Walks in rough energy landscapes: a network model

R G Margiotta, R Kühn, P Sollich, *J. Phys. A 2018*
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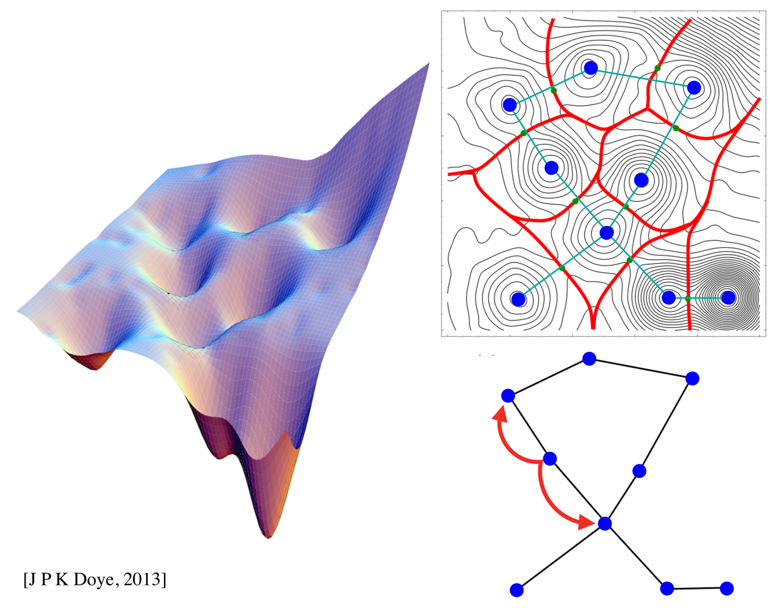
1. Introduction

We consider a glass as a point in configuration-space hopping between metastable energy minima idealised as point-like **traps** at the vertices of a network.
Two main ingredients define the problem: the **network structure** and the **hopping rates** between the traps.



2. Background

Motivated by deep minima distribution of real glasses the trap depth distribution is taken as exponential:

$$\rho_E(E) = e^{-E}\theta(E)$$

Bouchaud Trap model: rates only depend on the departing trap depth (energetic barriers - activated dynamics).

$$r_{ij} = \frac{1}{N}\exp(-\beta E_j)$$

Glass transition: the average trapping time (prop. to the inverse transition rate) blows up for *T*<1:

$$\tau = \exp(\beta E_j) \qquad \rho_\tau(\tau) = T\tau^{-(T+1)}$$

This model has been studied primarily for mean field connectivity, i.e. on a fully connected network, and related (degree based) approximations.

3. Aims & methodology

We want to investigate the slow dynamics of the trap model with sparse inter-trap connectivity, accounting for the entropic effects generated by the network structure. **Starting point**: master equation for the probability distribution

$$\partial_t \mathbf{p}(t) = \mathbf{M}\mathbf{p}(t) \qquad \mathbf{p}(t) = \sum_\alpha e^{\lambda_\alpha t}\mathbf{r}_\alpha(\mathbf{l}_\alpha, \mathbf{p}(0))$$

The dynamics is determined by the spectral properties of **M.** These can be found with the **cavity method**.

Quantities of interest are:
- the eigenvalue spectrum of the master operator;
- modes localisation (IPR and other measures accounting for distance among vertices);

$$\text{IPR:} \quad I_2(\mathbf{v}) = \sum_i^N v_i^4 / (\sum_i^N v_i^2)^2 \propto N^{-t_2}$$

The density of states (DOS) can be written as

$$\rho(\lambda) = \lim_{\varepsilon\to 0}\frac{1}{\pi N}\sum_i^N \mathrm{Im}G_{ii}(\lambda_\varepsilon)$$

$$\mathbf{G}(\lambda_\varepsilon) = [\lambda_\varepsilon - \mathbf{M}]^{-1}$$

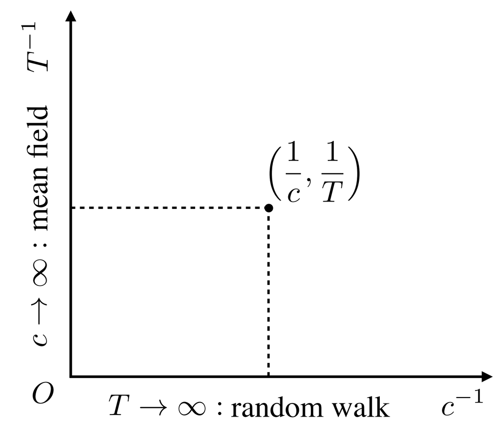
The cavity method allows to find the entries *Gii* recursively, on the cavity graph.

5. Results

Fixing the transition rates, energy distribution and network topology, the relevant model parameters reduce to the temperature T and the mean degree c.

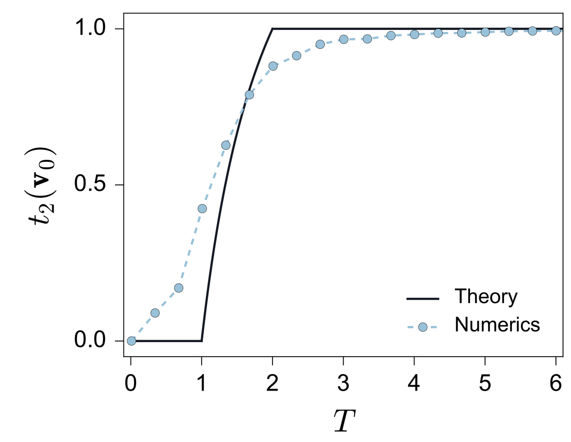
Accordingly there are two relevant limits:

c -> infinity (mean field limit);
T -> infinity (random walk limit).



5a. Ground State

The IPR of the ground state is independent of the network structure (Boltzmann distribution). **Two low-T regimes** are present:

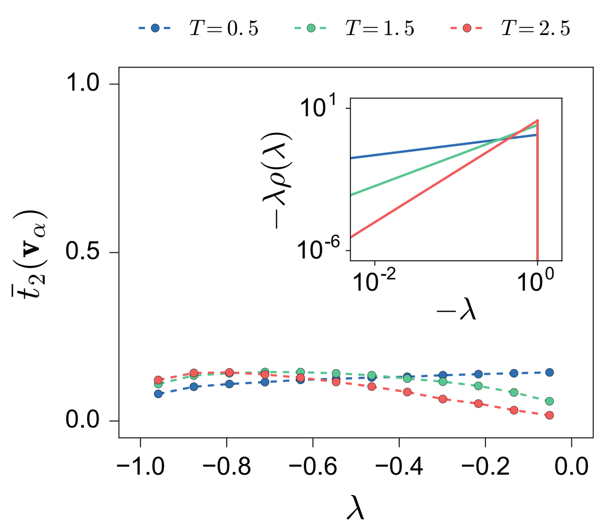


IPR :
N^{-1} if $T > 2$
$N^{-2+\frac{2}{T}}$ ow
N^0 if $T < 1$

5b. Mean field limit

Fully connected graph with Bouchaud transition rates. The master operator is diagonalisable.

$$\rho(\lambda) = T(-\lambda)^{T-1} \qquad u_{\alpha,i} \propto (\lambda_\alpha + 1/\tau_i)^{-1}$$

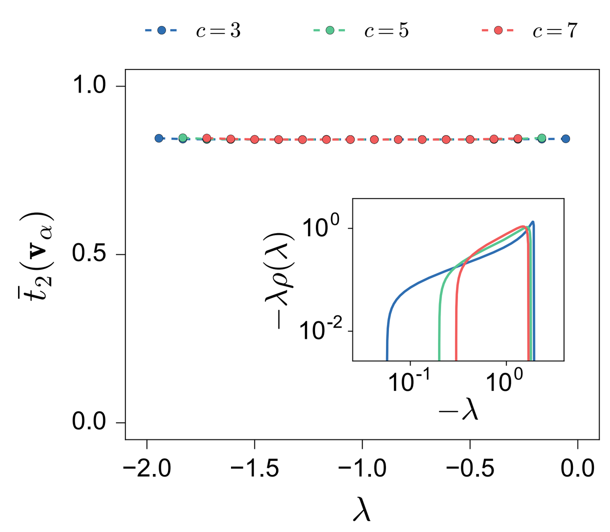


All **Eigenvectors** are **localised**.

5c. Random walk limit

Random regular graph at **infinite temperature.** Spectrum given by the Kesten-McKay law.

$$\rho(\lambda) = \frac{c}{2\pi}\sqrt{4\frac{c-1}{c^2} - \frac{\lambda+c}{c}} \Big/ \left(1 - \left(\frac{\lambda+c}{c}\right)^2\right)$$

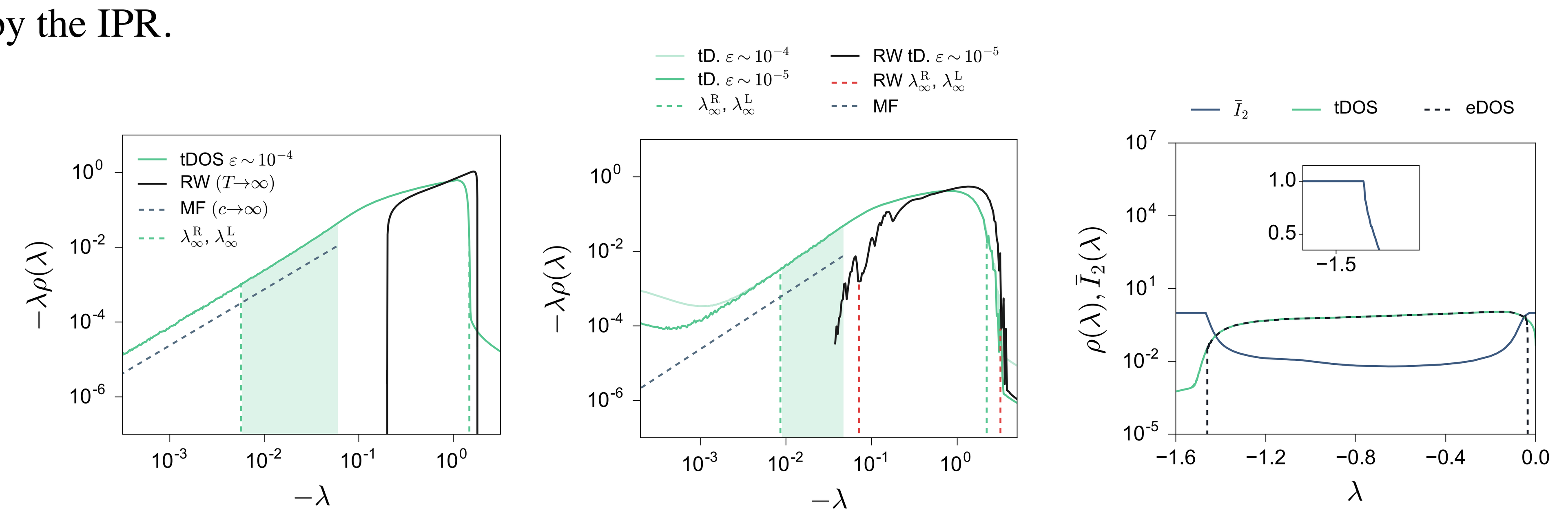


All **Eigenvectors** are **delocalised**.

5d. General case: network structure + glassiness

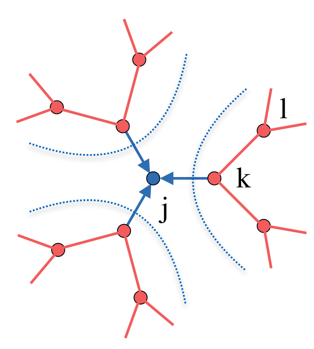
Random regular, Erdös-Rényi and scale-free graphs with Bouchaud rates. The epsilon dependence in the average for the density of states allows to distinguish between the total DOS, and the extended DOS, which only includes the de-localised eigenstates of the system covering the continuous part of the spectrum; this is confirmed by the IPR.

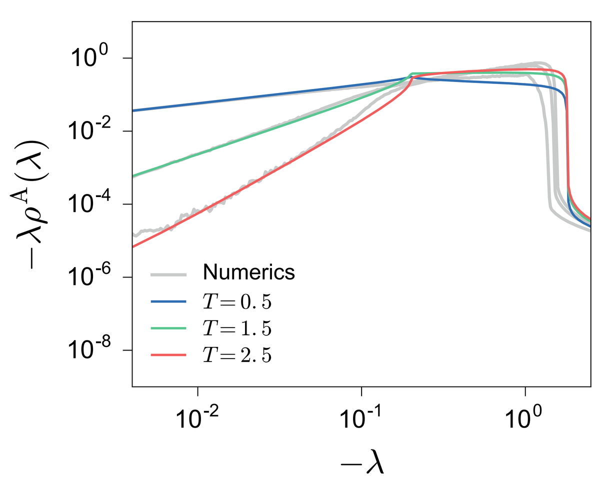
$T = 1.5$
$c = 5$



The **localisation-transition** shows up in the MF-like region -> we have three different regions: **MF-DOS** with **localised** modes**, MF-DOS** with **delocalised** modes and **RW-DOS** with **delocalised** modes.

Following the cavity construction we can perform a (“**high *T***”) analytical **approximation**: one cavity iteration is taken at finite temperature starting from the infinite temperature solution -> **only local disorder matters**. The low -λ power law tail is perfectly reproduced.





6. Conclusion & future directions

- Localisation transitions arise as non-trivial combination of glassiness and network effects.
- The three regimes in λ should correspond to three different regimes in time (eigenvalues are relaxation rates of the system).
- Spatial structure of eigenvectors? What is the nature/strength of the localisation? How does it affect the dynamics?
- Behaviour in time? Look at the local DOS which gives the return probability: **work in progress**.