Slow Relaxation and Equilibrium Dynamics in a 2 D Coulomb Glass: Demonstration of Stretched Exponential Energy Correlations

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with
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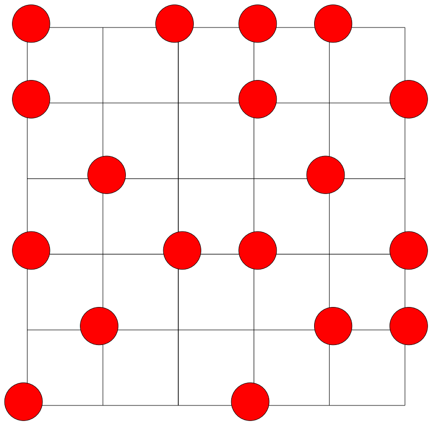
A simple model



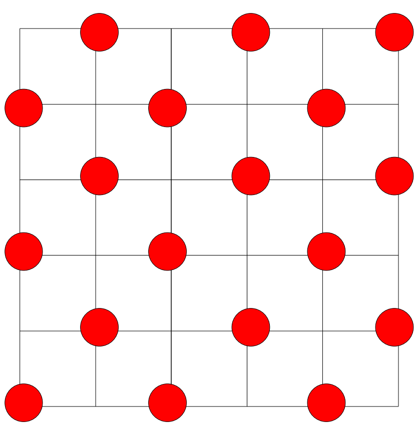
A square lattice with (typically) half as many electrons as lattice sites.

Electron energy:

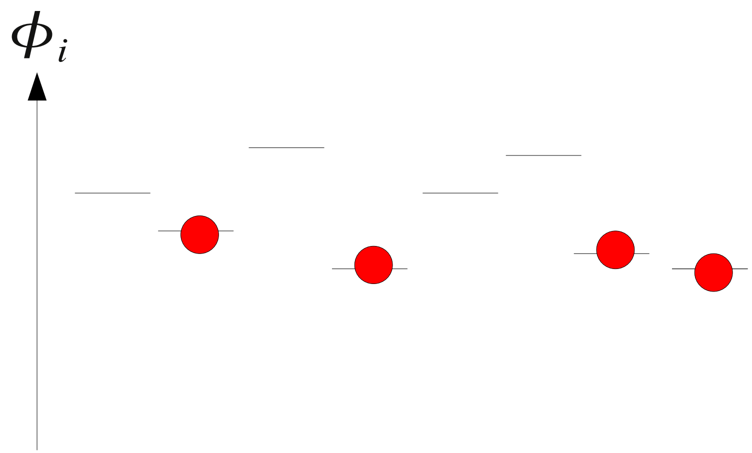
$$E_i = \phi_i + \sum_{j \neq i} \frac{e^2}{r_{ij}} (n_j - \nu)$$

Site energy, random in some interval [-U,U]

Coulomb energy from all the other electrons



Without disorder



Without interactions

With both

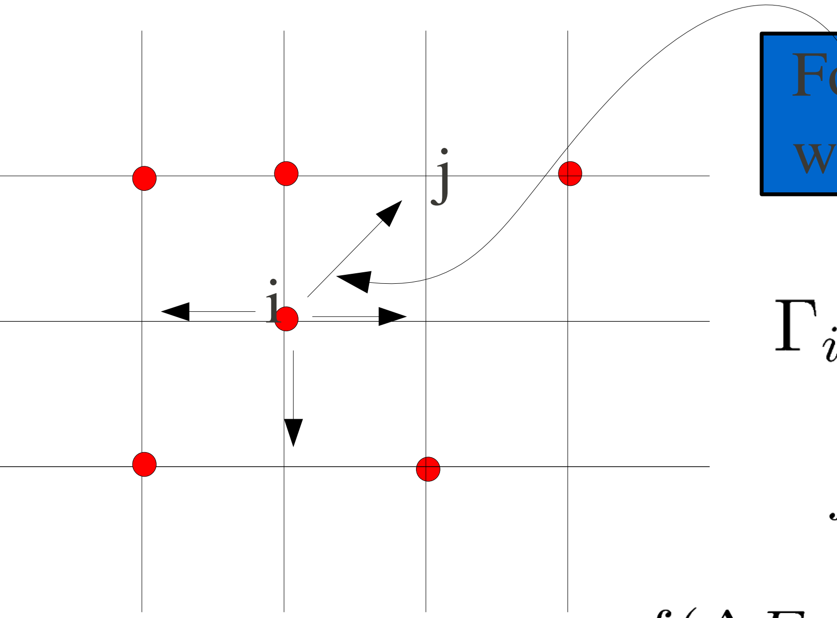
Metastable states

We can search for states (configurations) which are stable to all one-electron jumps. That is, the energy increases if we move one electron. Only for very small systems can we hope to find all such states.

Size	Number of metastable states
10 x 10:	29 - 114
15 x 15:	681 – 7832
20 x 20:	> 40000

The number of metastable states increases very rapidly with the size.
In simulations we typically use size 100x100.

Simulation of time evolution



For each possible transition (one electron jump) we can find a rate:

$$\Gamma_{i\to j} = t_0^{-1} e^{-2r_{i,j}/a_l} \frac{|\Delta E_{i\to j}|}{T_0} f(\Delta E_{i\to j}),$$

$$f(\Delta E_{i\to j}) = \frac{1}{e^{\Delta E_{i\to j}/T} - 1}, \qquad \Delta E_{i\to j} > 0.$$

$$f(\Delta E_{i\to j}) = 1 + \frac{1}{e^{|\Delta E_{i\to j}|/T} - 1}, \qquad \Delta E_{i\to j} < 0$$

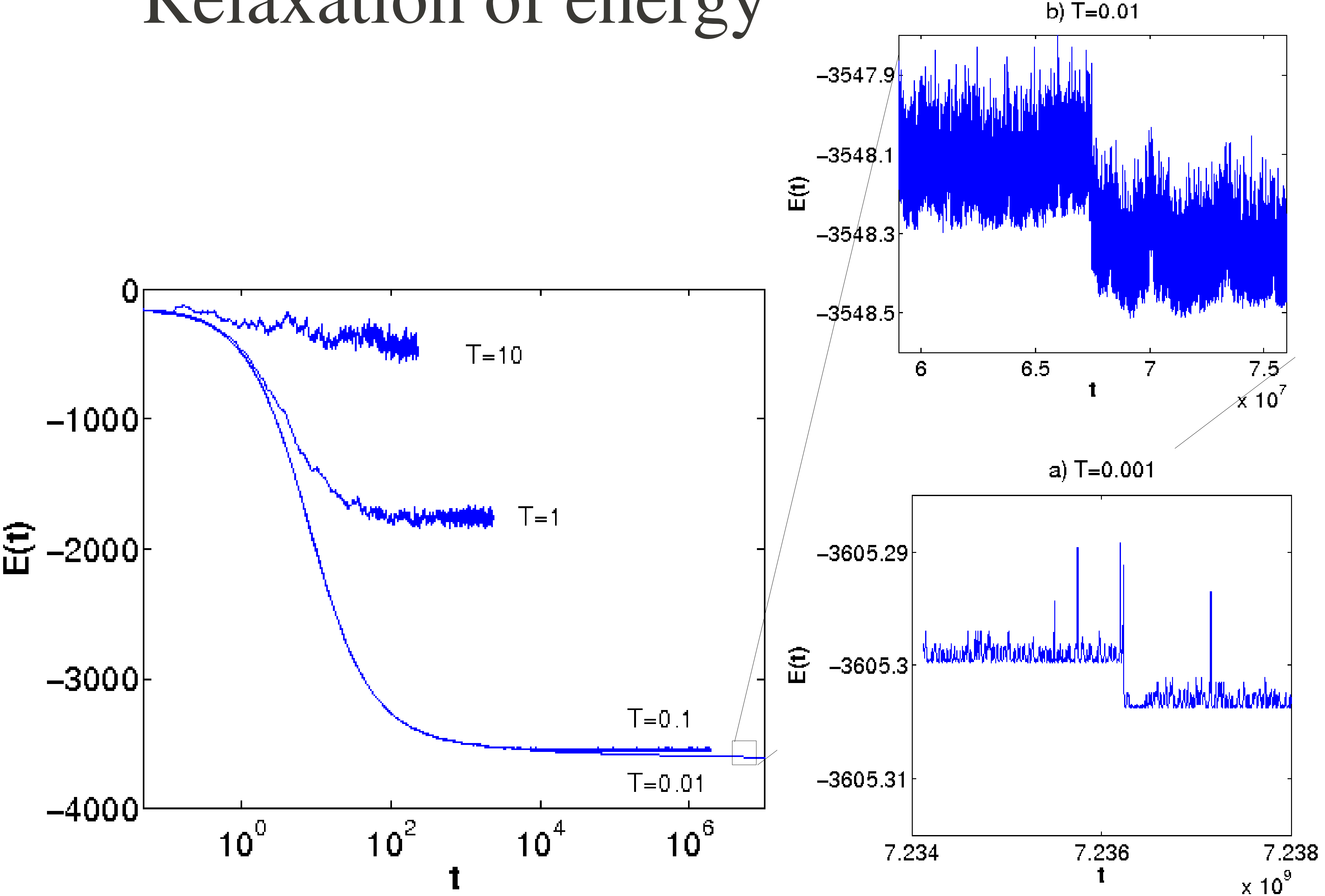
Approximately:

$$\Gamma \propto e^{-2r/a_l - \Delta E/T}$$

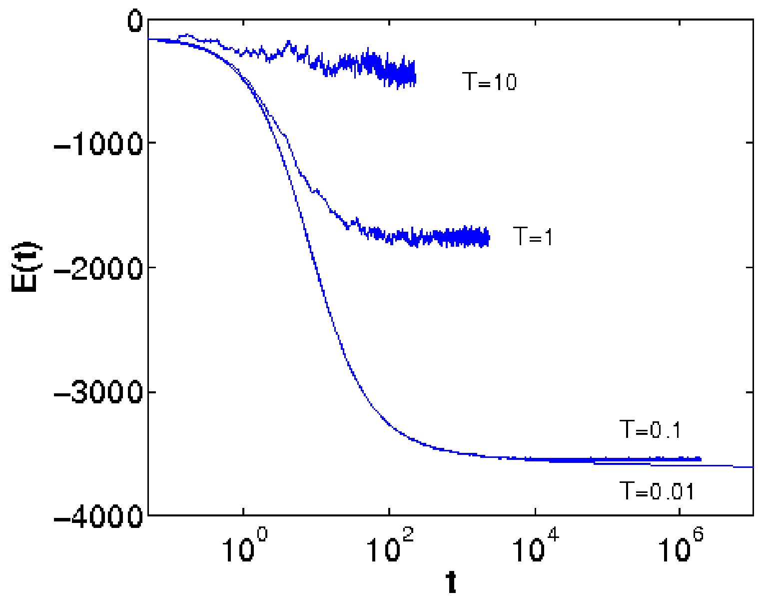
$$a_l = 2/3$$

Weighted by these rates, we select one electron to move, and where to move it. After each jump, all Coulomb energies have to be recalculated. This process is repeated many times ($10^6 - 10^8$).

Relaxation of energy



What is the shape of the relaxation curve?



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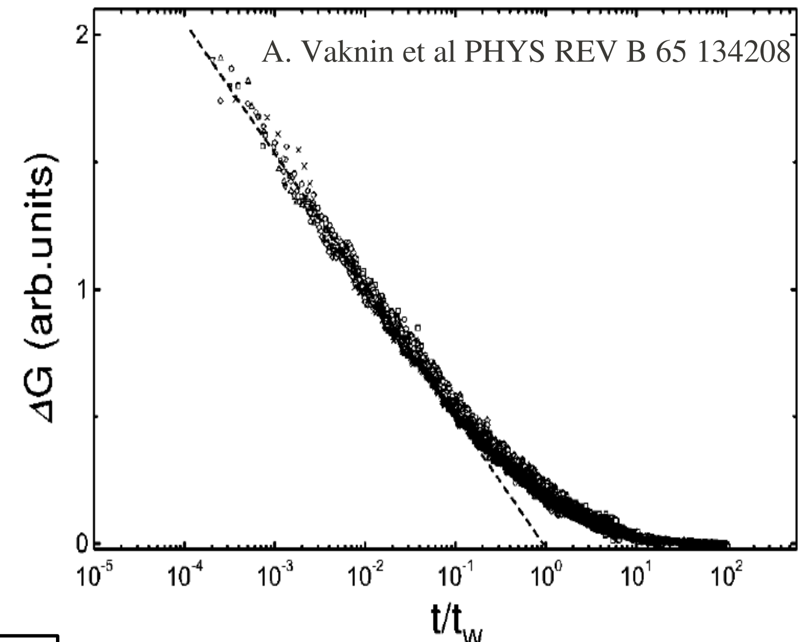

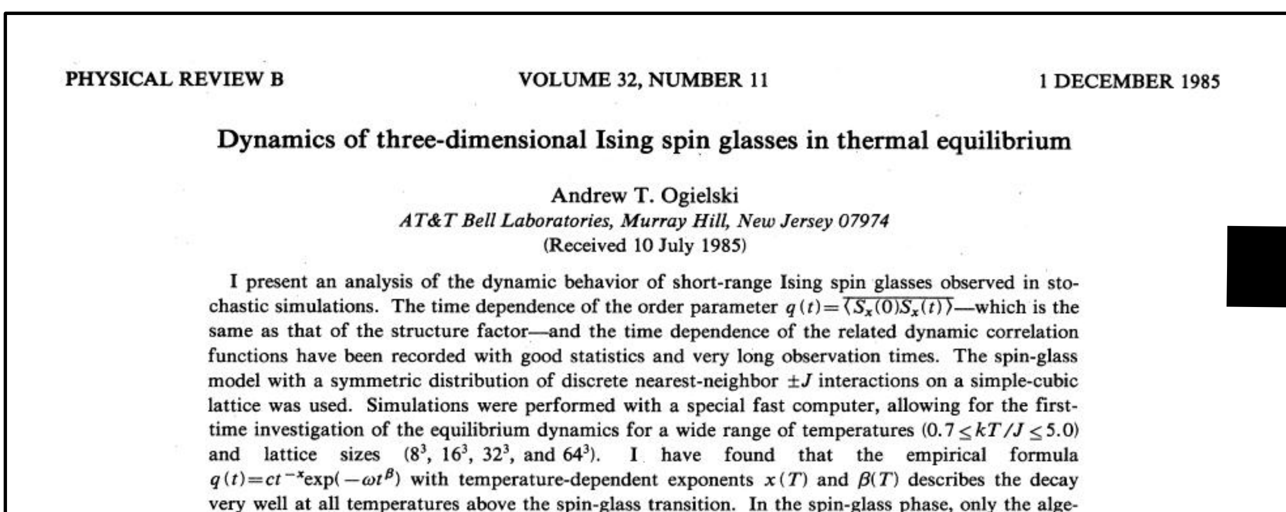

PHYSICAL REVIEW B VOLUME 32, NUMBER 11 1 DECEMBER 1985

Dynamics of three-dimensional Ising spin glasses in thermal equilibrium

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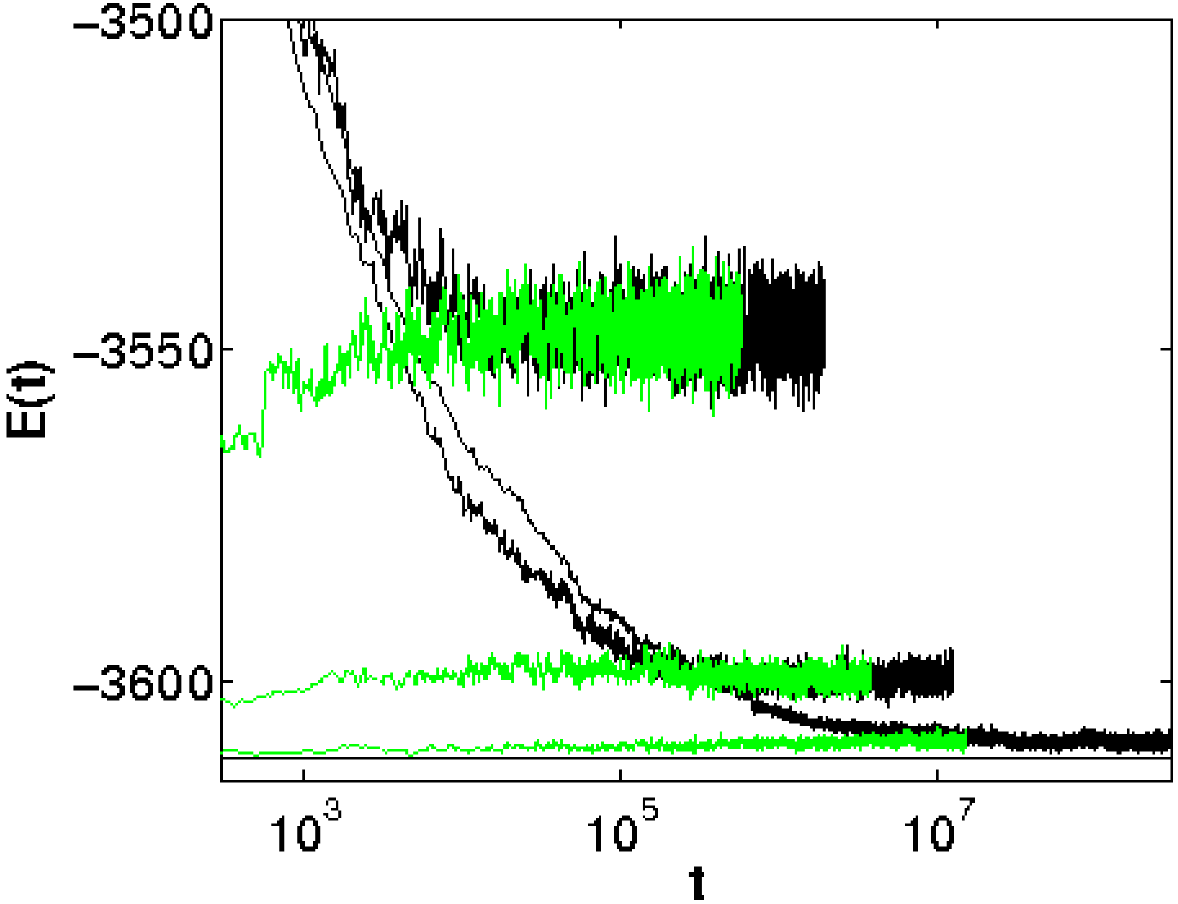
(Received 10 July 1985)

I present an analysis of the dynamic behavior of short-range Ising spin glasses observed in stochastic simulations. The time dependence of the order parameter $q(t)=\overline{\langle S_x(0)S_x(t)\rangle}$—which is the same as that of the structure factor—and the time dependence of the related dynamic correlation functions have been recorded with good statistics and very long observation times. The spin-glass model with a symmetric distribution of discrete nearest-neighbor $\pm J$ interactions on a simple-cubic lattice was used. Simulations were performed with a special fast computer, allowing for the first-time investigation of the equilibrium dynamics for a wide range of temperatures ($0.7 \le kT/J \le 5.0$) and lattice sizes (8^3, 16^3, 32^3, and 64^3). I have found that the empirical formula $q(t)=ct^{-x}\exp(-\omega t^{\beta})$ with temperature-dependent exponents $x(T)$ and $\beta(T)$ describes the decay very well at all temperatures above the spin-glass transition. In the spin-glass phase, only the alge-

Study the correlation function in equilibrium

Proof of equilibrium

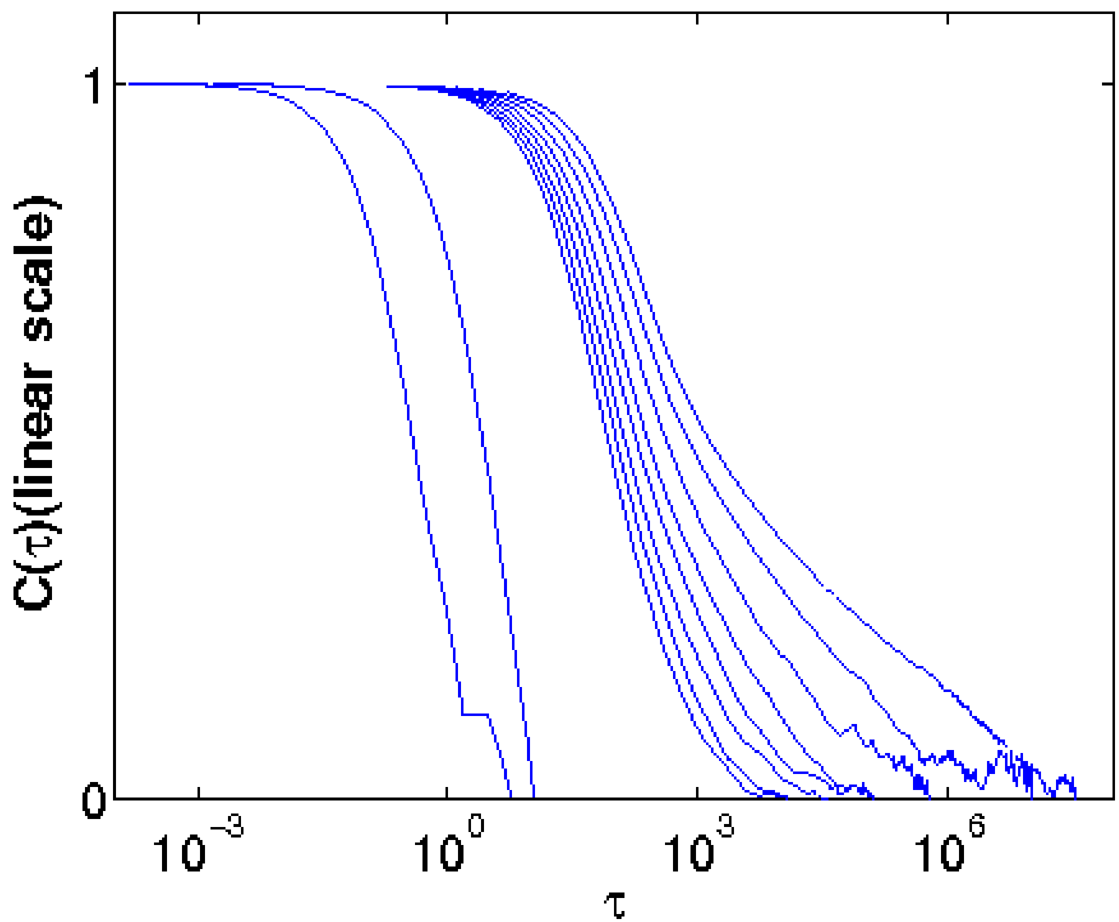


T = 0.03, 0.05, 0.1

Correlation function

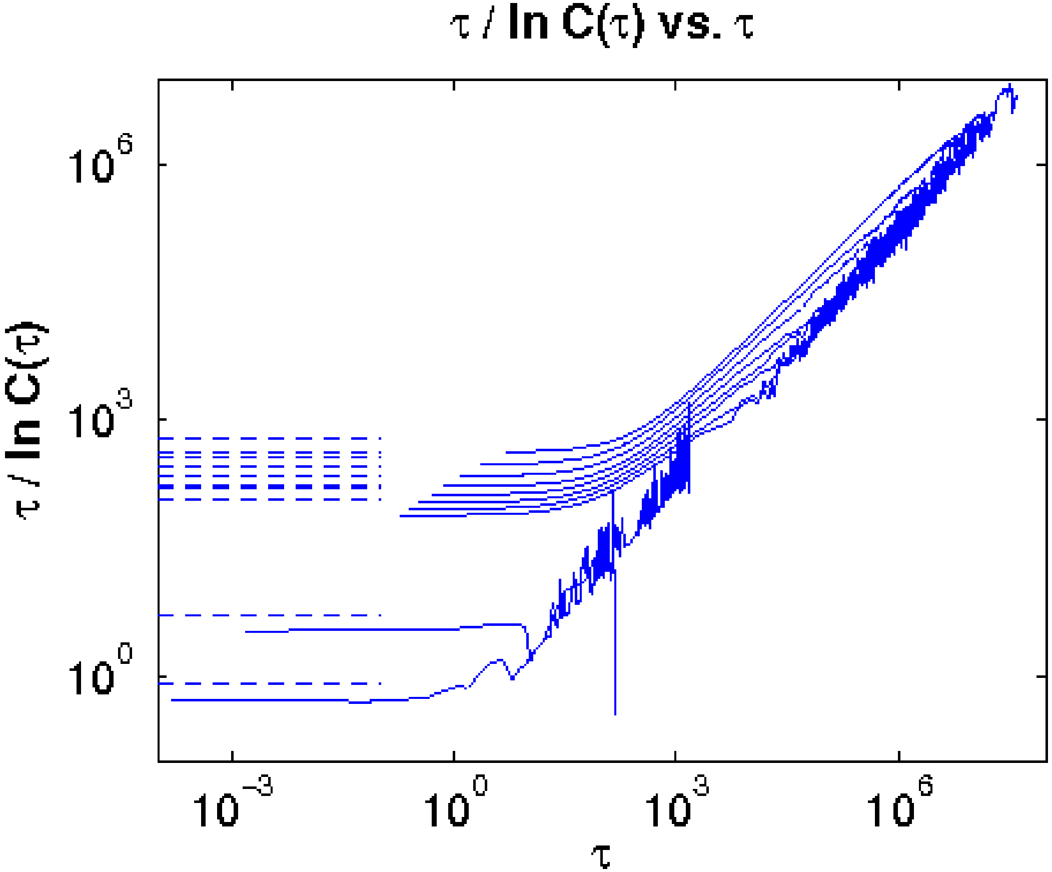
$$C(t, t+\tau) = \frac{1}{\sigma^2} \left\langle (E(t) - \bar{E})(E(t+\tau) - \bar{E}) \right\rangle$$

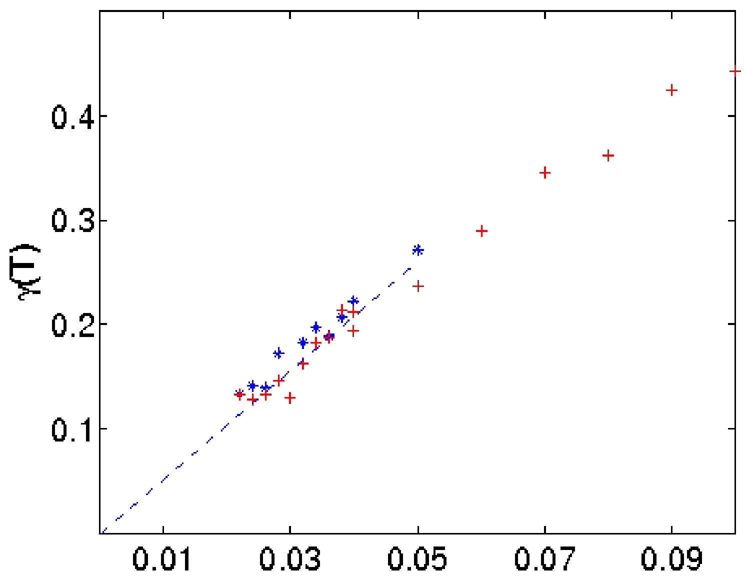
In equilibrium: $$C(\tau) = \frac{1}{\sigma^2} \left\langle (E(t) - \bar{E})(E(t+\tau) - \bar{E}) \right\rangle_t$$

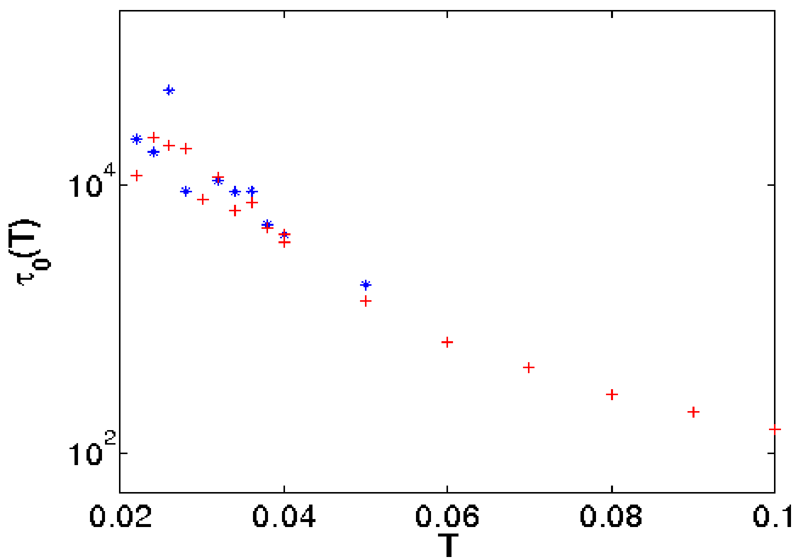


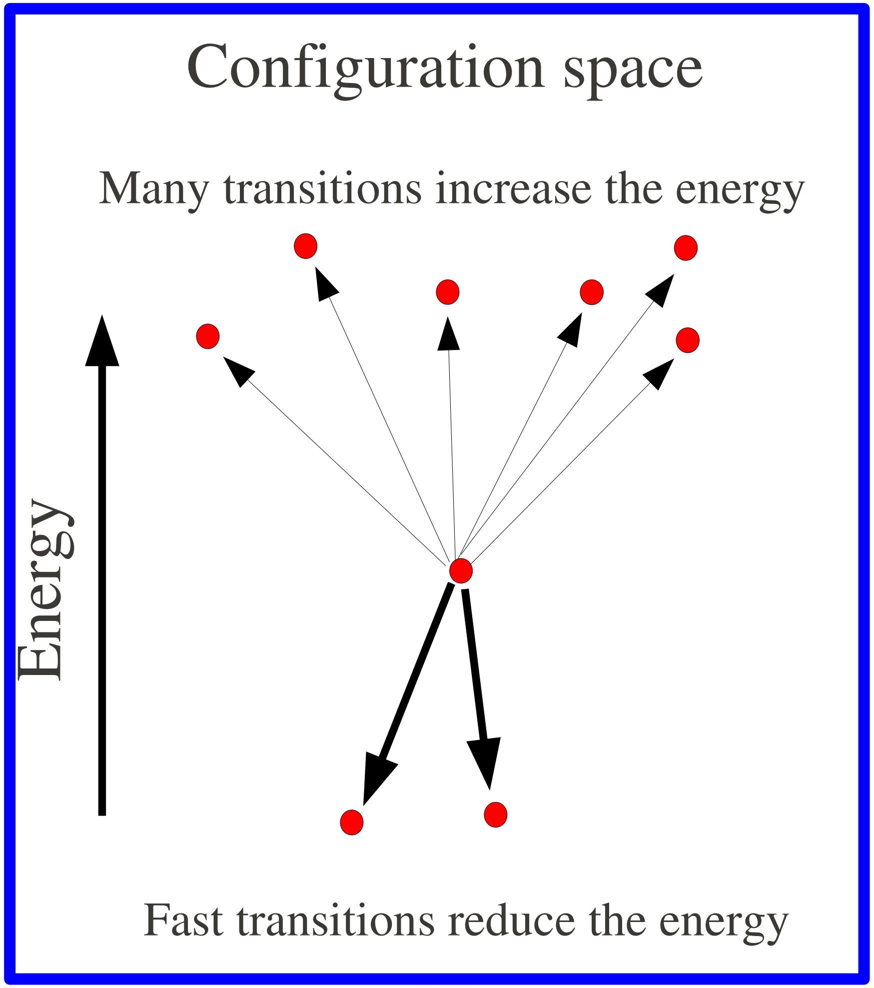
Stretched exponential behaviour

$$C(\tau) = Ae^{-(\tau/\tau_0)^\gamma}$$

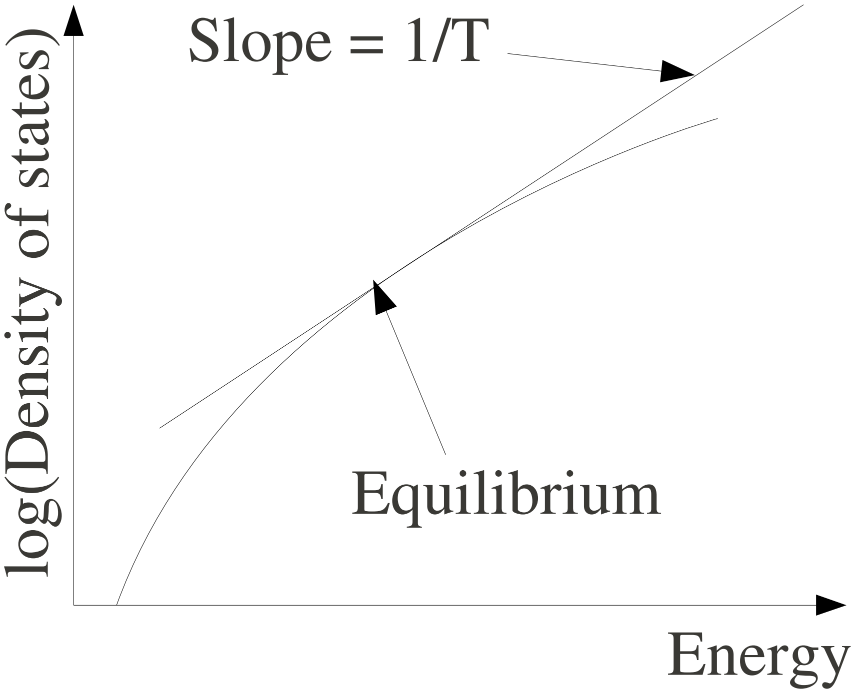








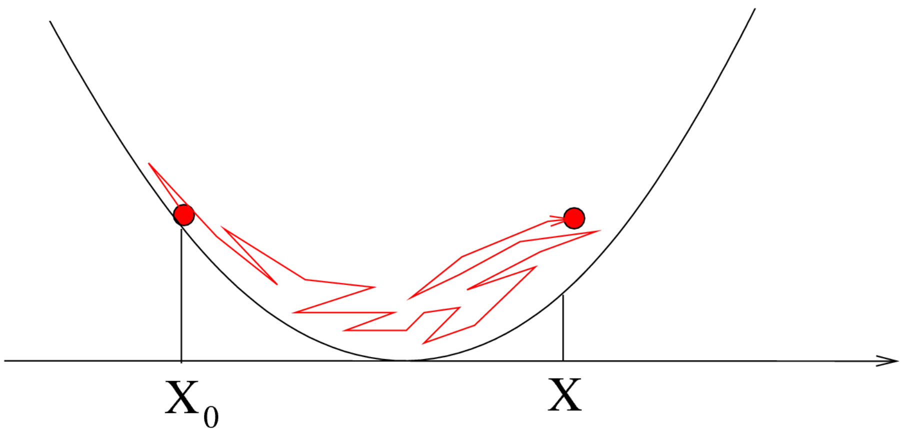
Equilibrium is the balance between the system wanting to reduce its energy and the increase of the density of states



Close to equilibrium it is like a random walk in a harmonic potential.

If there are no other constraints!

RW in a harmonic potential



$$u(x, x_0, t) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{c}{D(1 - e^{-2ct})}} e^{-\frac{(x - x_0 e^{-ct})^2 c}{2D(1 - e^{-2ct})}}.$$

S. Chandrasekhar, Rev. Mod. Phys. 15, 1–89 (1943)

$$C(t) = \int\int dE_0 dE \, E_0 E u(\infty) u(E, E_0, t) = e^{-ct}$$

There has to be some constraints in our dynamics

RW on fractal

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Random walks on fractals and stretched exponential relaxation

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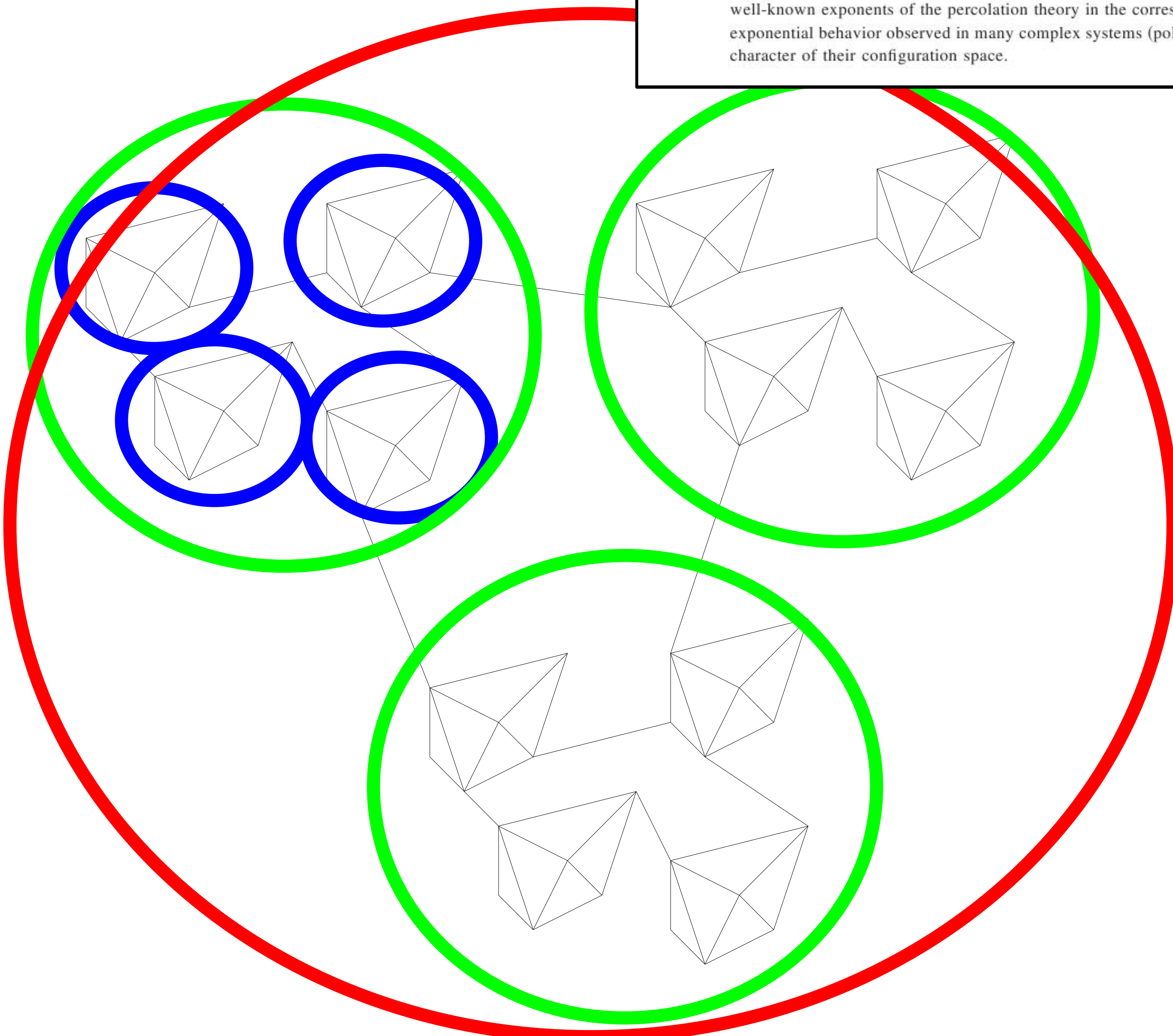
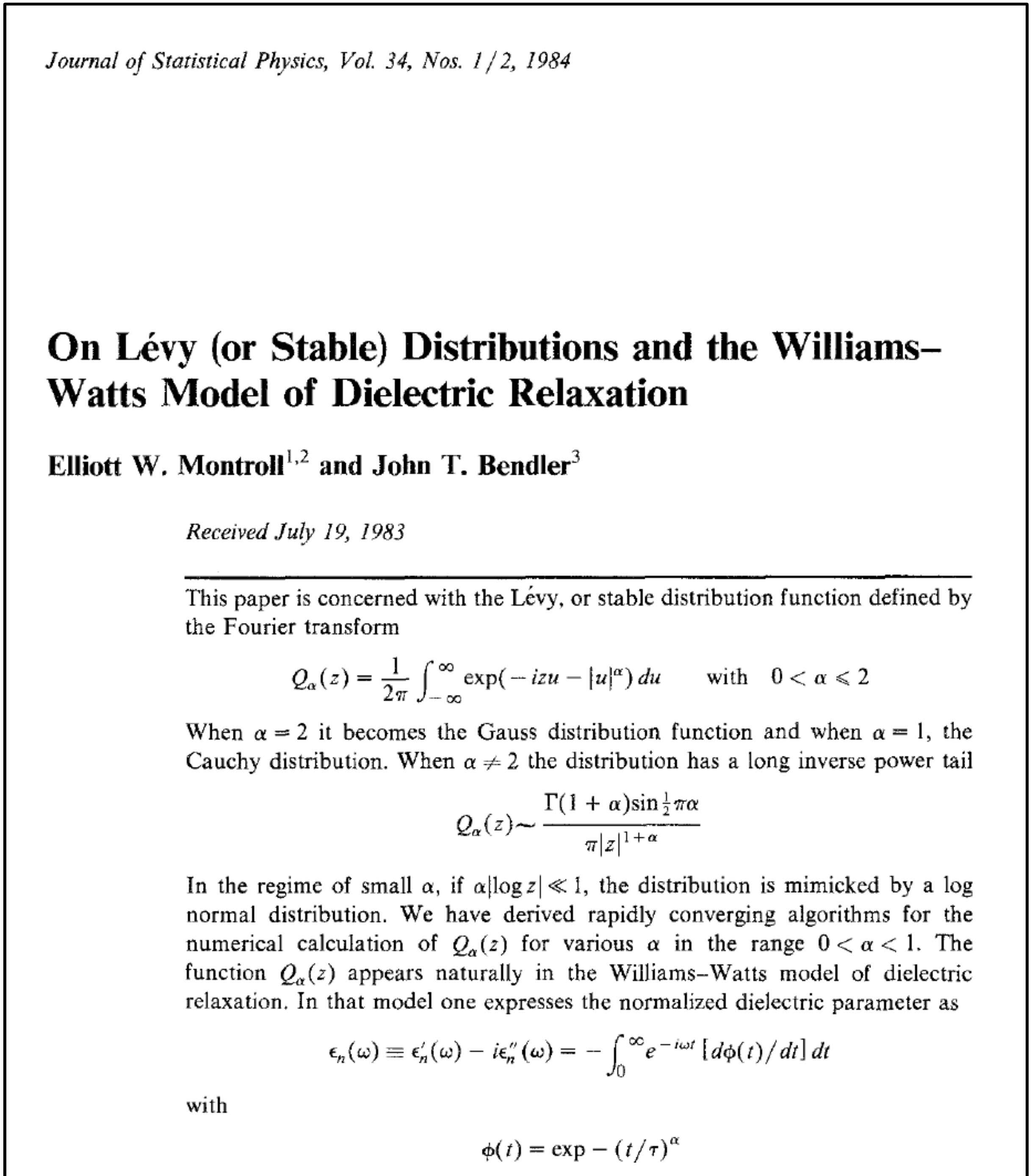
Stretched exponential relaxation $[\exp-(t/\tau)^{\beta_K}]$ is observed in a large variety of systems but has not been explained so far. Studying random walks on percolation clusters in curved spaces whose dimensions range from 2 to 7, we show that the relaxation is accurately a stretched exponential and is directly connected to the fractal nature of these clusters. Thus we find that in each dimension the decay exponent β_K is related to well-known exponents of the percolation theory in the corresponding flat space. We suggest that the stretched exponential behavior observed in many complex systems (polymers, colloids, glasses, . . .) is due to the fractal character of their configuration space.





Journal of Statistical Physics, Vol. 34, Nos. 1/2, 1984

On Lévy (or Stable) Distributions and the Williams–Watts Model of Dielectric Relaxation

Elliott W. Montroll[1,2] and John T. Bendler[3]

Received July 19, 1983

This paper is concerned with the Lévy, or stable distribution function defined by the Fourier transform

$$Q_\alpha(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-izu - |u|^\alpha)\,du \qquad \text{with} \quad 0 < \alpha \leqslant 2$$

When $\alpha = 2$ it becomes the Gauss distribution function and when $\alpha = 1$, the Cauchy distribution. When $\alpha \neq 2$ the distribution has a long inverse power tail

$$Q_\alpha(z) \sim \frac{\Gamma(1+\alpha)\sin\frac{1}{2}\pi\alpha}{\pi|z|^{1+\alpha}}$$

In the regime of small α, if $\alpha|\log z| \ll 1$, the distribution is mimicked by a log normal distribution. We have derived rapidly converging algorithms for the numerical calculation of $Q_\alpha(z)$ for various α in the range $0 < \alpha < 1$. The function $Q_\alpha(z)$ appears naturally in the Williams–Watts model of dielectric relaxation. In that model one expresses the normalized dielectric parameter as

$$\epsilon_n(\omega) \equiv \epsilon_n'(\omega) - i\epsilon_n''(\omega) = -\int_0^\infty e^{-i\omega t}\,[d\phi(t)/dt]\,dt$$

with

$$\phi(t) = \exp-(t/\tau)^\alpha$$

Distribution of relaxation rates:

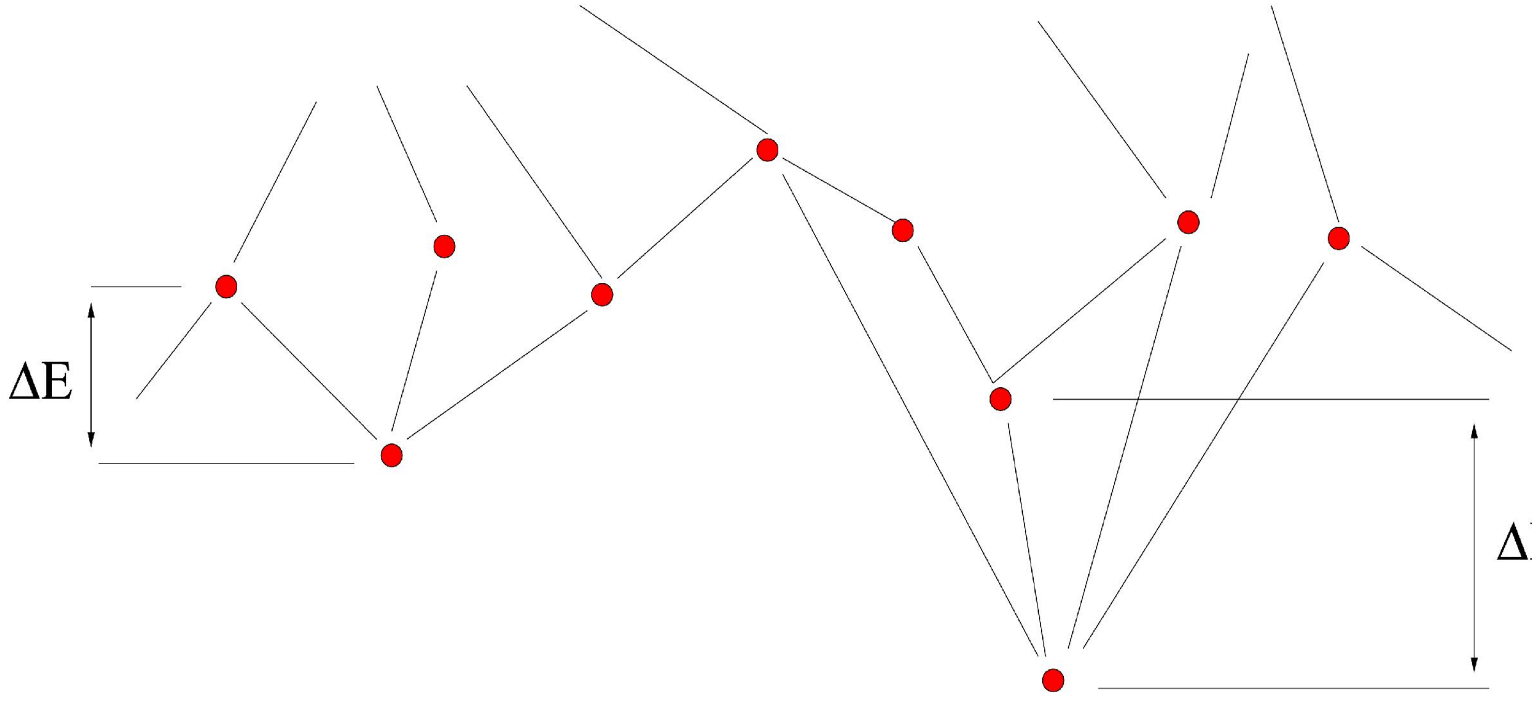
$$E(t) = \int d\lambda P(\lambda) e^{-\lambda t}$$

Question:
For which $P(\lambda)$ will $E(t)$ be stretched exponential?

Answer:

$$P(\lambda) = \text{Stable Levy distribution}$$

These arise from sums of random variables with inverse power-law tail distributions.



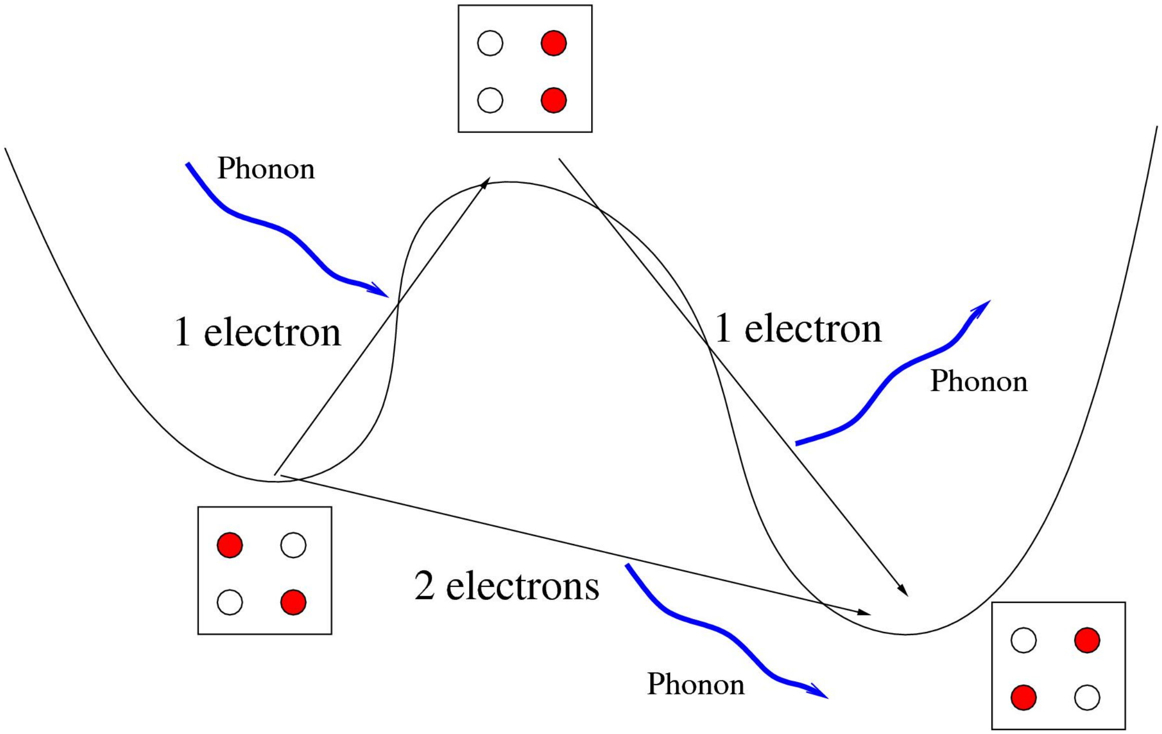
Time to escape from a trap of depth ΔE: $\tau = \tau_0 e^{\Delta E / T}$

Assume the distribution: $p(\Delta E) = e^{-\Delta E / T_0}$

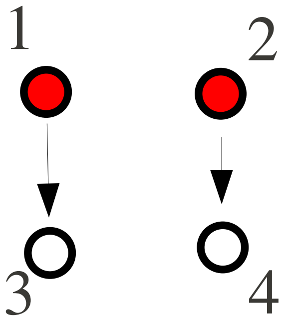
Then: $p(\tau) = 1/\tau^{(1+\beta)}$ $\beta = T / T_0$

Two-electron transitions

With
Miguel Ortuno and Andres Somoza
University of Murcia



Moving two electrons at the same time can avoid energy barriers



6 states with 2 electrons on 4 sites:

$$\left|\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}\right\rangle \quad \left|\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}\right\rangle \quad \left|\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}\right\rangle \quad \left|\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}\right\rangle \quad \left|\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}\right\rangle \quad \left|\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}\right\rangle$$

Tunneling as a perturbation:

$$\Delta H = \sum_{i<j} t_{ij} c_i^\dagger c_j + \text{h.c.}$$

$$t_{ij} = e^{-r_{ij}/a}$$

Perturbed eigenstates:

$$\left|\widetilde{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}}\right\rangle = \left|\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}\right\rangle + \frac{t_{23}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}}}\left|\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}\right\rangle + \frac{t_{24}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}}}\left|\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}\right\rangle + \frac{t_{13}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}}}\left|\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}\right\rangle + \frac{t_{14}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}}\left|\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}\right\rangle$$
$$+ \frac{1}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}}}\left[\frac{t_{23}t_{14}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}}} + \frac{t_{13}t_{24}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}}} + \frac{t_{13}t_{24}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}}} + \frac{t_{23}t_{14}}{E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}}\right]\left|\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}\right\rangle$$

$$\left|\widetilde{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}}\right\rangle = \left|\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}\right\rangle + \frac{t_{14}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}}}\left|\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}\right\rangle + \frac{t_{13}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}}}\left|\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}\right\rangle + \frac{t_{24}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}}}\left|\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}\right\rangle + \frac{t_{23}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}}\left|\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}\right\rangle$$
$$+ \frac{1}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}}}\left[\frac{t_{23}t_{14}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}}} + \frac{t_{13}t_{24}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}}} + \frac{t_{13}t_{24}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}}} + \frac{t_{23}t_{14}}{E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}}\right]\left|\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}\right\rangle$$

Phonon assisted transitions between these:

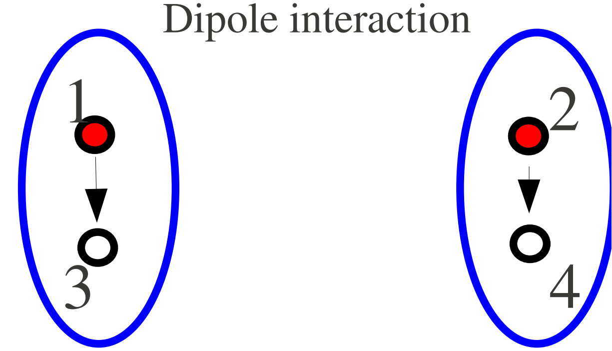
$$\left|\left\langle\widetilde{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}}\right| H_{\text{e-ph}} \left|\widetilde{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}}\right\rangle\right|^2 \qquad H_{\text{e-ph}} = \sum_{\mathbf{q}} \sum_i c_i^\dagger c_i \left(e^{-i\mathbf{q}\mathbf{r}_i}\gamma_{\mathbf{q}} b_{\mathbf{q}} + \text{h.c.}\right)$$

Transition rate:

$$E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}} + E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}} = V_{12} - V_{23} + V_{34} - V_{14}$$

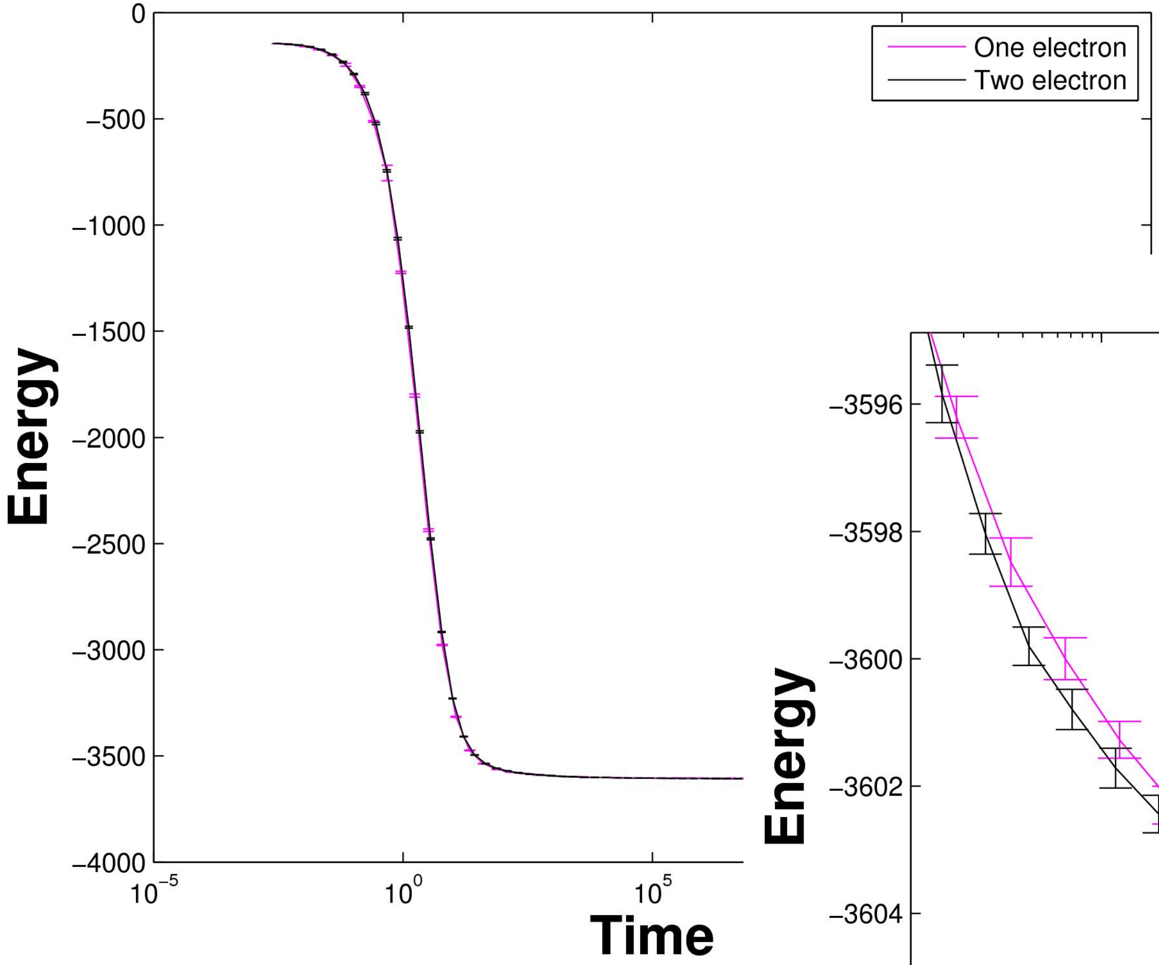
$$\Gamma_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix} \to \begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} = \frac{1}{\tau_0}\min(1, e^{-\Delta E/T})\left[|t_{13}t_{24}|^2\left(E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}} + E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}\right)^2\right.$$
$$+ |t_{23}t_{14}|^2\left(E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}} + E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}\right)^2$$
$$\left. + t_{13}t_{24}t_{23}t_{14}\left(E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\bullet&\circ\end{smallmatrix}} + E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\circ&\bullet\end{smallmatrix}}\right)\left(E_{\begin{smallmatrix}\circ&\circ\\\bullet&\bullet\end{smallmatrix}} - E_{\begin{smallmatrix}\bullet&\circ\\\bullet&\circ\end{smallmatrix}} + E_{\begin{smallmatrix}\bullet&\bullet\\\circ&\circ\end{smallmatrix}} - E_{\begin{smallmatrix}\circ&\bullet\\\circ&\bullet\end{smallmatrix}}\right)\right]$$

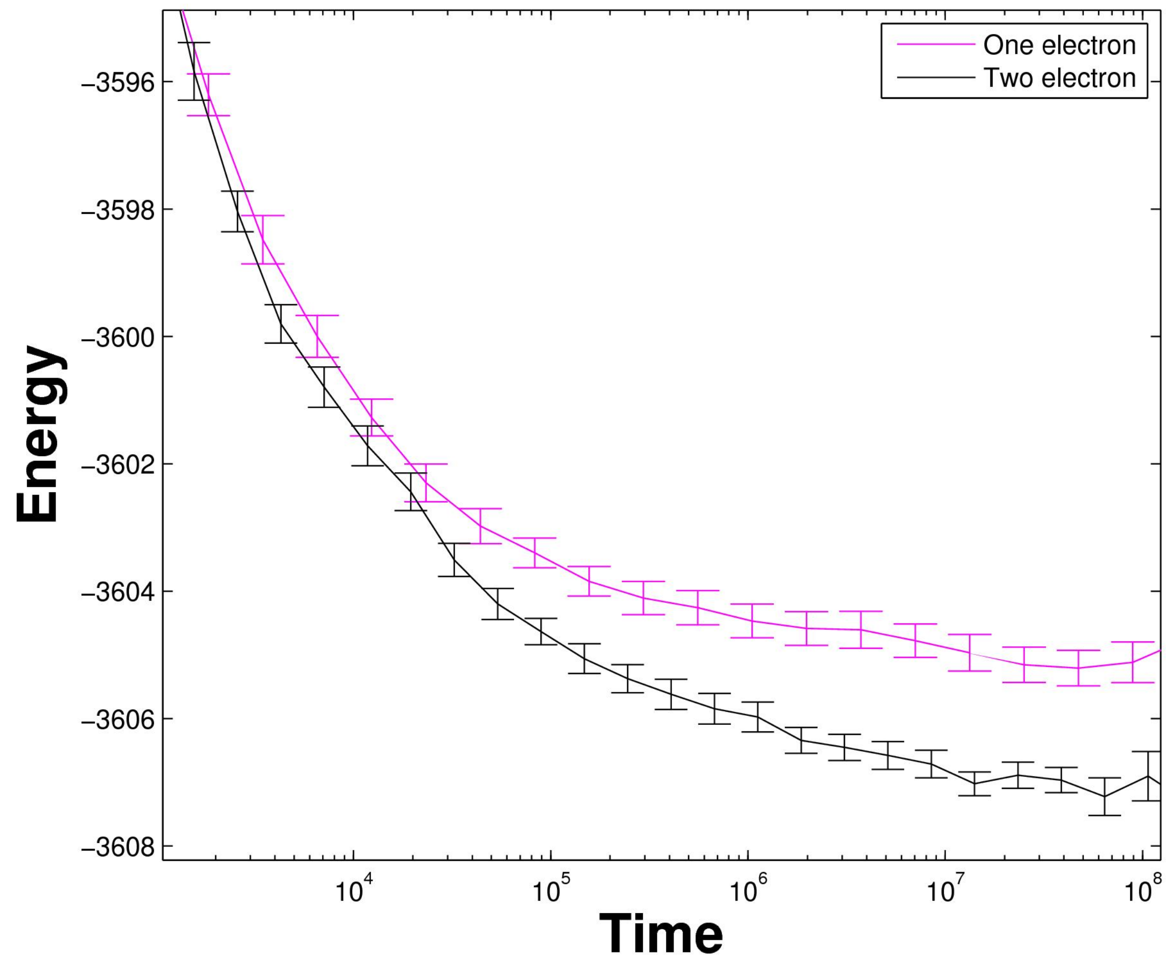
Dipole interaction

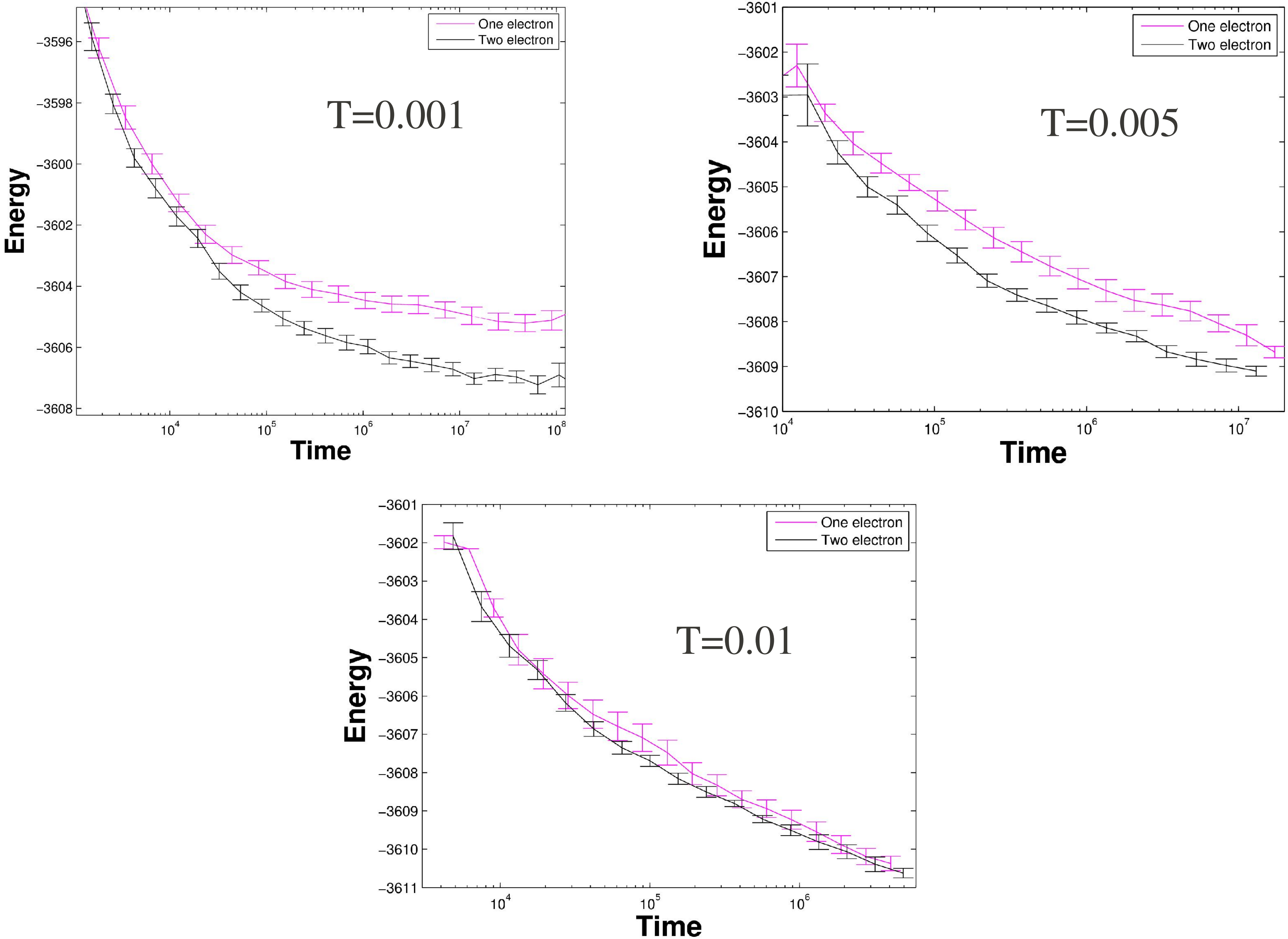


Relaxation of energy

T = 0.001, random initial state

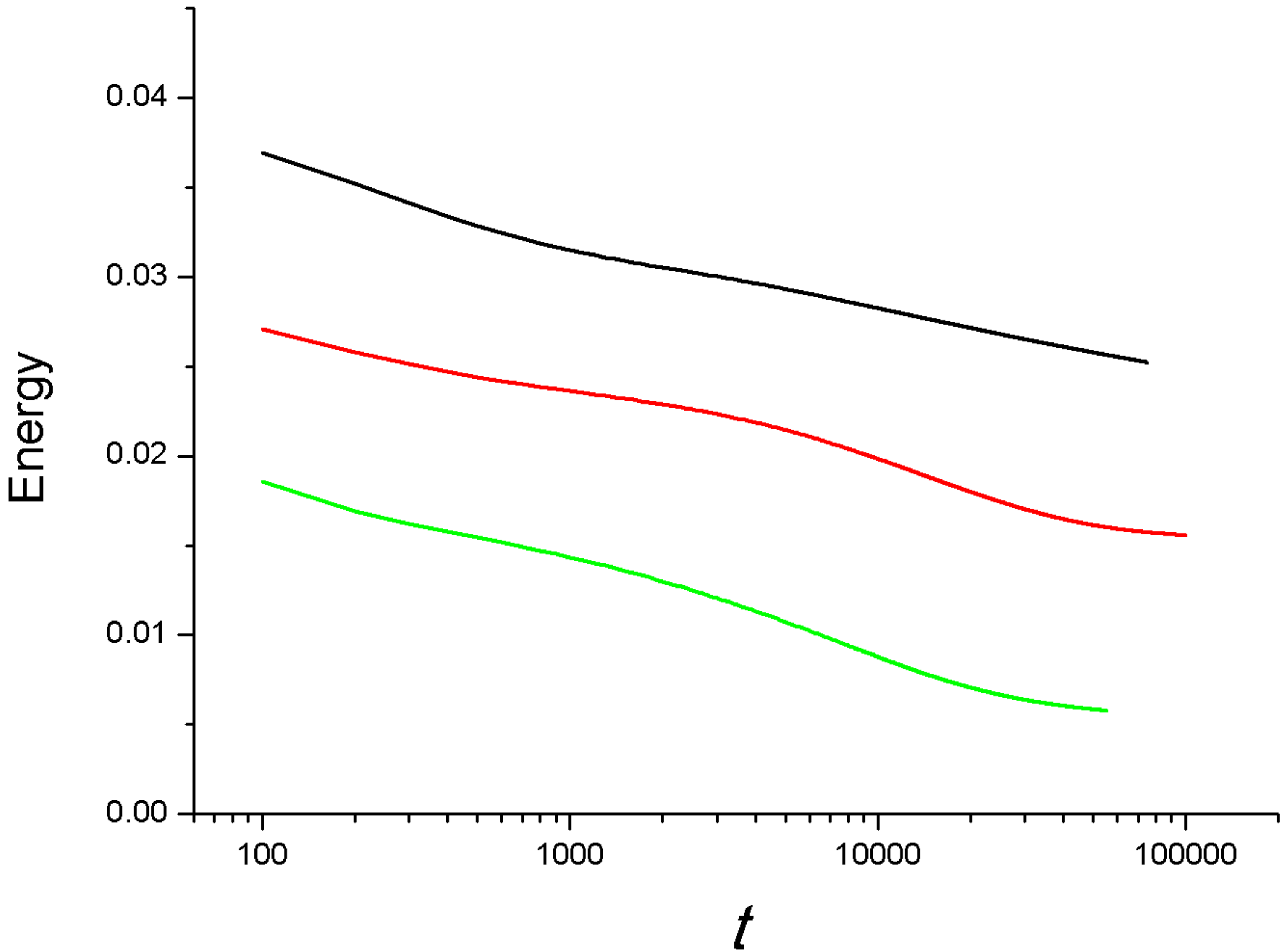


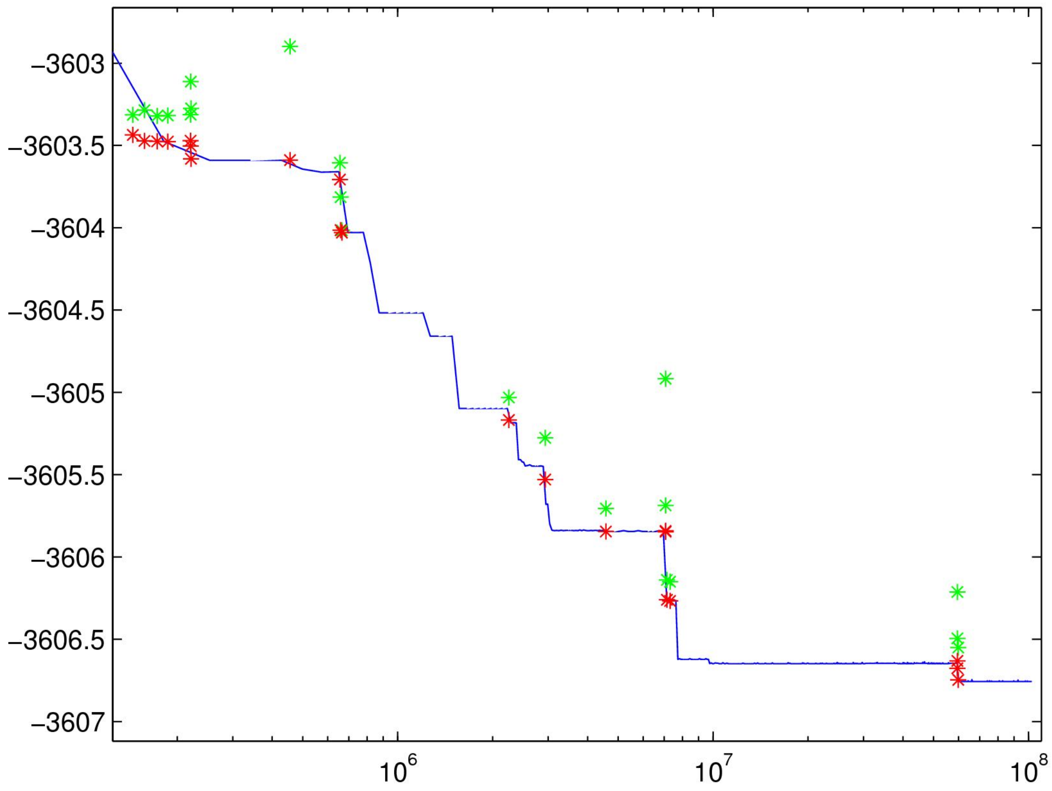




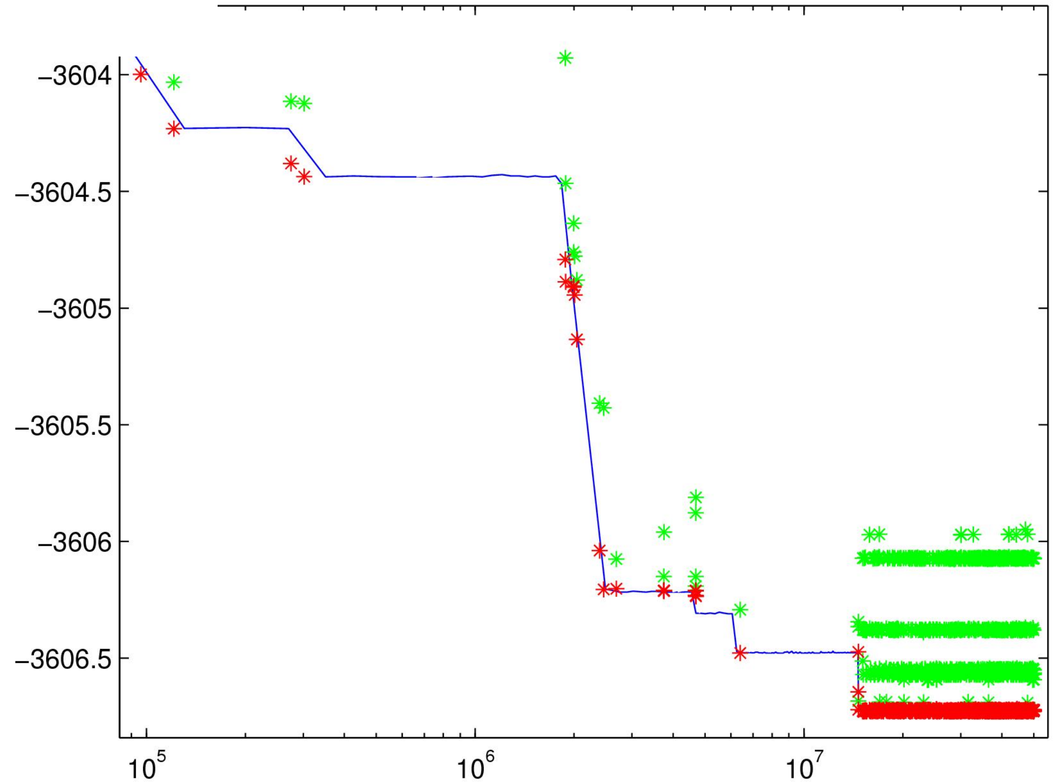
T=0.001
One electron
Two electron
Energy
Time
T=0.005
One electron
Two electron
Energy
Time
T=0.01
One electron
Two electron
Energy
Time

Master equation

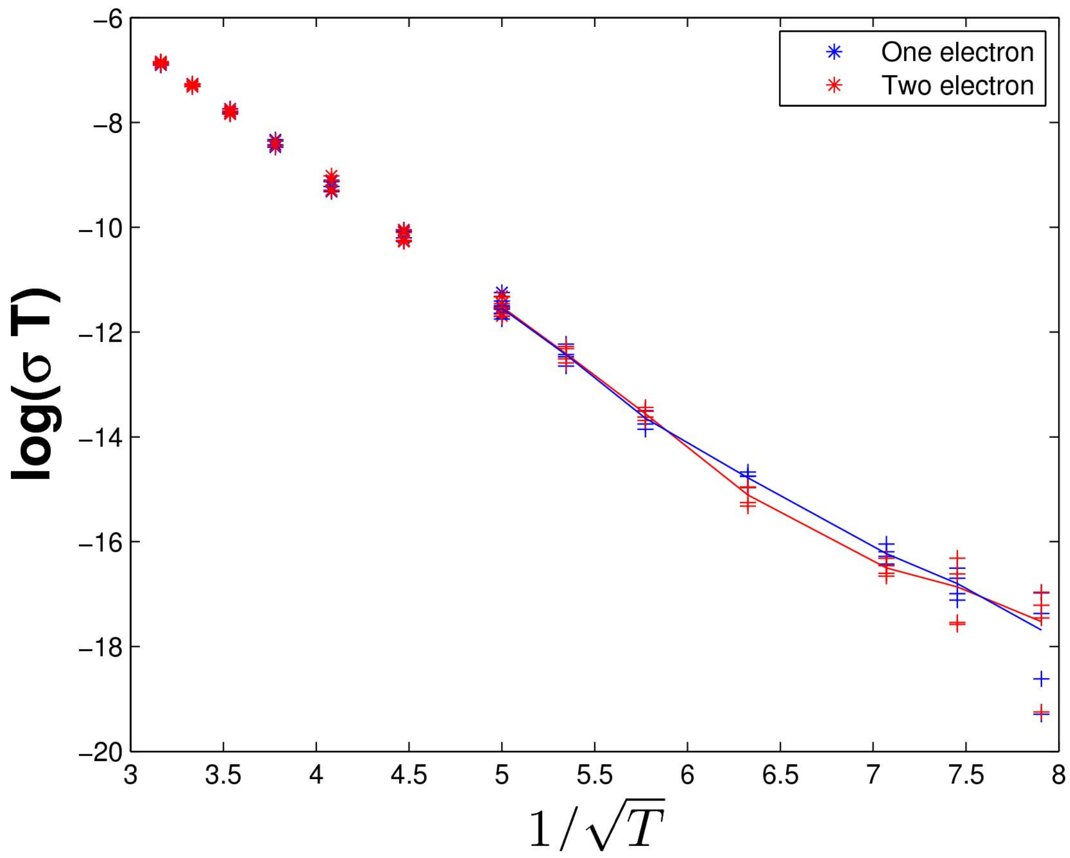




Two-electron jumps are correlated with sudden drops in the energy.



Conductance



Summary

- At temperatures above T=0.02 we can demonstrate that the system reaches equilibrium
- At temperatures above but close to this temperature, the correlation function shows a stretched exponential law.
- This might be explained by a fractal structure of the configuration space or a broad distribution of trapping times.
- Two-electron transitions facilitates relaxation by letting the system escape from traps.