On some physical applications of random hierarchical matrices

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Structure of the talk

1. Physical motivations for the consideration of random block-hierarchical matrices, of their statistical and dynamic properties;

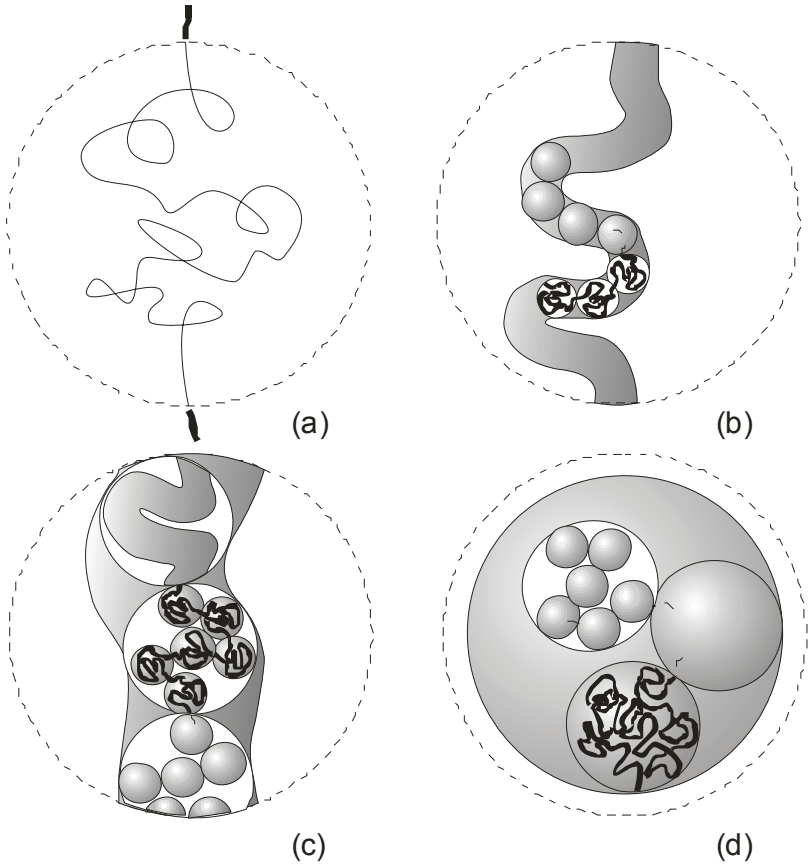
2. Kinetic random block-hierarchical matrices in “basin-to-basin” protein dynamics;

3. Random block-hierarchical matrices as adjacency matrices of random hierarchical graphs.

Physical motivations for the consideration of random block-hierarchical matrices

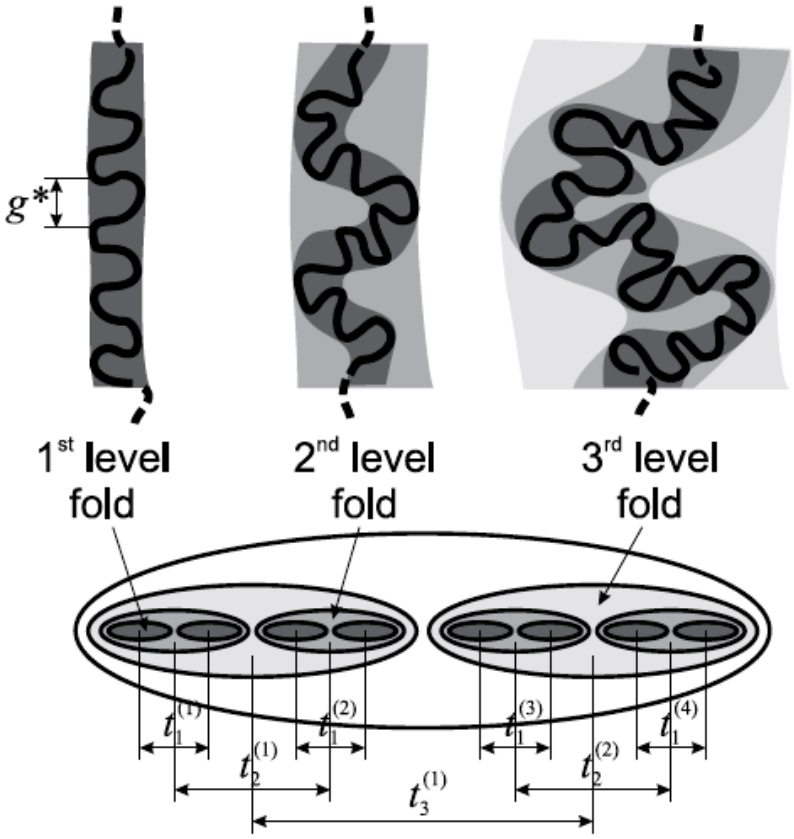
I. Contact map of the polymer collapse

Collapsed (globular) state of unknotted ring polymer chain after a temperature jump from θ–temperature to T ($T<\theta$)



A.Grosberg, E.Schakhnovich, S.N, 1988

Three subsequent stages of the hierarchical contact map (adjacency matrix) construction



(a)

$$T=\begin{array}{|cc|cc|cccc|}
\hline
0 & t_1^{(1)} & t_2^{(1)} & t_2^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
t_1^{(1)} & 0 & t_2^{(1)} & t_2^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
\hline
t_2^{(1)} & t_2^{(1)} & 0 & t_1^{(2)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
t_2^{(1)} & t_2^{(1)} & t_1^{(2)} & 0 & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
\hline
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & 0 & t_1^{(3)} & t_2^{(2)} & t_2^{(2)} \\
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_1^{(3)} & 0 & t_2^{(2)} & t_2^{(2)} \\
\hline
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_2^{(2)} & t_2^{(2)} & 0 & t_1^{(4)} \\
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_2^{(2)} & t_2^{(2)} & t_1^{(4)} & 0 \\
\hline
\end{array}$$

(b)

II. “Basin-to-basin” kinetics in disordered complex systems

Myoglobin (Mb) = 153 amino acids that form a globular protein. The energy landscape (EL) in Mb is organized in a **hierarchy of a number of tiers**.

The top tier, **CS0** = major conformations, **A0**; **A1**; **A3**. In **A1** a histidine 64, is inside the protein, in **A0** it extends into the solvent.

Within each of these **CS0** there exist a large number of **CS1α**; within each **CS1α** there are again substates which called **CS1β** and so on…

H. Frauenfelder et al, Science **254** (1991) 1598;
P.W. Fenimore, et al, Physica A **351** (2005) 1

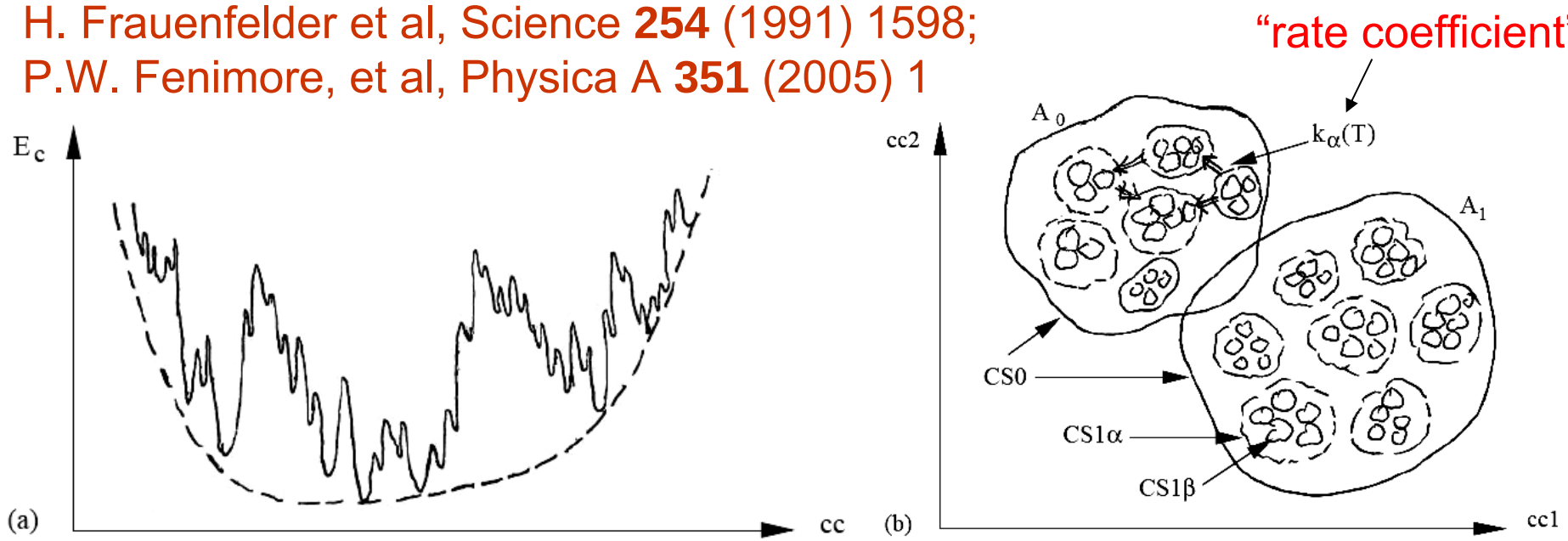


Fig. 1. (a) 1D cross section through the energy landscape of Mb. E_c is the conformational energy as a function of a confomational coordinate cc. (b) The 2D cross section through the EL already gives a better picture and shows that many paths lead from one particular substate to another one.

Kinetic random block-hierarchical matrices in "basin-to-basin" protein dynamics

Stochastic motion in a *regular* ultrametric Energy Landscape is usually encoded in a Parisi-type transition matrix:

$$T = \begin{array}{|cc|cc|cccc|}
\hline
\varepsilon & q_1 & q_2 & q_2 & q_3 & q_3 & q_3 & q_3 \\
q_1 & \varepsilon & q_2 & q_2 & q_3 & q_3 & q_3 & q_3 \\
\hline
q_2 & q_2 & \varepsilon & q_1 & q_3 & q_3 & q_3 & q_3 \\
q_2 & q_2 & q_1 & \varepsilon & q_3 & q_3 & q_3 & q_3 \\
\hline
q_3 & q_3 & q_3 & q_3 & \varepsilon & q_1 & q_2 & q_2 \\
q_3 & q_3 & q_3 & q_3 & q_1 & \varepsilon & q_2 & q_2 \\
\hline
q_3 & q_3 & q_3 & q_3 & q_2 & q_2 & \varepsilon & q_1 \\
q_3 & q_3 & q_3 & q_3 & q_2 & q_2 & q_1 & \varepsilon \\
\hline
\end{array}$$

Since T is a transition matrix, one has the "conservation" condition:

$$\varepsilon + q_1 + 2q_2 + 4q_3 + \ldots = 0$$

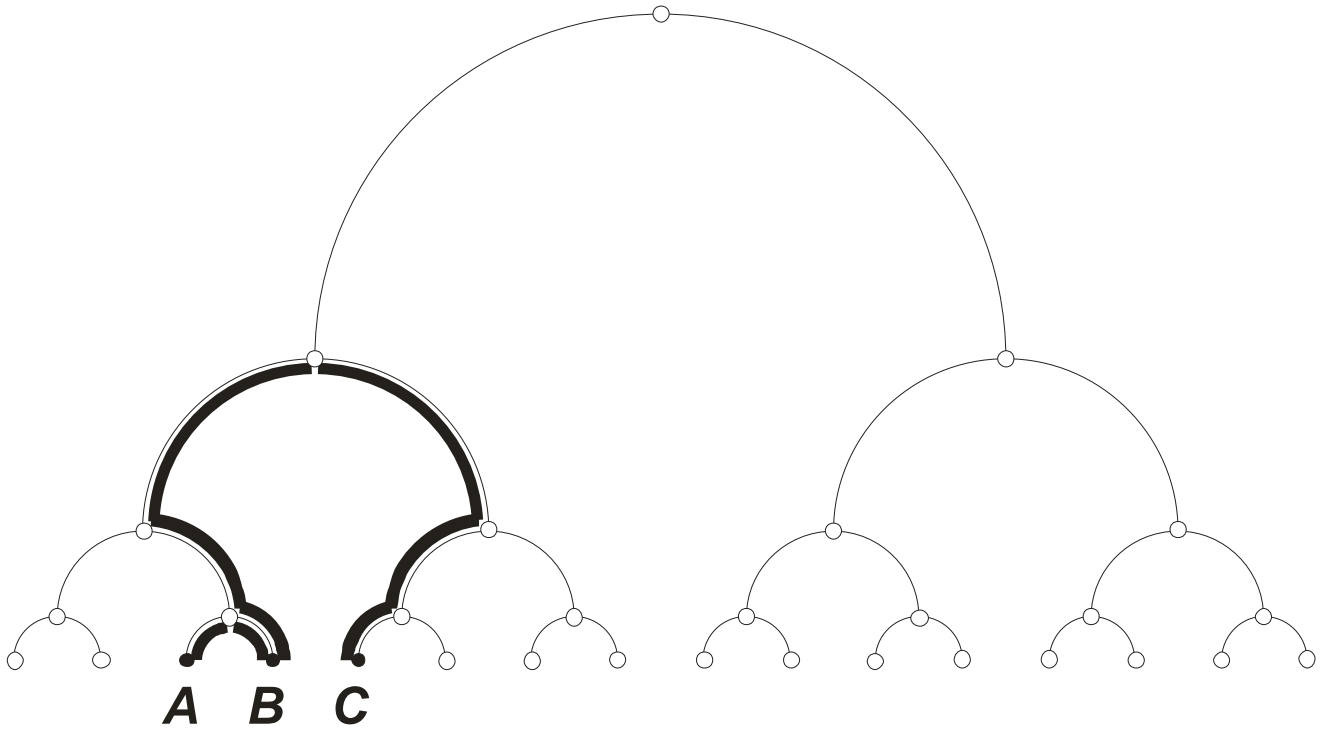
Why we should know the eigenvalues of the Parisi matrix?

The eigenvalues of the Parisi matrix determine a hierarchy of relaxation times of the entire system, hence, define the **kinetics constrained to an ultrametric landscape**.

Transition between two basins = passage time **over the highest barrier** separating these basins, i.e. transitions between two local minima obey the «strong triangle inequality»

$$|| AB | + | BC || \leq \max(| AB |, \ | BC |)$$

typical for ultrametric (*p*-adic) systems:



Eigenvalues of kinetic *regular* Parisi matrix

(A.Ogielski, D.Stein, 1985):

$$\lambda_\gamma = -p^\gamma T^{(\gamma)} - (1-p^{-1}) \sum_{\gamma'=\gamma+1}^{\Gamma} p^{\gamma'} T^{(\gamma')}; \qquad \left(T^{(\gamma)} \equiv q_\gamma = p^{-(\alpha+1)\gamma}\right)$$

where γ $(1 \le \gamma \le \Gamma)$ is the hierarchical level of the Parisi matrix of size $N = p^\Gamma$.

$$\lambda_\gamma = -p^\gamma p^{-(\alpha+1)\gamma} - (1-p^{-1}) \sum_{\gamma'=\gamma+1}^{\Gamma\to\infty} p^{\gamma'} p^{-(\alpha+1)\gamma'} = -p^{-\gamma\alpha} \frac{p^{(\alpha+1)}-1}{p^{(\alpha+1)}-p}; \qquad (\alpha>0)$$

$$\lambda_\gamma = -1-(\Gamma-\gamma)\frac{p-1}{p}; \qquad (\alpha=0)$$

We consider below p=2. Degeneracy of eigenvalues is:

$$\left\{\begin{array}{l} 2^{\Gamma-1} \text{ eigenvalues } \lambda_1 \\ 2^{\Gamma-2} \text{ eigenvalues } \lambda_2 \\ \ldots \\ 2^0 \text{ eigenvalues } \lambda_\Gamma \text{ and one eigenvalue = 0} \end{array}\right| \Rightarrow \text{ totally } 2^\Gamma \text{ eigenvalues}$$

The information about the relaxation is characterized by the **survival probability**, $W(t,\Gamma)$, i.e. the probability to find a dynamical system in the initial state by the time *t*,

$$W(t,\Gamma) = (p-1)\sum_{\gamma=1}^{\Gamma} p^{-\gamma} e^{\lambda_\gamma t} + p^{-\Gamma}$$

For a *nonrandom* (i.e. *regular*) kinetic Parisi matrix of Γ hierarchy levels, the survival probability, $W(t,\Gamma)$, is

$$W(t,\Gamma) = (p-1)\sum_{\gamma=1}^{\Gamma\to\infty} p^{-\gamma} \exp\left(c_\alpha p^{-\gamma\alpha} t\right) \simeq \left(c_\alpha t\right)^{-1/\alpha}$$

where $c_\alpha = \dfrac{p^{(\alpha+1)}-1}{p^{(\alpha+1)}-p} \quad (\alpha > 0)$

Randomization of the kinetic Parisi-type matrix

$$T=\begin{array}{|cccc|cccc|}
\hline
\varepsilon^{(1)} & q_1^{(1)} & q_2^{(1)} & q_2^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} \\
q_1^{(1)} & \varepsilon^{(2)} & q_2^{(1)} & q_2^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} \\
q_2^{(1)} & q_2^{(1)} & \varepsilon^{(3)} & q_1^{(2)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} \\
q_2^{(1)} & q_2^{(1)} & q_1^{(2)} & \varepsilon^{(4)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} \\
\hline
q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & \varepsilon^{(5)} & q_1^{(3)} & q_2^{(2)} & q_2^{(2)} \\
q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_1^{(3)} & \varepsilon^{(6)} & q_2^{(2)} & q_2^{(2)} \\
q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_2^{(2)} & q_2^{(2)} & \varepsilon^{(7)} & q_1^{(4)} \\
q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_3^{(1)} & q_2^{(2)} & q_2^{(2)} & q_1^{(4)} & \varepsilon^{(8)} \\
\hline
\end{array}$$

Since T is a transition matrix, one has the "conservation" condition

$$\varepsilon + q_1 + 2q_2 + 4q_3 + \ldots = 0$$

for each column. It is supposed that

$$q_\gamma^{(n)} = e^{-u_\gamma^{(n)}}; \quad e^{-\left\langle u_\gamma^{(n)} \right\rangle} = p^{-(\alpha+1)\gamma}$$

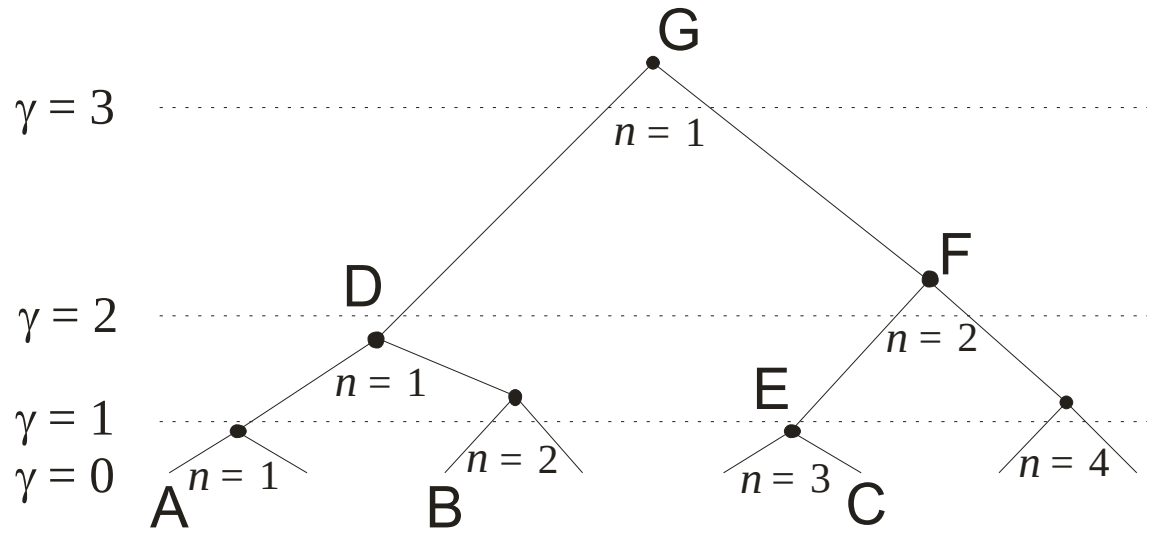
and

$$u_\gamma^{(n)} = \left\langle u_\gamma^{(n)} \right\rangle + \xi_\gamma^{(n)}; \quad \left| \xi_\gamma^{(n)} \right| \ll 1$$

1. The barriers of the same hierarchy level, coincide only on the order of magnitude. The transition rates between basins of the *same* hierarchical level have **random distribution around mean values** prescribed by the regular ultrametric hierarchy;
2. In the real experiments one deals not with individual proteins, but with **ensembles of molecules** in a sample.

Eigenvalues of kinetic *randomized* Parisi matrix (V.Avetisov, S.Kozyrev, V.Osipov, 2005):

The non-degenerated Parisi-type matrix corresponds to the transitions on the following non-uniform tree



General expression for eigenvalues of non-degenerated Parisi-type matrix:

$$\lambda_{\gamma,n} = -p^{\gamma}T^{(\gamma,n)} - (1-p^{-1})\underbrace{\sum_{\gamma'=\gamma+1}^{\Gamma} p^{\gamma'}T^{(\gamma',n')}}_{S}$$

where the sum Σ runs along the tree from the point (γ,n) to the root point, G.

Survival probability for complex systems described by randomized hierarchical matrices

(V.Avetisov, A.Bikulov, S.N, 2009):

To make the survival probability independent on initial points on a tree, we consider survival probability $\overline{W}(t,\Gamma)$ averaged over all positions of initial states:

$$\overline{W}(t,\Gamma)=(p-1)\sum_{\{\gamma,n\}}^{\Gamma} p^{-\gamma}e^{\lambda_{\gamma,n}t}+p^{-\Gamma}=(p-1)\sum_{\gamma=1}^{\Gamma} p^{-\gamma}Z(t,\gamma,\Gamma)+p^{-\Gamma}$$

where

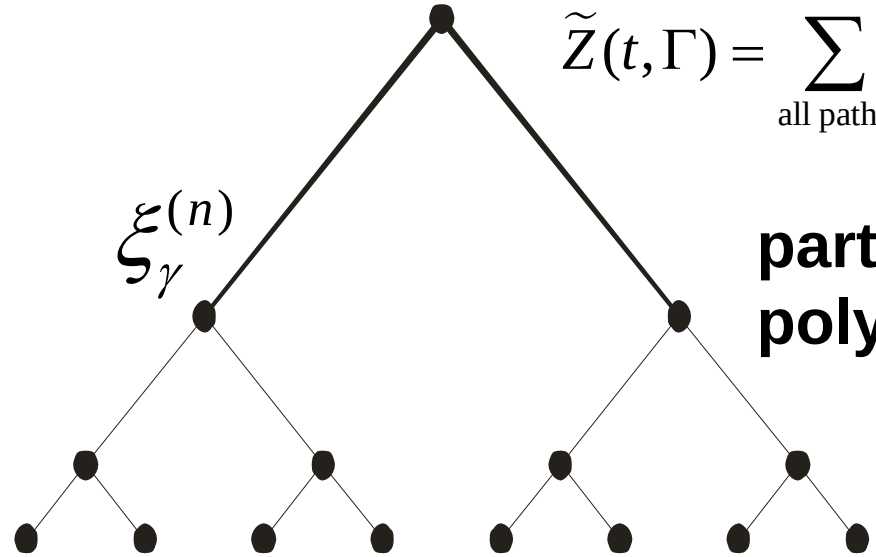
$$Z(t,\gamma,\Gamma)=\sum_{n=1}^{p^{\Gamma-\gamma}} e^{\lambda_{\gamma,n}t}=\widetilde{Z}(t,\gamma,\Gamma)e^{\nu_\gamma(\Gamma)t};\ \nu_\gamma(\Gamma)=p^{-\alpha\gamma}+\left(1-p^{-1}\right)\sum_{\gamma'=\gamma+1}^{\Gamma} p^{-\alpha\gamma'}$$

it is supposed that

$$T^{(\gamma,n)}\equiv q_\gamma^{(n)}\approx e^{-\left\langle u_\gamma^{(n)}\right\rangle}\left(1-\xi_\gamma^{(n)}+O\left(\xi_\gamma^{(n)}\right)^2\right);\ e^{-\left\langle u_\gamma^{(n)}\right\rangle}=p^{-(\alpha+1)\gamma}$$

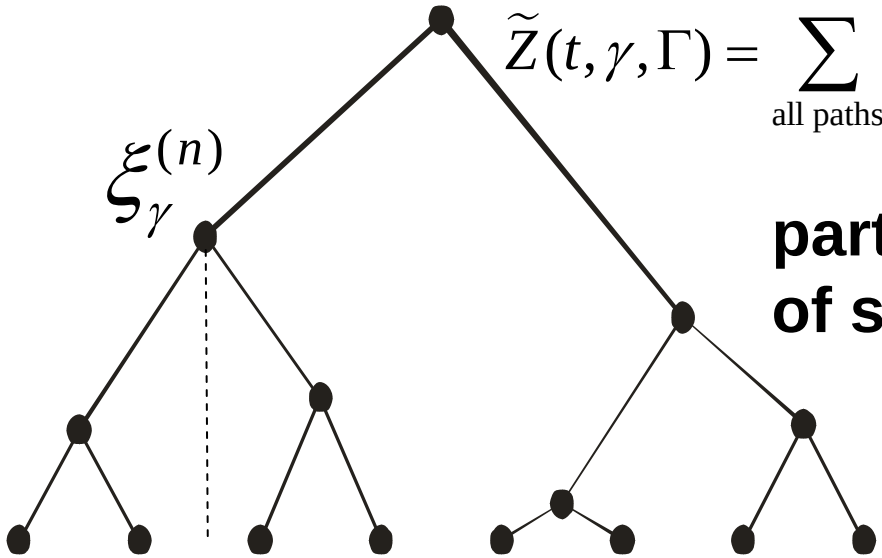
So, one has the following "partition function" of directed polymer:

$$\widetilde{Z}(t,\gamma,\Gamma)=\sum_{\text{all paths}}\exp\left\{t\left(p^{-\alpha\gamma}\xi_\gamma^{(n)}+\left(1-p^{-1}\right)\sum_{\gamma'=\gamma+1}^{\Gamma}p^{-\alpha\gamma'}\xi_{\gamma'}^{(n')}\right)\right\}$$



$$\widetilde{Z}(t,\Gamma)=\sum_{\text{all paths}}\exp\left\{-\beta\sum_{\gamma'=1}^{\Gamma}\xi_{\gamma'}^{(n')}\right\}$$

partition function of directed polymer



$$\widetilde{Z}(t,\gamma,\Gamma)=\sum_{\text{all paths}}\exp\left\{t\left(p^{-\alpha\gamma}\xi_\gamma^{(n)}+\left(1-p^{-1}\right)\sum_{\gamma'=\gamma+1}^{\Gamma}p^{-\alpha\gamma'}\xi_{\gamma'}^{(n')}\right)\right\}$$

partition function for computation of survival probability

The function $\widetilde{Z}(\Gamma)$ satisfies the stochastic recursion (B.Derrida, H.Spohn, 1988)

$$\widetilde{Z}(\Gamma) = \exp\left[t\left(1- p^{-1}\right) p^{-\alpha\Gamma} \xi_{\Gamma} \right] \sum_{j=1}^{p} \widetilde{Z}(\Gamma - 1)$$

For the generating function

$$G_m(x) = \left\langle \exp\left\{ -\widetilde{Z}(m) \exp\left[t\left(1- p^{-1}\right) p^{-\alpha m} x \right] \right\} \right\rangle$$

one gets recursion relation

$$G_{m-1}(x) = \int d\xi P(\xi) \left[G_m\left(p^{-\alpha}(x+\xi) \right) \right]^p$$

equipped by initial condition

$$G_{\Gamma}(x) = \exp\left\{ -\exp\left[t\left(1- p^{-1}\right) p^{-\alpha\Gamma} x \right] \right\}$$

The case $\alpha > 0$ is a “contracting map”. Here we consider $\alpha = 0$, which is formally identical to the Derrida-Spohn model of the **directed polymer on the disordered tree** and is related to the Kolmogorov-Petrovsky-Piscounov (KPP) equation.

Interpretation

The overlap between two trajectories starting from the common root point can be: i) 0 (with probability 1) for $t < t_{cr}$, and ii) either 0 (with prob. $\pi(t) = \text{const}/t$) or 1 (with prob. $1-\pi(t)$) for $t > t_{cr}$

For $t < t_{cr}$ the overlap of two trajectories is 0 and the boundary of the Cayley tree is uniform. The escape probability from any basin at the boundary is independent on the specific point and **the kinetics happens as for nonrandom Parisi matrix**.

For $t > t_{cr}$ the overlap of the trajectories signals the "probabilistic non-uniformity" of the boundary: with the probability $1-\pi(t)$ the boundary has a “lacunary” structure such that **the escape from some boundary basins is locked and the kinetics is confined in these basin for infinitely long time**.

Random block-hierarchical adjacency matrices of random hierarchical graphs (contact maps)

(V.Avetisov, A.Chertovich, O.Vasilyev, S.N, 2009)

$$T = \begin{array}{|cc|cc|cccc|}
\hline
0 & t_1^{(1)} & t_2^{(1)} & t_2^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
t_1^{(1)} & 0 & t_2^{(1)} & t_2^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
\hline
t_2^{(1)} & t_2^{(1)} & 0 & t_1^{(2)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
t_2^{(1)} & t_2^{(1)} & t_1^{(2)} & 0 & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} \\
\hline
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & 0 & t_1^{(3)} & t_2^{(2)} & t_2^{(2)} \\
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_1^{(3)} & 0 & t_2^{(2)} & t_2^{(2)} \\
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_2^{(2)} & t_2^{(2)} & 0 & t_1^{(4)} \\
t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_3^{(1)} & t_2^{(2)} & t_2^{(2)} & t_1^{(4)} & 0 \\
\hline
\end{array}$$

Now there is no “conservation condition” in matrix T .

What is the density of eigenvalues $\rho(\lambda)$ for such a matrix for some typical distributions of matrix elements?

Each hierarchical level represents the local graph with binomial distribution on elements of adjacency matrix:

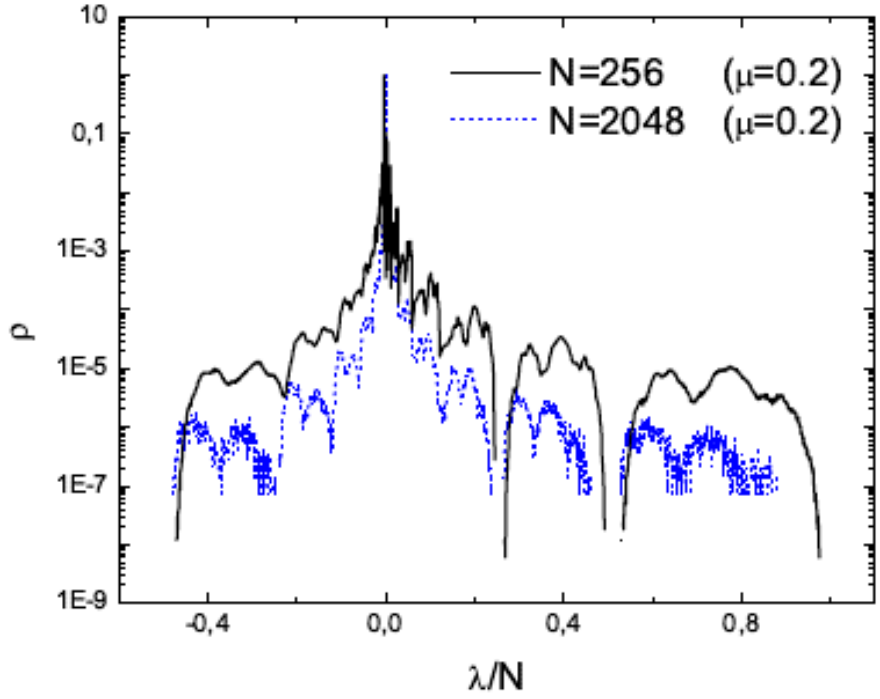
$$t_{\gamma}^{(n)} = \begin{cases} 1 & \text{with the probability } q_{\gamma} \\ 0 & \text{with the probability } 1 - q_{\gamma} \end{cases}$$

The adjacency matrix of the graph is completely determined by the set $\{Q\} = \{q_1, q_2, ..., q_{\Gamma}\}$ where $q_{\gamma} = e^{-\mu\gamma}$

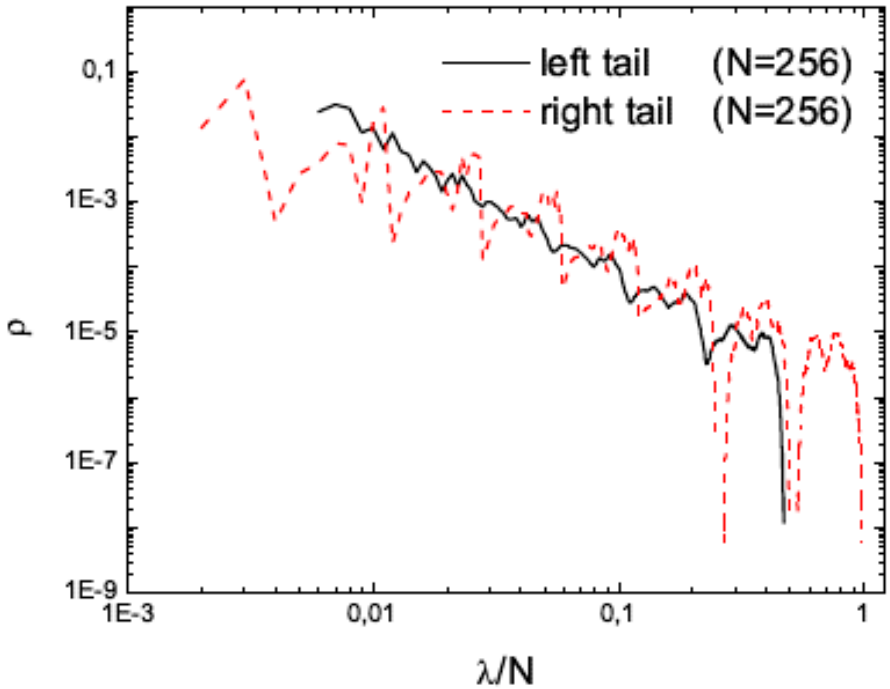
Spectral density for $\mu = 0.2$

(a) Semi–log plot of the distribution of eigenvalues $\rho(\lambda)$ for $N = 256$ (solid line) and $N = 2048$ (dashed line);

(b) The left– and right–hand tails of $\rho(\lambda)$ for $N = 256$ in log–log coordinates.

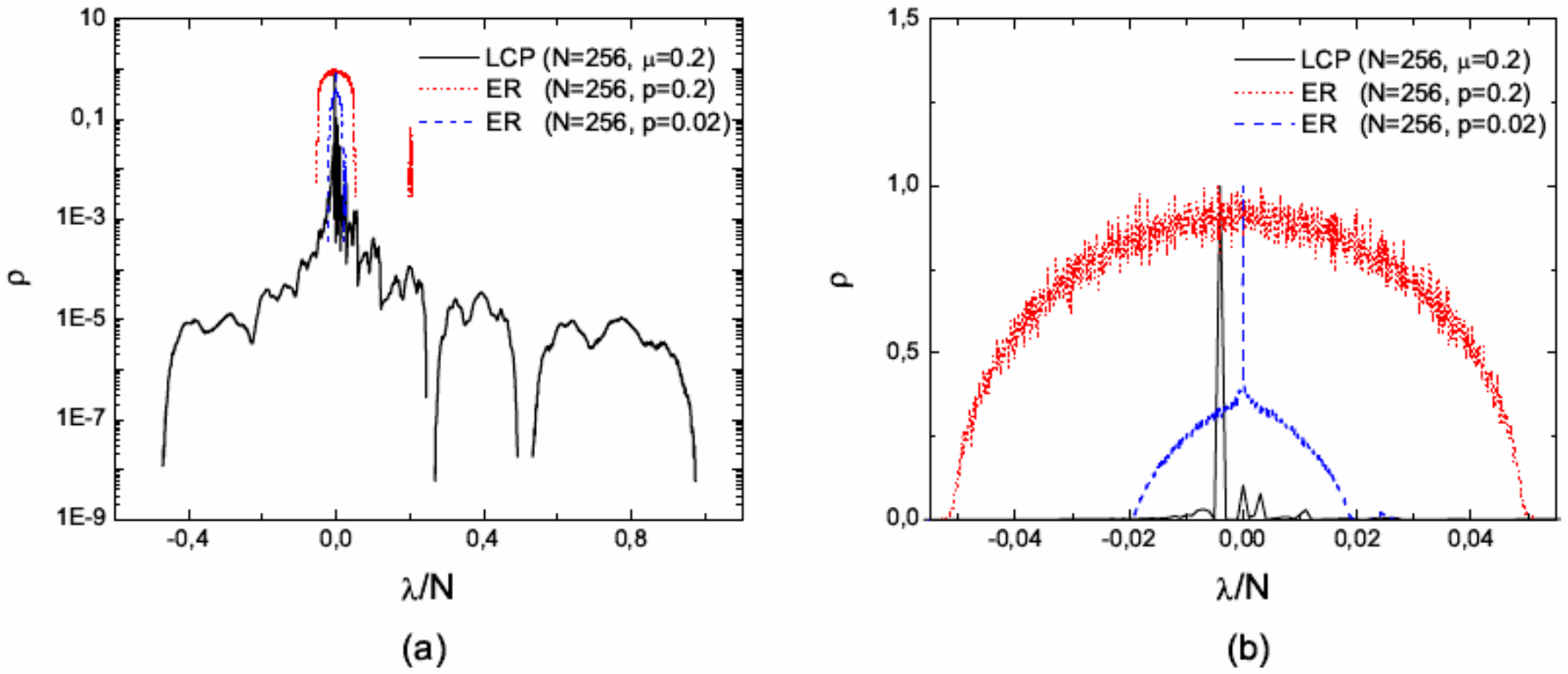


(a)



(b)

Comparison of spectral densities of random hierarchical and Erdös-Rényi random graphs



(a) The semi–log plot of the spectral densities for: random hierarchical graphs for $N = 256$ and $\mu = 0.2$ (**solid line**), random Erdös-Rényi graphs for $N = 256$ and $p = 0.2$ (**dotted line**), for $N = 256$ and $p = 0.02$ (**dashed line**);

(b) The central part of the figure (a) in the linear scale.

Spectral density of *randomized* hierarchical adjacency matrices: conjectures and analytic results

Instead of binomial distribution on the elements of hierarchical matrix, we consider Gaussian distribution

$$P\left(t_\gamma^{(n)}\right)=\frac{1}{\sqrt{\pi\sigma_\gamma^2}}\exp\left(-\frac{\left(t_\gamma^{(n)}-\left\langle t_\gamma^{(n)}\right\rangle\right)^2}{\sigma_\gamma^2}\right);\quad \left\langle t_n^{(\gamma)}\right\rangle=0;\quad \left\langle\left(t_n^{(\gamma)}\right)^2\right\rangle=\sigma_\gamma^2=p^{-2\nu\gamma}$$

where ν is a parameter ($\nu>0$).

Reminder:

For ***regular normalized*** Parisi matrix one had

$$\overline{\lambda}_\gamma=-2^\gamma T^{(\gamma)}-2^{-1}\sum_{\gamma'=\gamma+1}^{\Gamma}2^{\gamma'}T^{(\gamma')}$$

For ***regular non-normalized*** Parisi matrix (contact map) one has

$$\lambda_\gamma=-2^\gamma T^{(\gamma)}+2^{-1}\sum_{\gamma'=1}^{\gamma}2^{\gamma'}T^{(\gamma')}$$

Conjecture about the spectrum of *randomized non-normalized* hierarchical matrix

Suppose that

$$\lambda_{\gamma,n} = -2^{\gamma} T^{(\gamma,n)} + 2^{-1} \underbrace{\sum_{\gamma'=1}^{\gamma} 2^{\gamma'} T^{(\gamma',n')}}_{S}$$

Problem with $\lambda_{\gamma,n}$: the sum S runs from γ=1 to γ. There are many such trajectories on the tree, while for normalized Parisi-type matrix the sum runs from γ to Γ and such a path is **unique**.

With $\lambda_{\gamma,n}$ we compute the spectral density, $\rho_G(\lambda)$, and we get

$$\rho_G(\lambda) = \frac{1}{p^{\Gamma}} \sum_{\{\gamma,n\}} \left\langle \delta(\lambda - \lambda_{\gamma,n}) \right\rangle_{P\left(t_{\gamma}^{(n)}\right)} = \frac{1}{\sqrt{\pi}} \sum_{\gamma=1}^{\Gamma} p^{-\gamma} \frac{1}{\sqrt{u_{\gamma}^2}} \exp\left(-\frac{\lambda^2}{u_{\gamma}^2} \right)$$

where

$$u_{\gamma}^2 = p^{2(\gamma-1)} \sigma_{\gamma}^2 + \left(1 - p^{-1}\right) \sum_{\gamma'=1}^{\gamma-1} p^{2\gamma'} \sigma_{\gamma'}^2 = \frac{p-2}{p} p^{2(1-\nu)\gamma} + \frac{(p-1)^2}{p - p^{\gamma}} \left(p^{2(1-\nu)\gamma} - 1 \right)$$

For p=2 and $\Gamma \to \infty$ we get the following expression for the spectral density

$$\rho_G(\lambda) \simeq \frac{1}{\sqrt{\pi}} \sum_{\gamma=1}^{\infty} 2^{-(2-\nu)\gamma} \exp\left(-\lambda^2 \frac{4-4^{\nu}}{4^{-(1-\nu)\gamma} - 1} \right)$$

using that

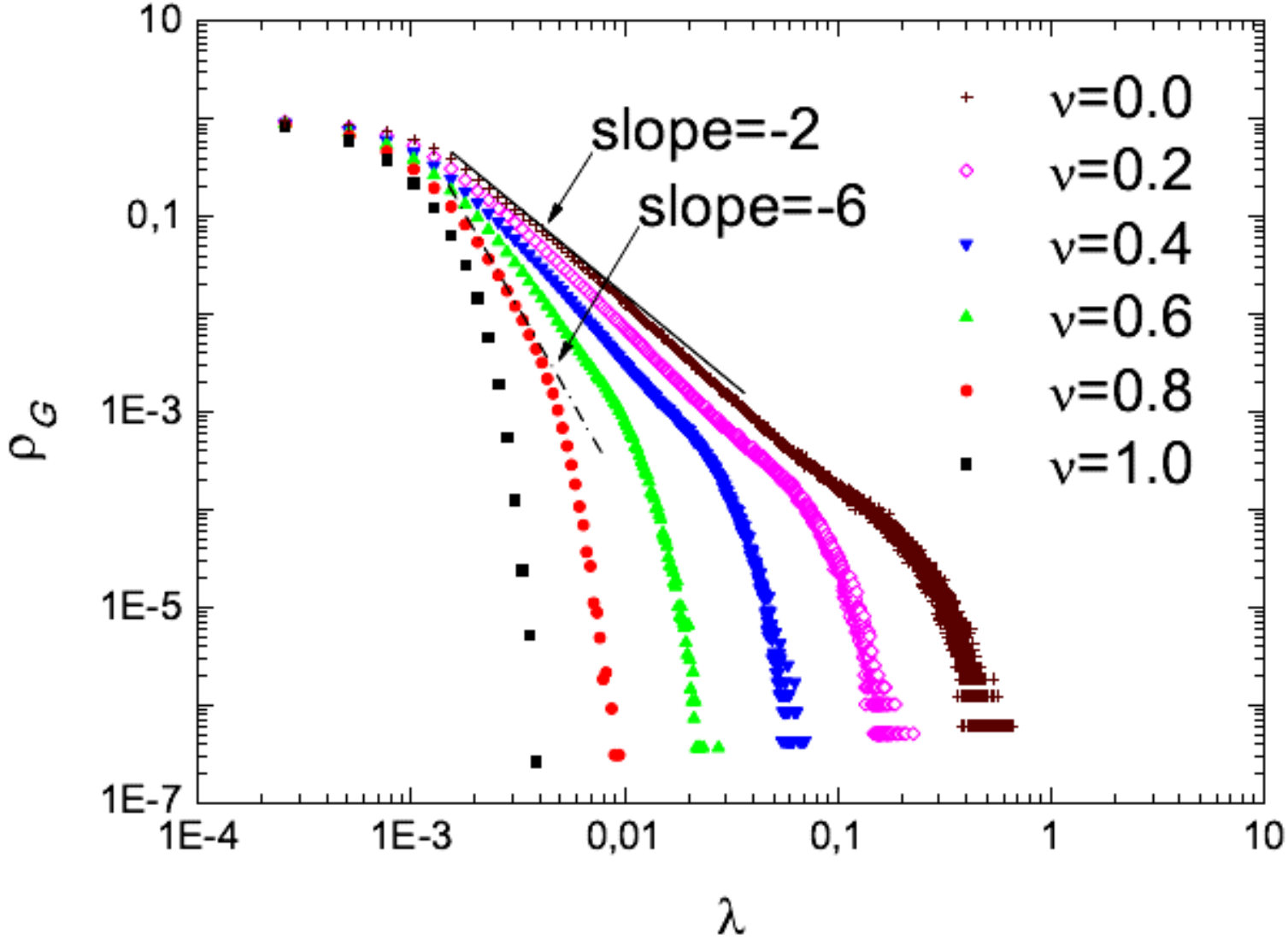
$$\sum_{\gamma=1}^{\infty} p^{-c_1\gamma} \exp\left(-p^{-c_2\gamma} u\right)\Big|_{t\to\infty} \simeq u^{-c_1/c_2}$$

and substituting $c_1 = 2-\beta$; $c_2 = 2(1-\beta)$, we arrive finally at the asymptotic expression:

$$\rho(\lambda)\big|_{\lambda\to\infty} \simeq |\lambda|^{-\frac{2-\nu}{1-\nu}}$$

For ν >1 there is a termination of the power-law tail and the asymptotics becomes exponential.

Numerical verification of the power-law behavior for Gaussian distribution of $2^8 \times 2^8$ hierarchical adjacency matrix



A posteriori supporting arguments:

1. Extensive numerical simulations for spectral density support our conjecture;

2. In the sum S the lower limit of the summation can be shifted from $\gamma = 1$ to $\gamma \to -\infty$. Asymptotically the result for u_γ^2 remains unchanged if $0 < \nu < 1$. Such a change in summation means that the computation of the spectral density involves the summation along the infinite paths running from $-\infty$ to the hierarchical level γ. We expect that for $\sigma_\gamma = p^{-\nu\gamma}$ due to the convergence of the sum

$$u_\gamma^2 = p^{2(\gamma-1)}\sigma_\gamma^2 + \left(1 - p^{-1}\right) \sum_{\gamma' \to -\infty}^{\gamma-1} p^{2\gamma'} \sigma_{\gamma'}^2$$

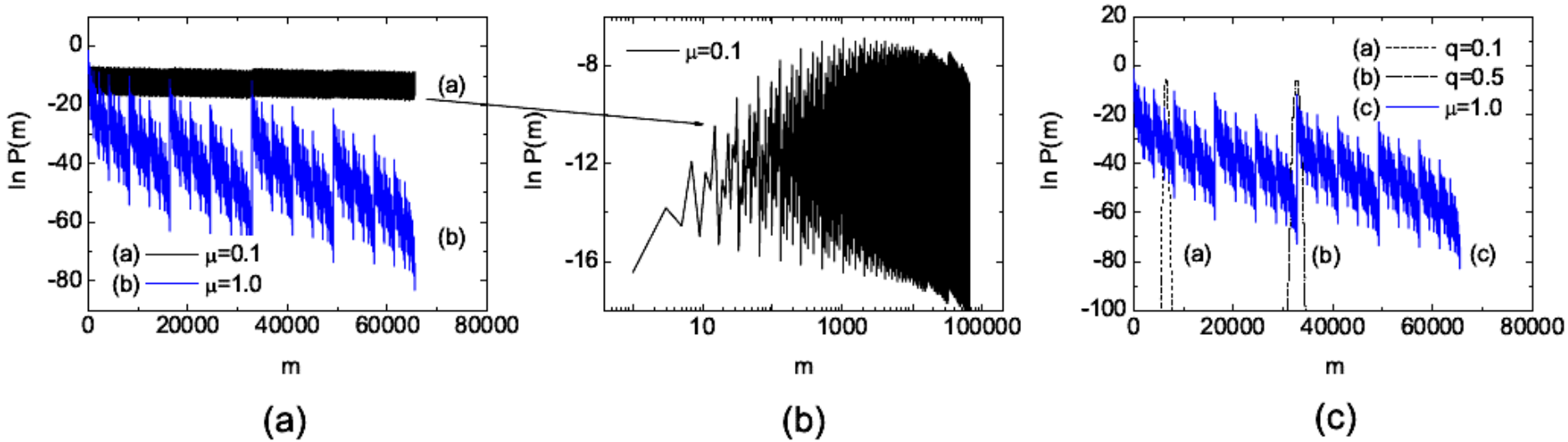
for $0 < \nu < 1$, the eigenvalues do not depend on each particular path on a Cayley tree.

Vertex degree distribution in random hierarchical graphs has fractal structure

$$P(m) = \sum_{\{t_1,\ldots,t_\Gamma\}} \left[\prod_{\gamma=1}^{\Gamma} q_\gamma\left(t_\gamma\right) \right] \Delta\left(\sum_{\gamma=0}^{\Gamma} p^\gamma t_{\gamma+1} - m \right)$$

where the binomial distributions $q_\gamma\left(t_\gamma\right)$ have the form

$$q_\gamma\left(t_\gamma\right) = p^{-\mu\gamma}\delta_{q_\gamma\left(t_\gamma\right),1} + (1 - p^{-\mu\gamma})\delta_{q_\gamma\left(t_\gamma\right),0}$$



The family of distributions $P(m)$ for Γ=16 and μ = 0.1; 1.0