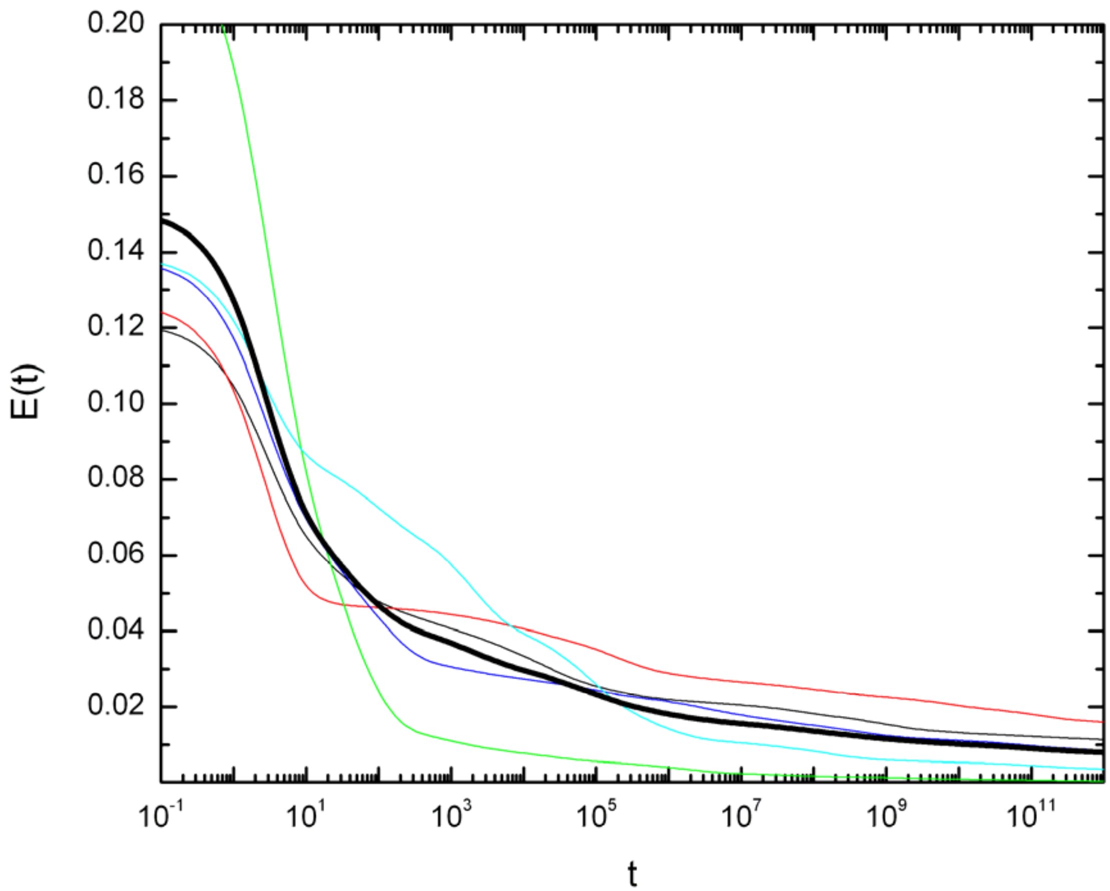
N=1000, M=100000, T=0.002.



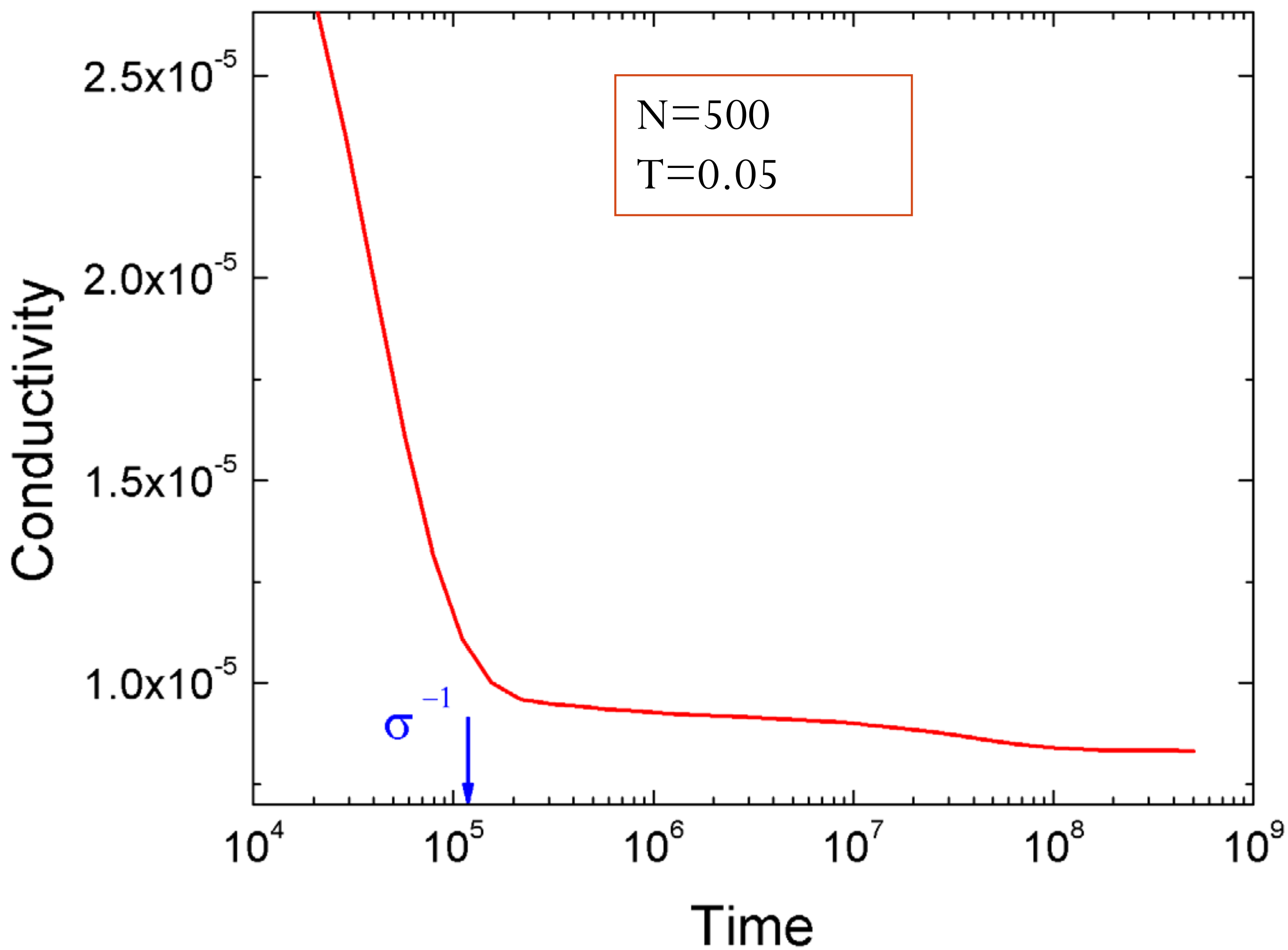
Heating from low temperature



N=1000, 2×10^5 configurations T=0.001



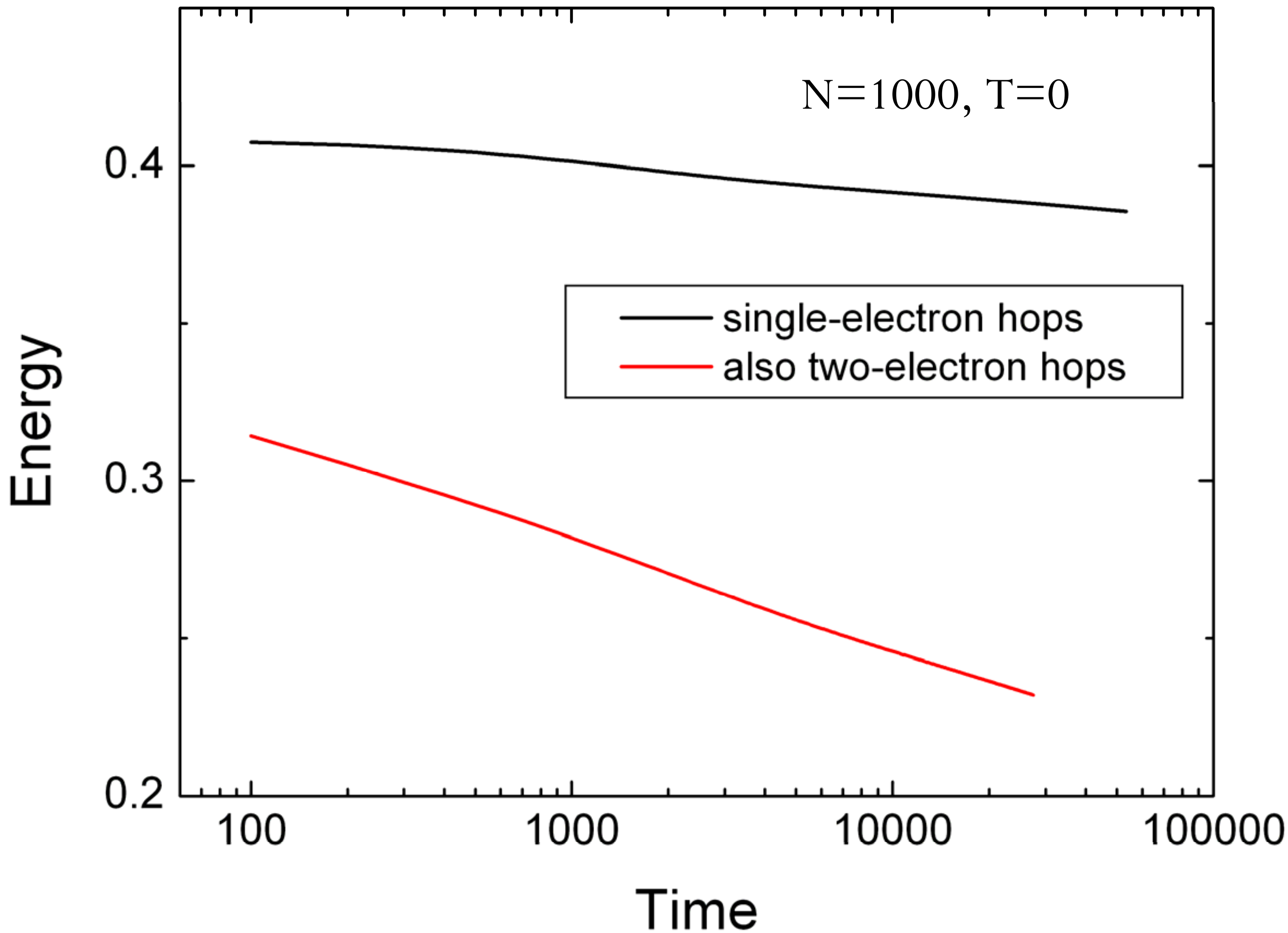
Conductance



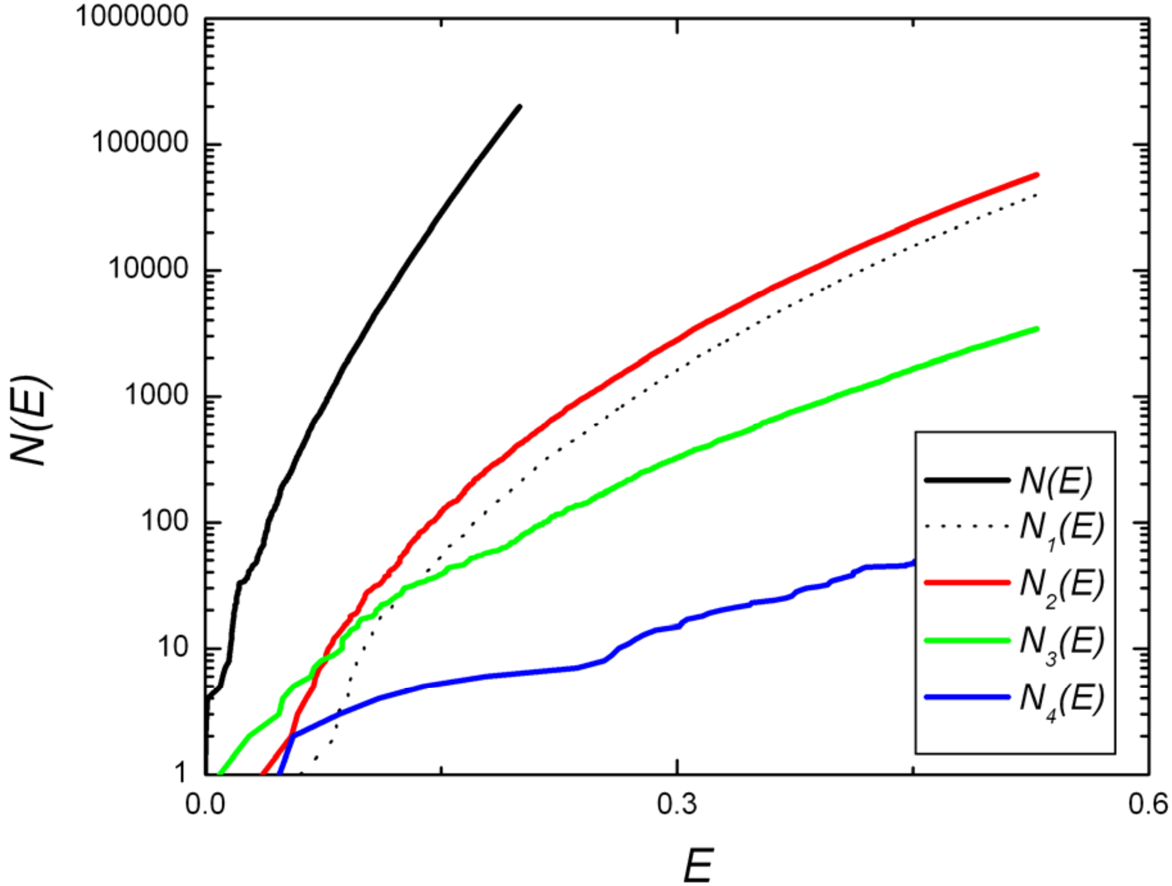
Direct search for cluster information

- Instead of calculating all low energy configurations, we directly search for configurations stable with respect one-electron hops shorter than a given distance.
- We store up to 250000 "metastable" states.
- The range of energies increases by a factor 10.

Two-electrons hops



Valley stability



Conclusions

- The Master Equation is an expensive but useful tool to get information hardly available from MonteCarlo.
- The effective temperatures in glassy systems may be explained without resorting to any thermalization mechanism.
- Many-electron hops are important in relaxation. Collective hops of several electrons may be necessary .
- The ME permits a possible implementation of "some" quantum effects.