Statistical Physics of Disordered Systems

Random Matrices, Anderson Model, Trap models and Computational Methods

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Disordered systems

What is disorder?

Frozen heterogeneity that is a background random potential for the fluctuating degrees of freedom.

Introduction to Quenched Disorder, Leo Radzihovsky

Examples:

- Spin Glasses
- Neural Networks
- Trap Models
- Anderson Model

Fluctuating variable:

- Spins
- Weights
- Configuration (trap)
- Configuration (position)

Heterogeneity:

- Spins couplings
- Data
- Traps energies
- On–site energies

Example: mean–field spin glass

Hamiltonian of the *Sherrington-Kirkpatrick model*

$$H(\vec{\sigma};\boldsymbol{J}) = -\sum_{i<j} J_{ij}\sigma_i\sigma_j\,; \quad \sigma_i = \pm 1$$

with $P(J_{ij}) = \mathcal{N}(0,1)$ i.i.d. *random* variables.

Thermodynamics:

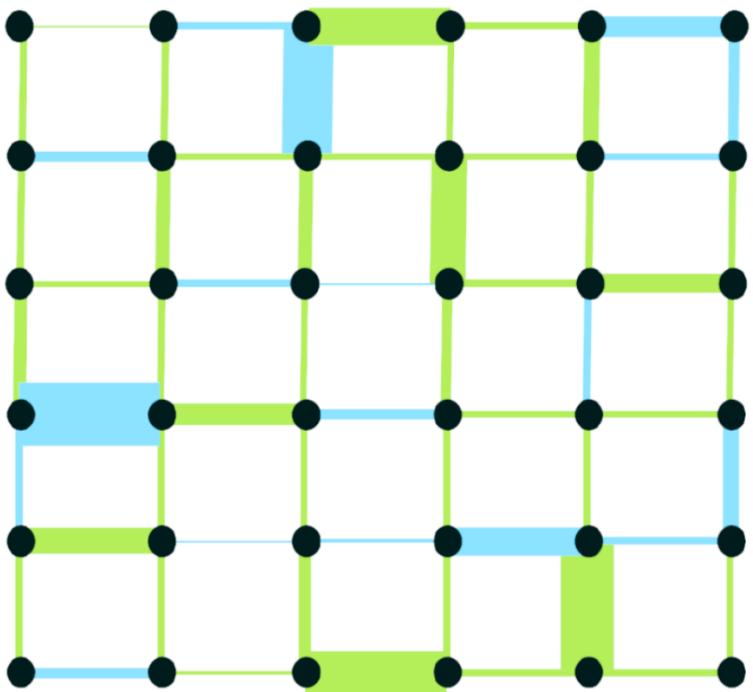
$$\langle F \rangle_J = \int \prod_{i<j} dJ_{ij} P(J_{ij}) F(\boldsymbol{J}) = -k_B T \left\langle \log \sum_{\{\sigma_i=\pm 1\}_{i=1}^N} \mathrm{e}^{\beta H(\vec{\sigma};\boldsymbol{J})} \right\rangle_J$$

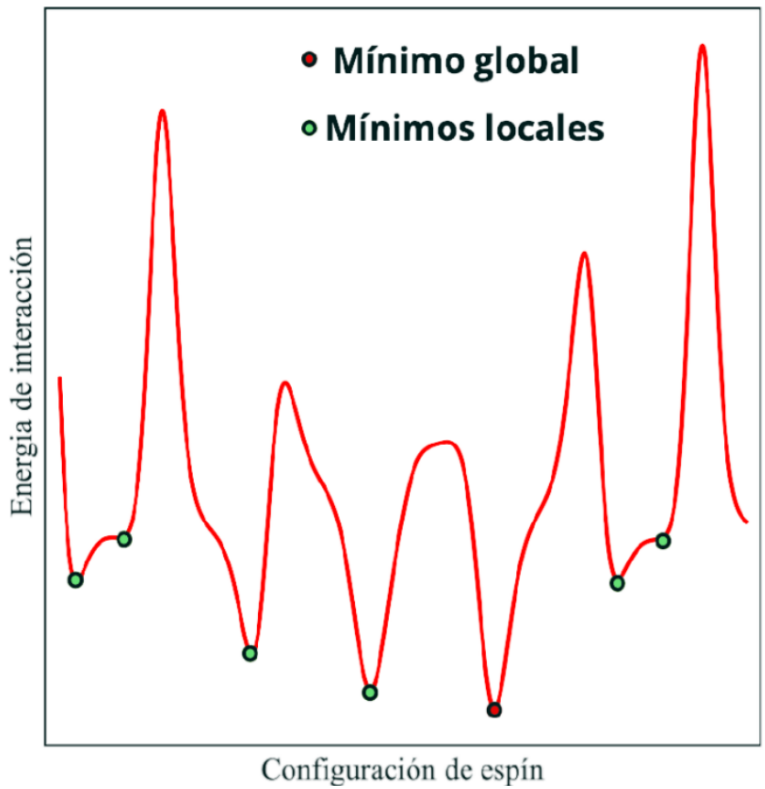
New set of tools: Replica trick, replica symmetric breaking, **cavity method** ...

Disordered systems

2021 Nobel Prize in Physics awarded to **Giorgio Parisi**:

For the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales





Pérez Castillo, I. (2022) *Vidrios de espín y sistemas complejos*. Bol. Rev. Mex. Fís.

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Cavity method: inference

Method for inference on graphs. Given

$$P(\mathbf{x}) = P(x_1, x_2, x_3, \cdots, x_N)$$

aims to estimate marginal distribution

$$P(x_i) = \int \prod_{j \neq i} dx_j P(\mathbf{x})$$

Non–disordered example (1D Ising chain)

$$P(\vec{\sigma}) = \frac{1}{\mathcal{Z}} \mathrm{e}^{-\beta H(\vec{\sigma})} = \frac{1}{\mathcal{Z}} \mathrm{e}^{\beta\left(\sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} + h \sum_{i=1}^{N} \sigma_i\right)}$$

estimate from this $\langle \sigma_i \rangle = \sum_{\sigma_i} \sigma_i P(\sigma_i)$.

Cavity method and spectral density

Given a random symmetric matrix $\mathbf{M}$, we want to estimate its spectral density

$$\rho_{\mathbf{M}}(\lambda) = \frac{1}{N}\sum_{i=1}^{N}\delta(\lambda - \lambda_i[\mathbf{M}])\,.$$

(without diagonalizing $\mathbf{M}$)
Smart (but convoluted) workaround:

- construct the resolvent $\mathbf{G}(z) = (z\mathbf{I} - \mathbf{M})^{-1}$

  $$\text{use: } z = \lambda - i\epsilon \implies \mathbf{G}(\lambda - i\epsilon) = ((\lambda - i\epsilon)\mathbf{I} - \mathbf{M})^{-1}$$

- use it as the covariance matrix of an *auxiliary* (complex) Gaussian distribution

  $$P(\mathbf{x}) = \frac{\mathrm{e}^{-\frac{i}{2}\mathbf{x}^T\mathbf{G}^{-1}\mathbf{x}}}{Z(\mathbf{G},\lambda)} = \frac{1}{Z(\mathbf{G},\lambda)}\mathrm{e}^{-\frac{i}{2}\sum_{k,j}x_j((\lambda-i\epsilon)\delta_{k,j}-M_{kj})x_k}$$

  Diagonal elements $G_{jj}(\lambda - i\epsilon)$ determine spectral density

Cavity method and spectral density

Sokhotski–Plemelj formula: $\delta(x) = \frac{1}{\pi} \lim_{\epsilon \to 0^+} \mathrm{Im}\left\{ \frac{1}{x - i\epsilon} \right\}$

Let $\lambda_\varepsilon = \lambda - \mathrm{i}\varepsilon$. We use the *Edwards formula:*

$$\rho_{\mathbf{M}}(\lambda) = -\frac{2}{\pi N} \lim_{\epsilon \to 0^+} \mathrm{Im}\left\{ \frac{\partial}{\partial \lambda} \ln Z(\mathbf{G}, \lambda_\epsilon) \right\}, \quad \left(\boldsymbol{G}(\lambda_\varepsilon) = \left(\lambda_\varepsilon \boldsymbol{I} - \boldsymbol{M} \right)^{-1} \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\pi N} \sum_{i=1}^{N} \mathrm{Im}\, G_{ii}(\lambda_\varepsilon) = \lim_{\varepsilon \to 0} \frac{1}{\pi N} \mathrm{Im}[\mathrm{Tr}\, \mathbf{G}(\lambda_\epsilon)]$$

Can be converted to calculating local variances of a distribution on network:

$$G_{jj} = \mathrm{i} \int \mathrm{d}x_j \, x_j^2 P(x_j) = \mathrm{i} \left\langle x_j^2 \right\rangle$$

Cavity method lets us do this recursively on locally tree-like networks (ok for $N \to \infty$)

Cavity method: Exercise 2 (zeros in the diagonal)

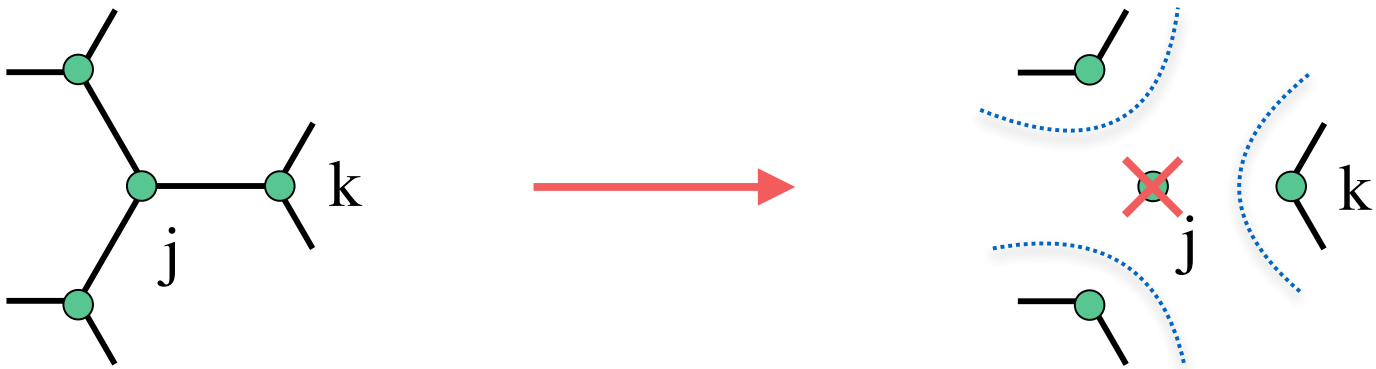
Marginals in terms of cavity distributions as

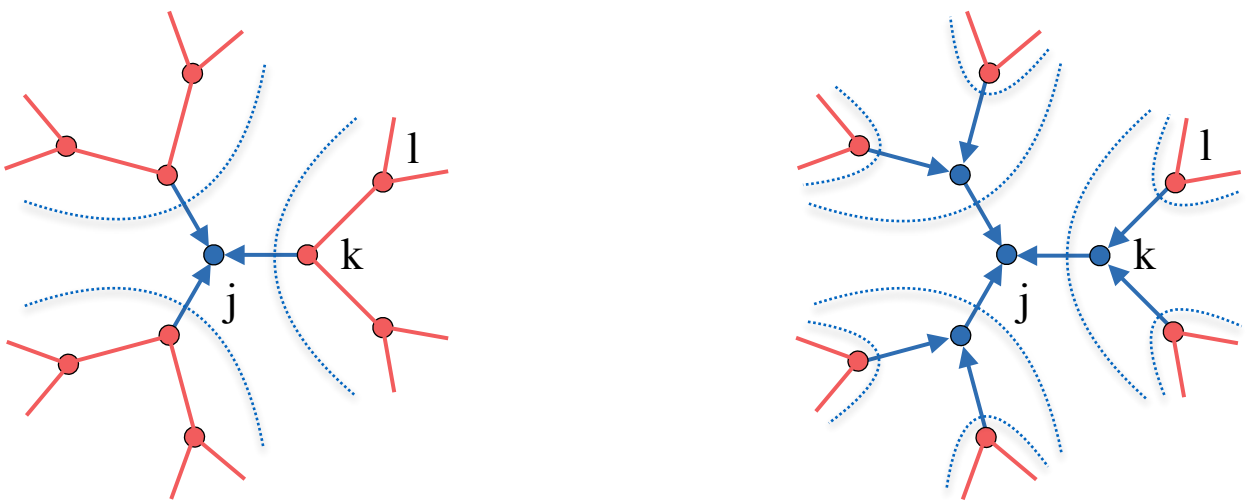
$$P(x_j) \propto \mathrm{e}^{-\frac{i}{2}(\lambda - i\epsilon)x_j^2} \int d\mathbf{x}_{\partial j}\, \mathrm{e}^{ix_j \sum_{k\in\partial j} x_k M_{kj}}\, P^{(j)}(\mathbf{x}_{\partial j})$$

$P^{(j)}(\mathbf{x}_{\partial j})$ denotes the probability distribution of the variables $\{x_k\}$ on the nodes that are neighbours of j on the RRG.
Tree–like approximation:

$$P^{(j)}(\mathbf{x}_{\partial j}) = \prod_{k\in\partial j} P^{(j)}(x_k)$$

Cavity method in pictures





Cavity method

Relation for cavity distributions:

$$P^{(j)}(\mathbf{x}_k) \propto \mathrm{e}^{-\frac{i}{2}(\lambda - i\epsilon)x_k^2} \prod_{l \in \partial k \setminus j} \int dx_l \, \mathrm{e}^{i x_k x_l M_{kl}} P^{(k)}(x_l)$$

Relation for marginals:

$$P(x_j) \propto \mathrm{e}^{-\frac{i}{2}(\lambda - i\epsilon)x_j^2} \prod_{k \in \partial j} \int dx_k \, \mathrm{e}^{i x_j x_k M_{kj}} P^{(j)}(x_k)$$

Those are equations for distributions, that lead to equations for the variances once a *Gaussian ansatz* is employed:

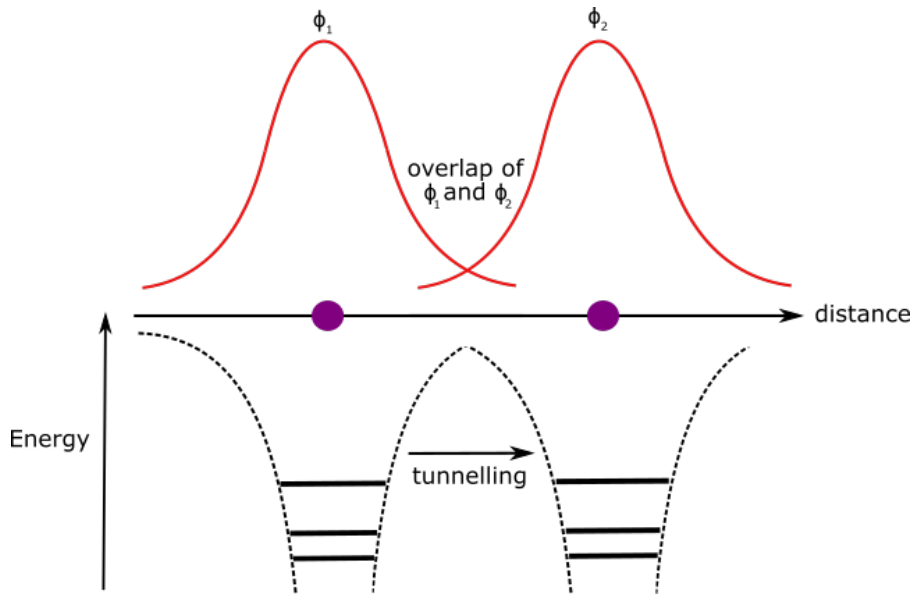
$$P^{(j)}(\mathbf{x}_k) \propto \mathrm{e}^{-\frac{1}{2}\omega_k^{(j)} x_k^2} \qquad P(x_j) \propto \mathrm{e}^{-\frac{1}{2}\omega_j x_j^2}$$

Notice that $G_{jj} = \frac{i}{\omega_j}$

Plan

Simple model for Electron transport

Tight–binding model



Electron wavefunctions of atoms separated by a certain distance. The potential wells generated by the nuclei are also shown. Because of the overlap tunelling among barriers is possible
https://www.quickquantum.co.uk/tight-binding-model/

Tight–Binding Model

Single electron in a lattice:

$$H = \frac{\boldsymbol{p}^2}{2m} + \sum_j V(\boldsymbol{r} - \boldsymbol{R}_j)$$

Last term: interaction with nucleus at (lattice site) j.
Basis: single orbital on lattice site n: $|n\rangle$ (solve isolated problem). Then generic elements can be written as:

$$H_{nm} = \langle n|H|m\rangle = E_0\delta_{m,n} - t\sum_{k\in\partial n}\delta_{k,m}$$

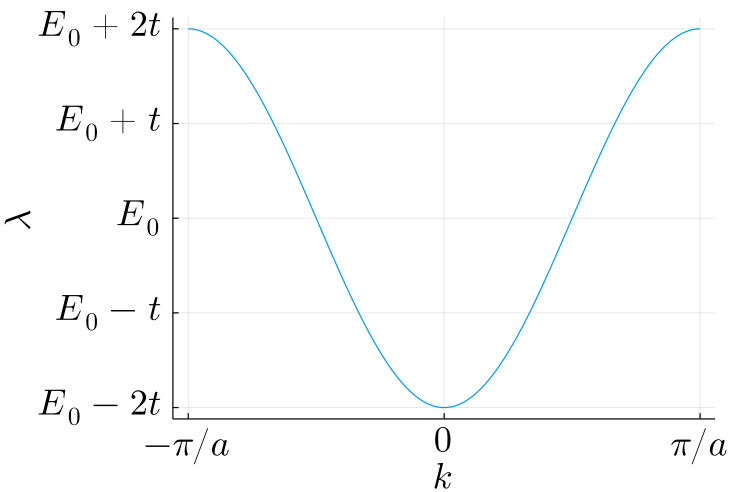
∂n : neighbours of site n.
E_0 is the on–site energy, t the tunneling amplitude.

Tight–Binding Model

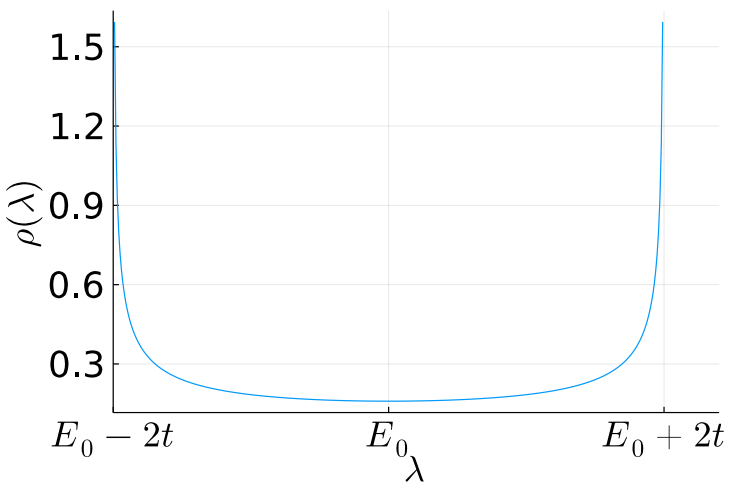
In a 1D (periodic) array

$$H_{ij} = E_0\delta_{ij} - t\left(\delta_{i,j+1} + \delta_{i,j-1}\right) = E_0 I_{ij} - tA_{ij}$$

- Distribution of eigenvalues: Density of States
- Periodicity+ Bloch's theorem: Dispersion relation



Dispersion Relation:
$\lambda = E_0 - 2t\cos(ka)$ with
$|\Psi\rangle = \sum_j \frac{e^{-ikja}}{\sqrt{N}}|j\rangle$



Density of states:
$\rho(\lambda) = 1/(\pi\sqrt{4 - ((\lambda - E_0)/t)^2})$

Tight–Binding model

Features

- Band of energies
- Width of the band proportional to t
- DOS: eigenvalue spectrum of the (shifted–scaled) adjacency matrix (Kesten–McKay law)
- Eigenvectors: extended or delocalized [1]: good model of a conductor

[1] More discussion later

Anderson Model

What if we introduce **DISORDER** in the tight–binding model?

Hamiltonian $(t = 1)$

$$H = \sum_{i=1}^{N} E_i c_i^\dagger c_i - \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$$
$$= \mathrm{diag}(E_1, \cdots, E_N) - \mathbf{A}$$

with

$$\rho(E) = \frac{1}{W} \Theta \left(\frac{W}{2} - |E| \right)$$

- H becomes a *random matrix*

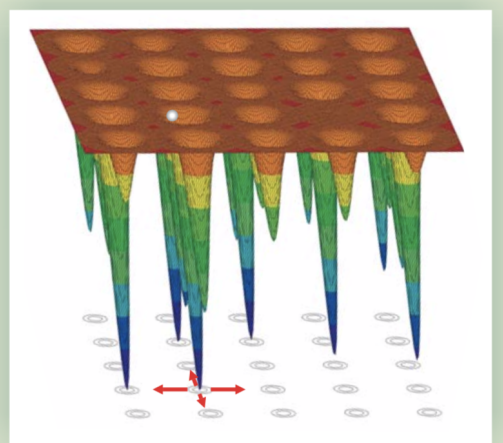


Figure 3. The Anderson model. Imagine an electron (silver) hopping on a two-dimensional lattice with random potential energies at each site. Quantum mechanics allows the electron to tunnel from one site to another through large energy barriers as depicted by the red arrows. The electron's energy thus changes randomly, although at each lattice site the spatial extent of its wavefunction (sketched below the potential) is assumed constant, leading to a constant tunneling rate. On an ordered lattice with all wells the same depth, the electron would be completely mobile for a range of energies. But here, a critical amount of randomness in the well depths localizes the electron, although on a scale larger than the lattice constant. For another perspective of what occurs as a lattice changes from perfect to disordered, see this month's cover.

Fifty years of Anderson Localization, Physics Today, 2009

Anderson Model

Localization transition

- 1D: Localization happens regardless the amount of disorder
- 2D: RG analysis suggests same as for 1D
- 3D and more: critical value W_c depends on the dimension and the energy λ
- Infinite Dimensions (Bethe lattice): *Your task!*

Localization in Anderson Model

Phase Diagram

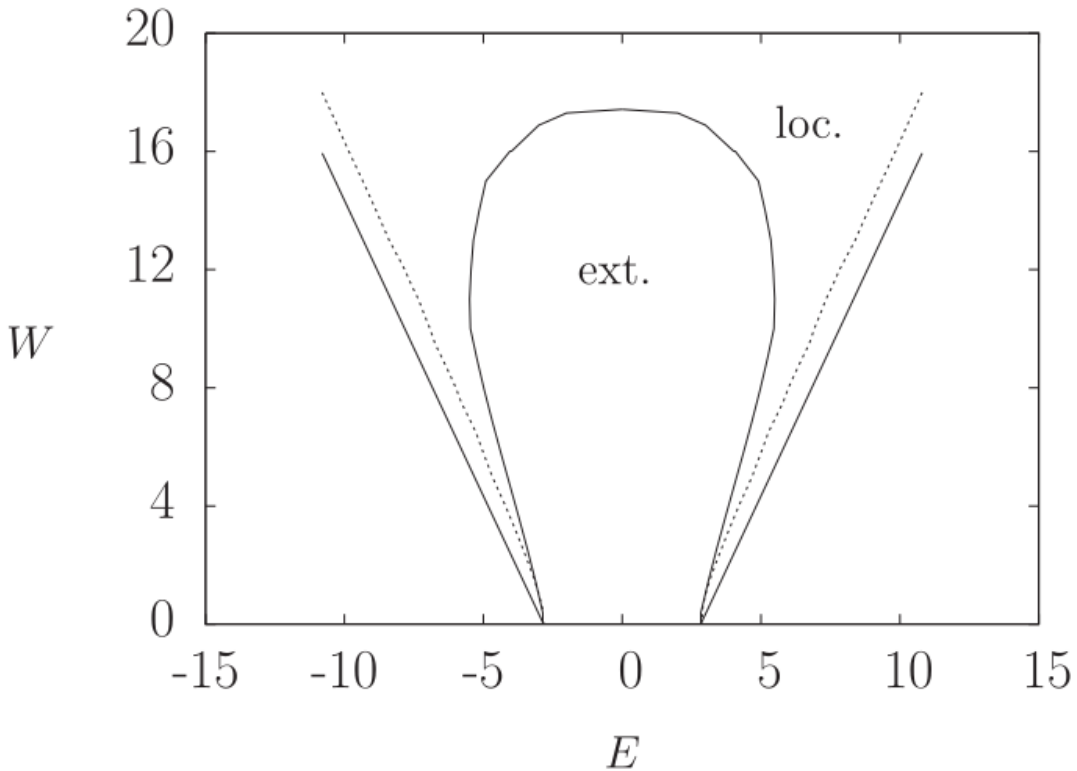
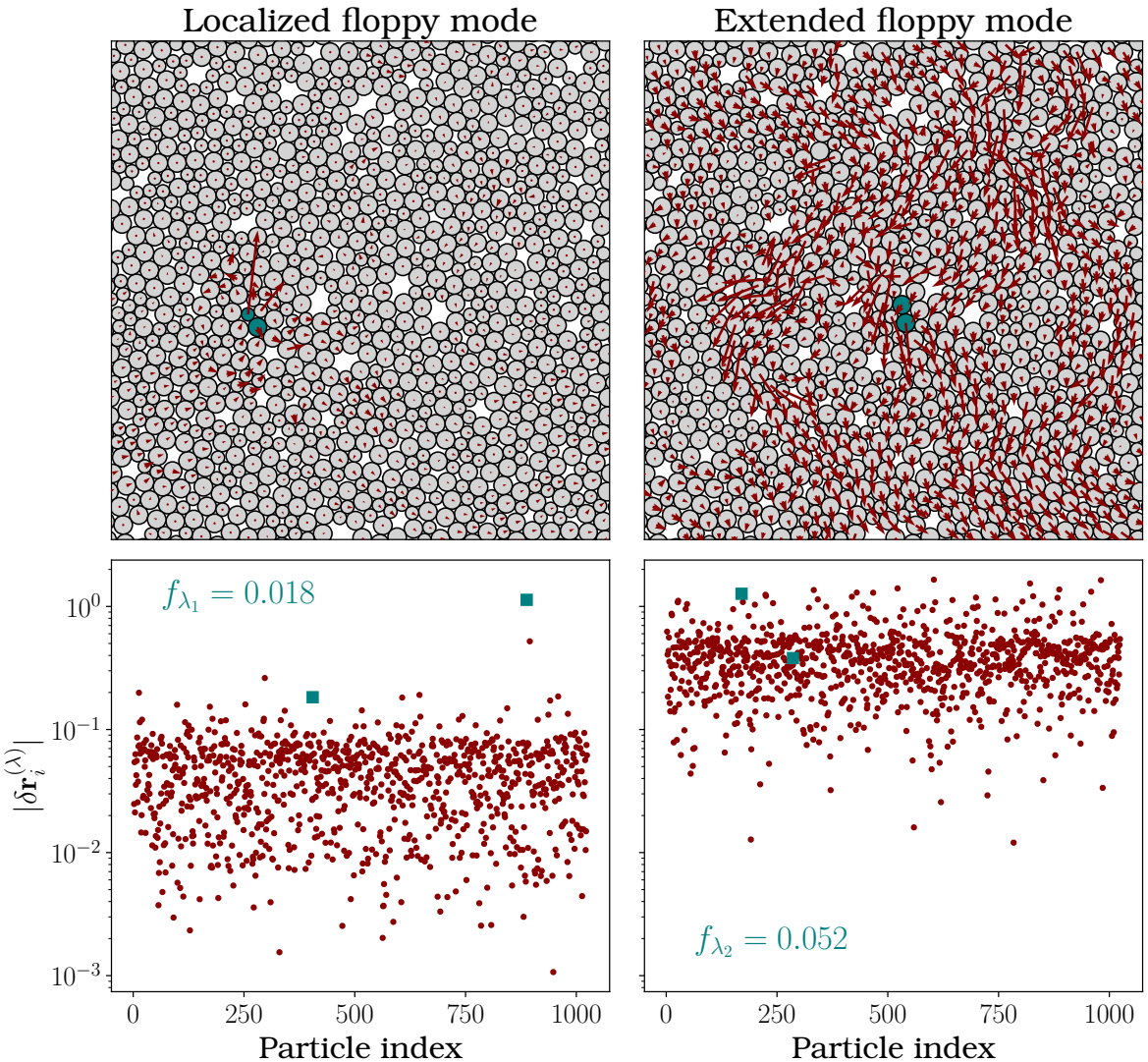


Fig. 1. Phase diagram for the Bethe lattice with connectivity $k+1=3$. The innermost solid line indicates the mobility edge between extended and localized states, the outermost solid line being the edge of the density of states $E=\pm(2\sqrt{k}+W/2)$. The dashed line is the numerically observed edge, see the text for details.

Biroli, Semerjian, & Tarzia (2010). *Anderson model on Bethe lattices*. Progr. Theo. Phys. Suppl.

How Localization looks like in amorphous solids?

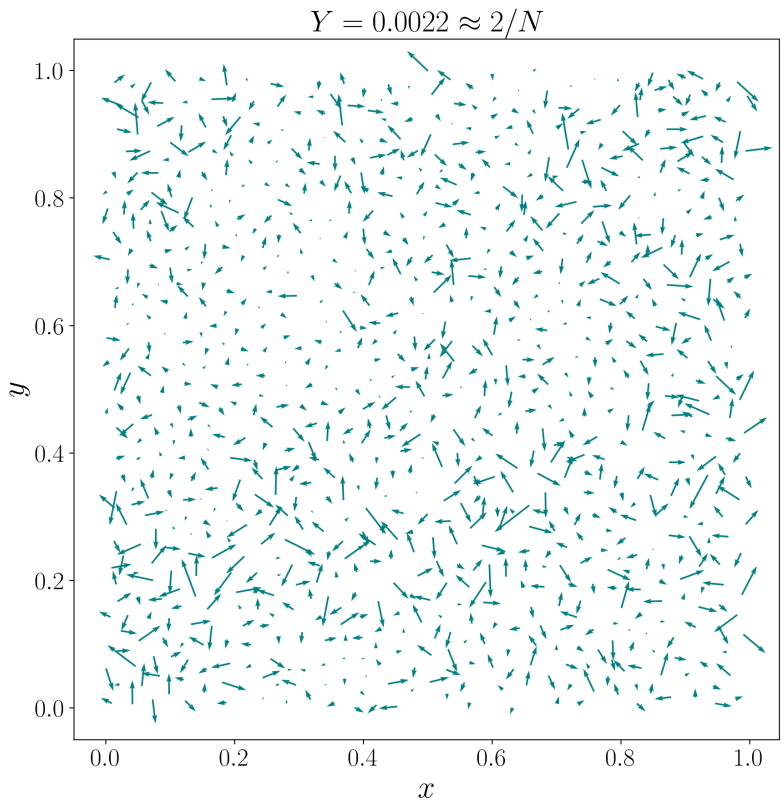
- Jammed packings: Critical behaviour ∼ phase transition.
- Heterogenous response to perturbations.
- Localized and extended modes have a clear spatial meaning.



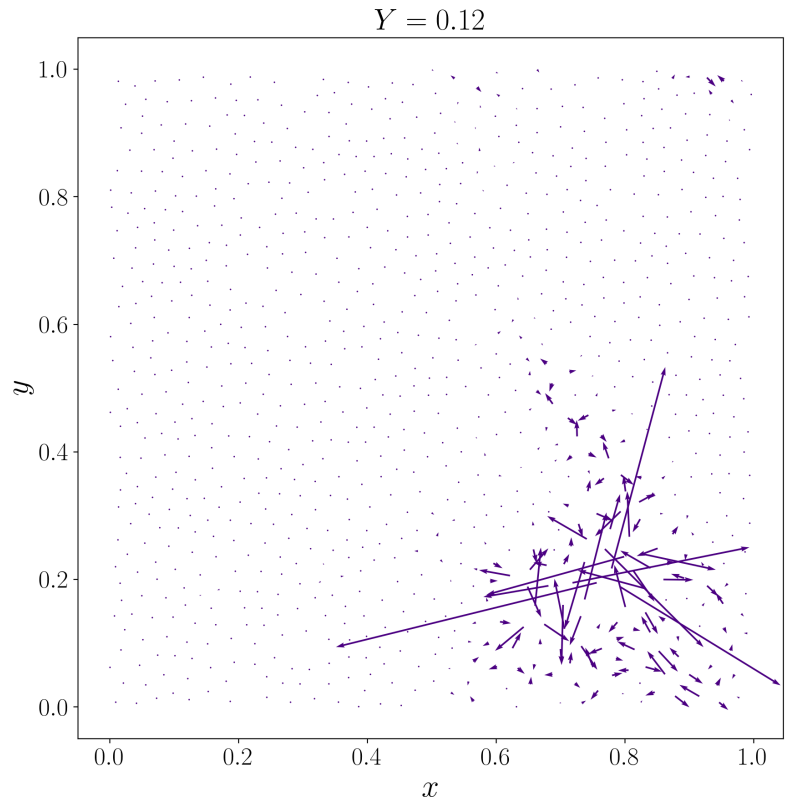
How Localization looks like in amorphous solids?

Given $H\,|V\rangle = \lambda\,|V\rangle$, the contribution to site i is $\mathbf{v}_i(\lambda) = \langle i|V\rangle$.

Inverse Participation Ratio: $Y(\lambda_k) = \dfrac{\sum_{i=1}^{N} |\mathbf{v}_i(\lambda_k)|^4}{\left|\sum_{i=1}^{N} |\mathbf{v}_i(\lambda_k)|^2\right|^2}$



Extended mode, $Y \sim 1/N$



Localized mode, $Y \sim 1$

Plan

Trap models

- Abstraction from landscape picture: hopping between traps
- Dynamics governed by distribution $\rho(E)$ of trap depths
- Simplest case: all traps accessible from each other, hop into random new trap each time
- But: no real-space picture
- Energy landscape vs dynamics
  - Intuitive picture of aging/non-equilibrium system: energetic, activation over increasingly large energy barriers, or entropic, fewer and fewer downhill directions
  - Trap models focus on distribution of energies in energy landscape
  - But connectivity of the landscape also (more?) important?
  - Only a few local rearrangements possible

Bouchaud trap model

- Traps $i = 1, \ldots, N$; trap i has depth $E_i > 0$; and $P_i(t)$ is prob. of being in a given trap at time t.
- Master operator $\boldsymbol{M}$: $M_{ij} = A_{ij} w_{ij}$ determined by connectivity and transition rates w_{ij}.
  - A: Adjecency matrix $\longleftrightarrow$ $A_{ij} = A_{ji} = 1$ only if $\langle ij \rangle$.
  - $k_i = \sum_{j \neq i} A_{ji}$ and $c = \langle k_i \rangle$.
  - Transition rates w_{ij}: how easy/likely is to go from trap $i \to j$
- Master Equation for evolution of $P_i(t)$:

$$\partial_t \boldsymbol{P} = \boldsymbol{M}\boldsymbol{P} \quad \Longleftrightarrow \quad \partial_t P_i(t) = \sum_{j=1}^{N} M_{ij} P_j(t), \quad M_{ii} = -\sum_{j \neq i} M_{ji}$$

- If $\boldsymbol{M}\boldsymbol{v}_\alpha = \lambda_\alpha \boldsymbol{v}_\alpha$, then general the solution is

$$\boldsymbol{P}(t) = \sum_{\alpha} e^{\lambda_\alpha t} \langle \boldsymbol{v}_\alpha | \boldsymbol{P}(0) \rangle \, \boldsymbol{v}_\alpha$$

Bouchaud trap model

- Trap i has depth $E_i > 0$
- Each hop is assumed to require activation to "top of landscape" ($\beta = 1/(k_{\mathrm{B}}T)$):

$$w_{i\to j} = \frac{1}{c}\, e^{-\beta E_i}$$

- Factor $1/c$ chosen to retrieve mean field model for $c \to \infty$
- Assume trap depth distribution $\rho_E(E) = e^{-E}$ $(E > 0)$
- Random graphs: Choose uniformly among networks with given p_k
- Simplest case: random regular graph, $p_k = \delta_{k,c}$

BTM Falling out of equilibrium

- Exit rate from trap i is $k_i/(c\tau_i) \sim 1/\tau_i := e^{-\beta E_i}$
- Lifetime scale $\tau_i = e^{\beta E_i}$ has prior distribution $\rho_\tau(\tau) = T\tau^{-T-1}$
- Dynamics satisfies detailed balance
- Equilibrium distribution is Boltzmann, $P_{\mathrm{eq},i} \propto e^{\beta E_i}$
- Eq. probability of being in traps of depth $E \ldots E + dE$ is $p_{\mathrm{eq}}(E) \propto \rho(E)e^{\beta E}$
- Grows with $E \to \infty$ for $\beta > 1$: glass transition, system ages into deeper and deeper traps

Plan

Summary

- Anderson and Bouchaud trap model are models of disordered systems
- Both are characterized by a random matrix ($N \times N$ dimensional)
  - Anderson: Hamiltonian

$$H_{ij} = E_i I_{ij} - t A_{ij}$$

  - Bouchaud: Master operator

$$M_{ij} = A_{ij} w_{ij} = \frac{A_{ij}}{c} \mathrm{e}^{-\beta E_j}$$

In both cases E is a random variable but sampled from different distributions. We are interested in:

- Density of states: distribution of eigenvalues
- Localization properties of associated eigenvectors

as $N \to \infty$ ...

Plan

Cavity method and Anderson model

For $\mathbf{M} = H$, the marginal precisions ω_j are determined by the equations (notice the presence of the diagonal elements):

$$\omega_j = i(\lambda - i\epsilon - E_j) + \sum_{k \in \partial j} \frac{1}{\omega_k^{(j)}}$$

Where the cavities satisfy the recursive relation

$$\omega_k^{(j)} = i(\lambda - i\epsilon - E_k) + \sum_{l \in \partial k \setminus j} \frac{1}{\omega_l^{(k)}}$$

Cavity equations in the thermodynamic limit

Consider a Random Regular Graph with connectivity c.
In the thermodynamic limit $N \to \infty$, the recursive equations become a self–consistent equation for the cavities distribution

$$P(\omega) = \int dE \rho(E) \prod_{l=1}^{c-1} dP(\omega_l)\, \delta\left(\omega - i(\lambda - i\epsilon - E) - \sum_{l=1}^{c-1} \frac{1}{\omega_l}\right)$$
$$= \left\langle \delta\left(\omega - i(\lambda - i\epsilon - E) - \sum_{l=1}^{c-1} \frac{1}{\omega_l}\right)\right\rangle_{\{\omega_l\},E}$$

Cavity variance $g = i/\omega$. Important: A specific matrix becomes non–relevant anymore.

Cavity method and Bouchaud trap model

Equation for cavity precisions:

$$\omega_k^{(j)} = ic((\lambda - i\epsilon)\tau_k + 1) + \sum_{l \in \partial k \setminus j} \frac{1}{\omega_l^{(k)}}$$

with lifetime $\tau_j = \mathrm{e}^{\beta E_j}$. Equation for marginal precisions:

$$\omega_j = ic((\lambda - i\epsilon)\tau_j + 1) + \sum_{k \in \partial j} \frac{1}{\omega_k^{(j)}}$$

The diagonal resolvent entries G_{jj} are then given by

$$G_{jj} = \frac{i\tau_j c}{\omega_j}$$

Localization

Distribution of marginal variances: $P(\mathrm{Im}G)$.
From Stieltjes-Perron formula:

$$\rho(\lambda) = \lim_{\epsilon\to 0} \frac{1}{\pi N} \sum_{i=1}^{N} \mathrm{Im}\, G_{ii}(\lambda_\varepsilon) \underbrace{=}_{\lim_{N\to\infty}} \lim_{\epsilon\to 0} \frac{1}{\pi} \langle \mathrm{Im}G \rangle$$

Abou–Chacra, Anderson and Thouless (1973) [2]:

$$\lim_{\epsilon\to 0} \mathrm{Im}G^{\mathrm{typ}}(\lambda) = \lim_{\epsilon\to 0} \mathrm{e}^{\langle \ln \mathrm{Im}G \rangle}$$

$$= \begin{cases} O(\epsilon) & \text{Localized eigenvector} \\ O(1) \approx \langle \mathrm{Im}G \rangle & \text{Extended eigenvector} \end{cases}$$

[2] A selfconsistent theory of localization, JPhysC

Localization

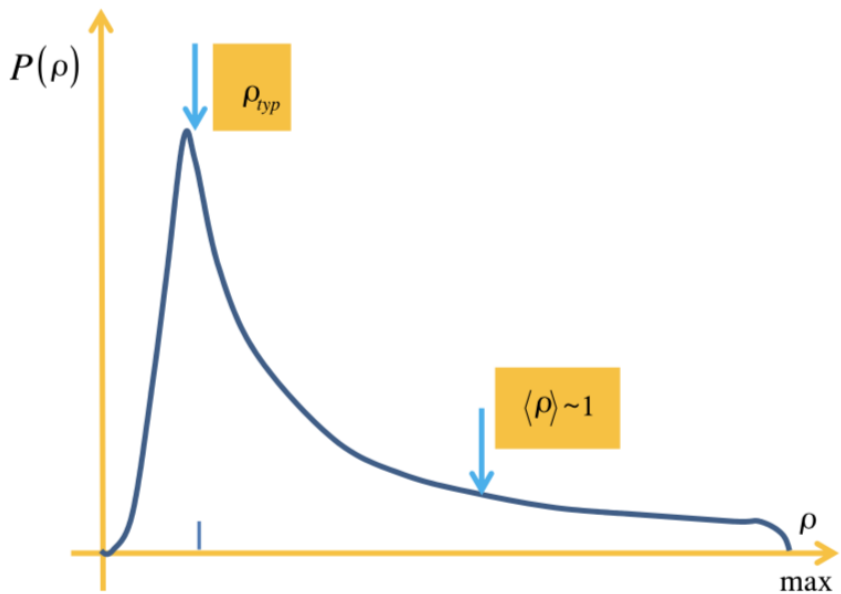


Fig. 2. (Color online) Distribution function of local density of states $P_0(\rho)$ for the non-ergodic extended states in the limit $\eta \to 0$ taken after the limit $N \to \infty$ (solid curve). The typical ρ_{typ} is much smaller than the average $\langle\rho\rangle$ and depends critically on disorder close to the Anderson transition.

Plan

Solving the Single Instance cavity equations

In general, the cavity equations that we consider will be of the form

$$\omega_k^{(j)} = h\left(\lambda_\epsilon, E_k, \sum_{l\in\partial k\setminus j} f\left(\omega_l^{(k)}\right)\right)$$

with f and h known functions.
Aim: find fixed point solution of this equation. Notice that (k, j) runs over all the edges ($\mathcal{E}$, considered as a directed network , i.e. $(k, j) \neq (j, k)$)

Solving the Single Instance cavity equations

[See Mézard & Montanari (2009), Chp. 14; and Susca *et al* SciPost Phys. (2021)]

1. Initialize all the $\{\omega_j^{(k)}\}_{j\in 1,\dots,N}^{k\in\partial j}$ as i.i.d. random variables with arbitrary distribution P; define `tolerance`
2. For $t \in \{0, \dots, t_{\max}\}$
   - For each $(k, j) \in \mathcal{E}$
     - Compute $\omega_k^{(j)}(t+1) = h(\lambda_\epsilon, E_k, \sum_{l\in\partial k\setminus j} f(\omega_l^{(k)}))$
     - Compute $\delta_j^{(k)} = |\omega_j^{(k)}(t+1) - \omega_j^{(k)}(t)|$
     - Update $\omega_j^{(k)}(t) \leftarrow \omega_j^{(k)}(t+1)$
   - Let $\Delta = \max_{j,k} \delta_j^{(k)}$ be the maximum change in precisions.
   - If $\Delta <$ `tolerance`, return $\{\omega_j^{(k)}(t)\}_{j\in 1,\dots,N}^{k\in\partial j}$
3. Return `not-converged`

Once the cavities $\omega_k^{(j)}$ are found, they must be plugged into the expression for the marginals ω_j.

Solving the Single Instance cavity equations

Convergence on trees [3]

Theorem

Consider a tree with diameter t^*. Then:

- *Irrespective of the initial condition, the SI cavity equations converge after at most t^* iterations.*
- *The fixed-point messages provide the exact marginals: for any variable node i, and any $t > t^*$, $\omega_{i,t} = \omega_i^*$ such that $P(x_i; \omega_i^*) = \int \prod_{j \neq i} dx_j P(\mathbf{x})$*

[3] c.f. Theorem 14.1, Mézard, Montanari

Solving the $N \to \infty$ limit

The self–consistent equation on a RRG:

$$P(\omega) = \left\langle \delta\left(\omega - h\left(\lambda_\epsilon, E, \sum_{l=1}^{c-1} f(\omega_l)\right)\right)\right\rangle_{\{\omega_l\},E}$$

is solved using the **Population Dynamics** (PD) algorithm.

1. Start with an initial (complex) population $\hat{P} = (\omega_1, \cdots, \omega_{N_p})$
2. Sweep-(i): Pick $c-1$ random elements $\{\omega_l\}$ from $\hat{P}$ and sample E from $\rho(E)$.
3. Sweep-(ii): Replace a random element of the population with $h\left(\lambda_\epsilon, E, \sum_{l=1}^{c-1} f(\omega_l)\right)$
4. Repeat steps (2) and (3) until equilibration is reached

With this procedure we can estimate $P(\omega)$ and hence $P(g)$

Evaluating the marginals (Measurment sweeps)

Marginal precisions are given by the distribution:

$$P(\Omega) = \left\langle \delta\left(\Omega - h\left(\lambda_\epsilon, E, \sum_{l=1}^{c} f(\omega_l)\right)\right)\right\rangle_{\{\omega_l\},E}$$

(*In these models:* Same h, but one extra ω_l)

1. Start with an equilibrated population $\hat{P}_{\rm eq} = (\omega_1, \cdots, \omega_{N_p})_{\rm eq}$
2. Pick c random elements $\{\omega_l\}$ from $\hat{P}_{\rm eq}$ and sample E from $\rho(E)$.
3. Generate a sample from $\Omega \sim P(\Omega)$ by evaluating $h\left(\lambda_\epsilon, E, \sum_{l=1}^{c} f(\omega_l)\right)$
4. Update one random element from $\hat{P}_{\rm eq}$ by evaluating steps 2 and 3 from the previous routine (PD sweep)
5. Repeat steps 2 to 4 for N times.

You can work (in principle) with $N \gg N_p$. To avoid introducing spurious correlations, do not do $N > N_p \times 1000$.