Nonequilibrium Statistical Physics of Complex Systems

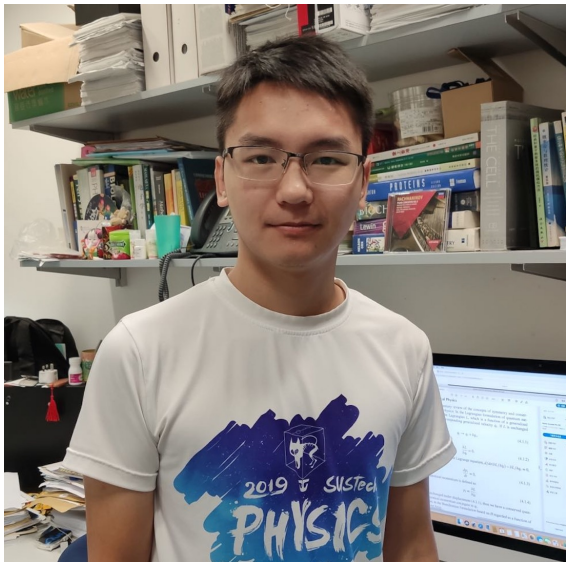
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Emergence of hidden order and its dynamical evolution in the annealed Sherrington-Kirkpatrick model

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Ding Wang, SUSTech/HKBU

Outline

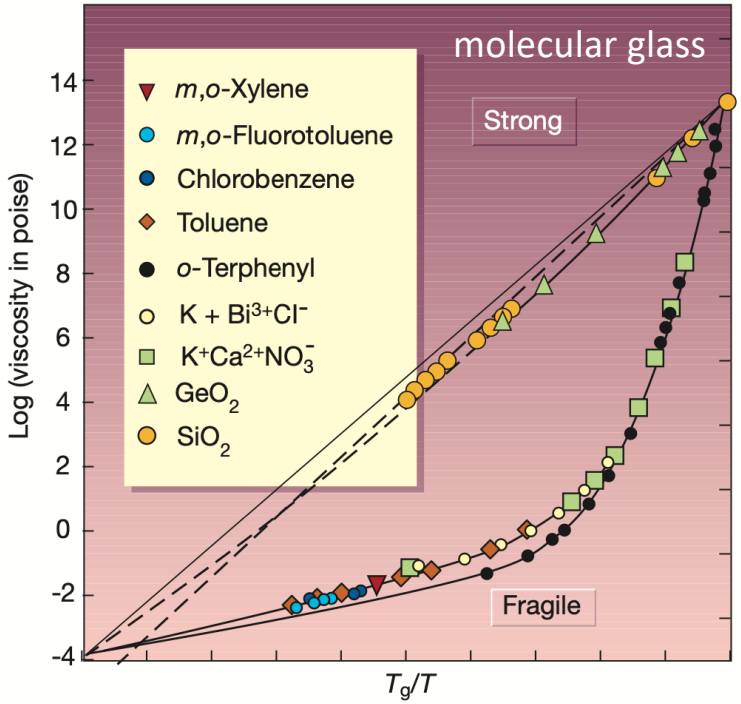
- Supercooled liquids and molecular glass
- A toy model: Sherrington – Kirkpatrick (SK) spin glass and the Nishimori line
- Random matrix formulation: gap opening and condensation at low temperatures
- Exact finite-size scaling at the spectral edge
- Separation of timescales and global reorganization near criticality

Ding Wang and LHT, arXiv 2405.14215

Supercooled liquids and molecular glass

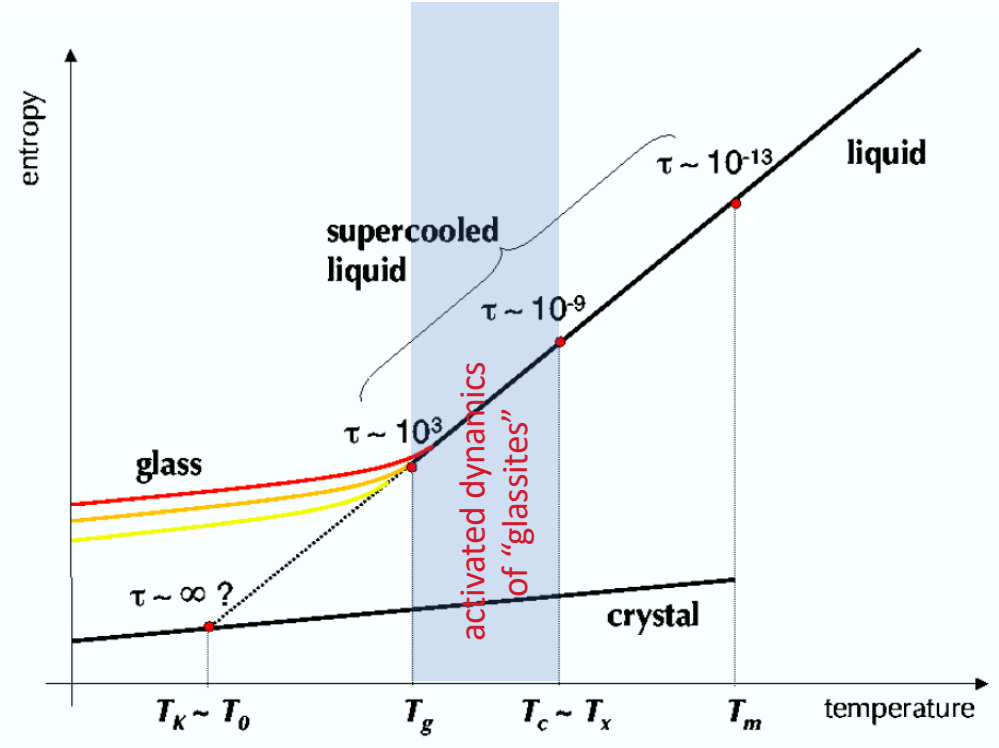


Is glass a frozen liquid?



Angell's plot showing super-Arrhenius divergence of viscosity near T_g for "fragile glass"

Debenedetti & Stillinger, *Nature* **410**, 259 (2001)



Andrea Cavagna, "Supercooled liquids for pedestrians", *Phys Reports* **476**: 51-124 (2009)

Dynamical Heterogeneities in Glasses, Colloids and Granular Media

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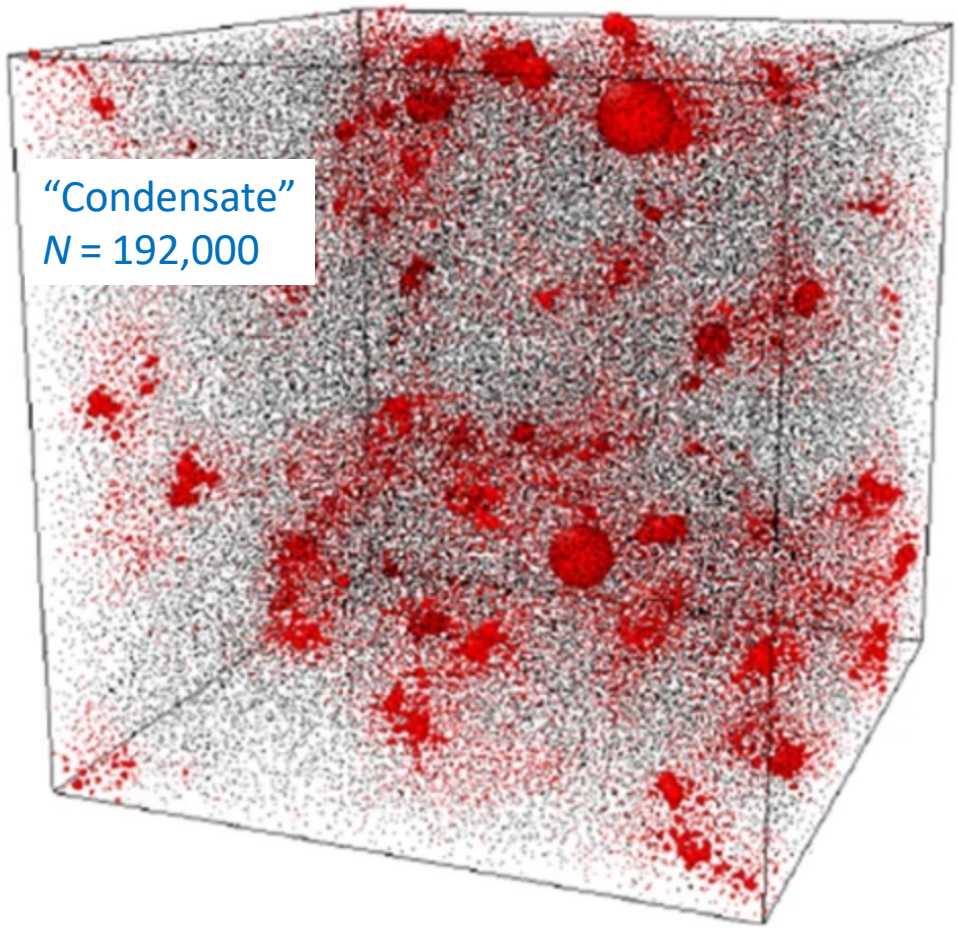
Review of intense theoretical efforts over two decades

In recent years, evidence has mounted that the dynamical slowing down of supercooled liquids, colloids and granular media might indeed be related to the **existence of genuine phase transitions**, but **of very peculiar nature**.

Contrasting with usual phase transitions, the dynamics of these materials dramatically slows down **with nearly no changes in their conventional structural properties.**

One of the most interesting consequences of these ideas is the existence of **dynamical heterogeneities**, which have been discovered to be, in the space-time domain, the **analog of critical fluctuations in standard phase transitions.**

Dynamic heterogeneity in 3D polydisperse soft spheres



L Wang, A Ninarello, P Guan, L Berthier, G Szamel, E Flenner, Low-frequency vibrational modes of stable glasses. *Nat Commun* **10**, 26 (2019)

Soft spots in deep quenched glass

More recent work and reviews

Y Nishikawa, M Ozawa, A Ikeda, P Chaudhuri, L Berthier Phys. Rev. X **12**, 021001 (2022)

LF Cugliandolo, Annu. Rev. Condens. Matter Phys. **15**: 177–213 (2024)

Biroli, G., & Bouchaud, J. P. (2023). The RFOT Theory of Glasses: Recent Progress and Open Issues. Comptes Rendus. Physique, 24(S1), 1-15.

Jean-Philippe Bouchaud (2024). Why is the Dynamics of Glasses Super-Arrhenius? arXiv:2402.01883

… extensive numerical simulations of the non-linear susceptibility of glasses, in particular in the aging regime, should shed important light on the mechanism at the origin of the **super-Arrhenius behaviour of the relaxation time.**

In any case, more imagination is still needed to come up with experimental, theoretical or numerical ideas that would allow to finally settle **the question of why glasses do not flow**.

Are we close to solving the

glass conundrum?

A toy model

Sherrington – Kirkpatrick spin glass and the Nishimori line

$$H(\{S_i\},\{J_{ij}\}) = -\sum_{1\le i<j\le N} J_{ij}S_iS_j\,, \qquad S_i = \pm 1$$

$$J_{ij} = \begin{cases} J/\sqrt{N}\,, & \text{prob } p \\ -J/\sqrt{N}, & \text{prob } 1-p \end{cases}$$

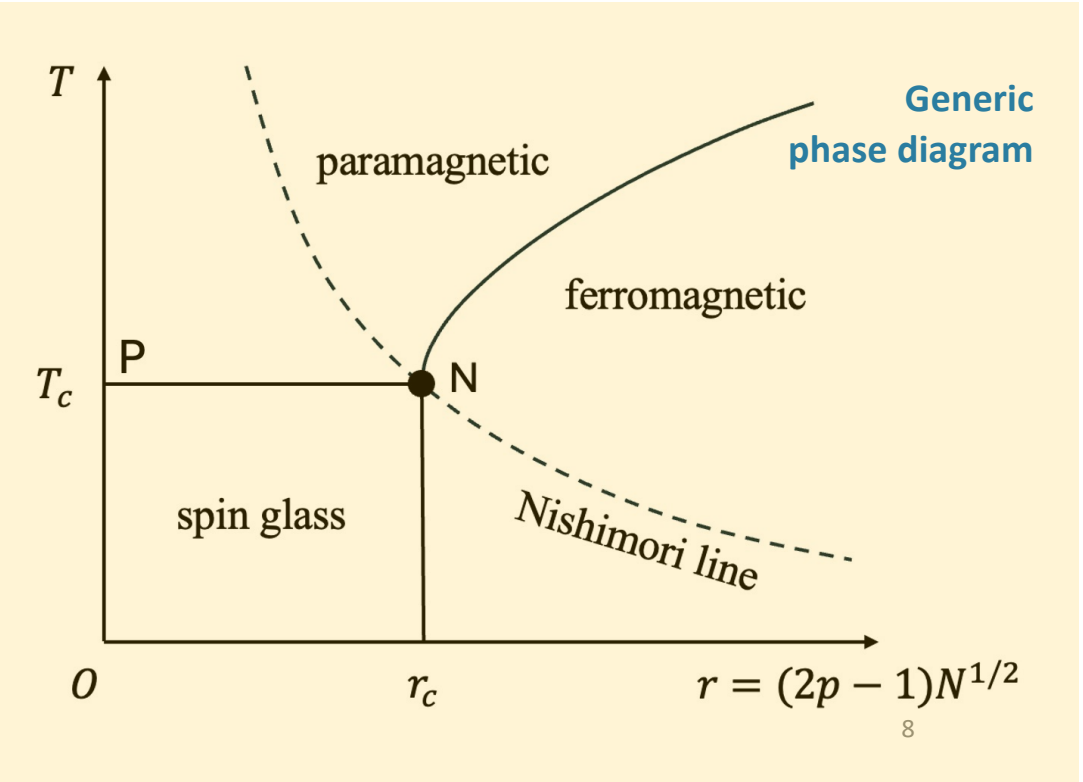
Energy change associated with a single spin flip:

$$\Delta E = \pm 2\sum_j J_{ij}S_j \simeq \pm 2J\left[\frac{2p-1}{\sqrt{N}}M + \eta\right]$$

Ferromagnetic coupling

"random field" of unit strength

$$M = \sum_j S_j$$



The Nishimori line

Annealed model:

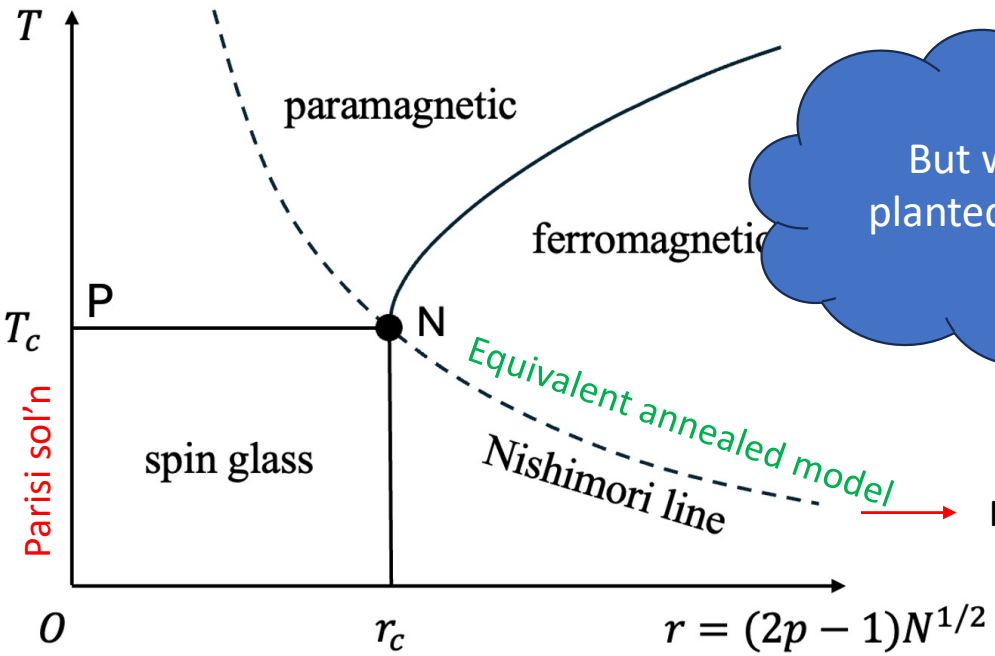
$$Z(\{J_{ij}\}) = \sum_{\{J_{ij}=\pm 1/\sqrt{N}\}} \sum_{\{S_i\}} e^{\beta \sum_{i<j} J_{ij} S_i S_j}, \qquad \beta = 1/T$$

no thermodynamic transition!

Nishimori line: $e^{2\beta/\sqrt{N}} = \frac{p}{1-p}$

- Along the Nishimori line, quenched averages are identical to those of the annealed model.

Hidden Mattis order in the annealed model $T < T_c = 1$ (first suggested by Kasai & Okiji (1983)



Mattis model: $J_{ij} = \frac{1}{N}\sigma_i^0 \sigma_j^0$

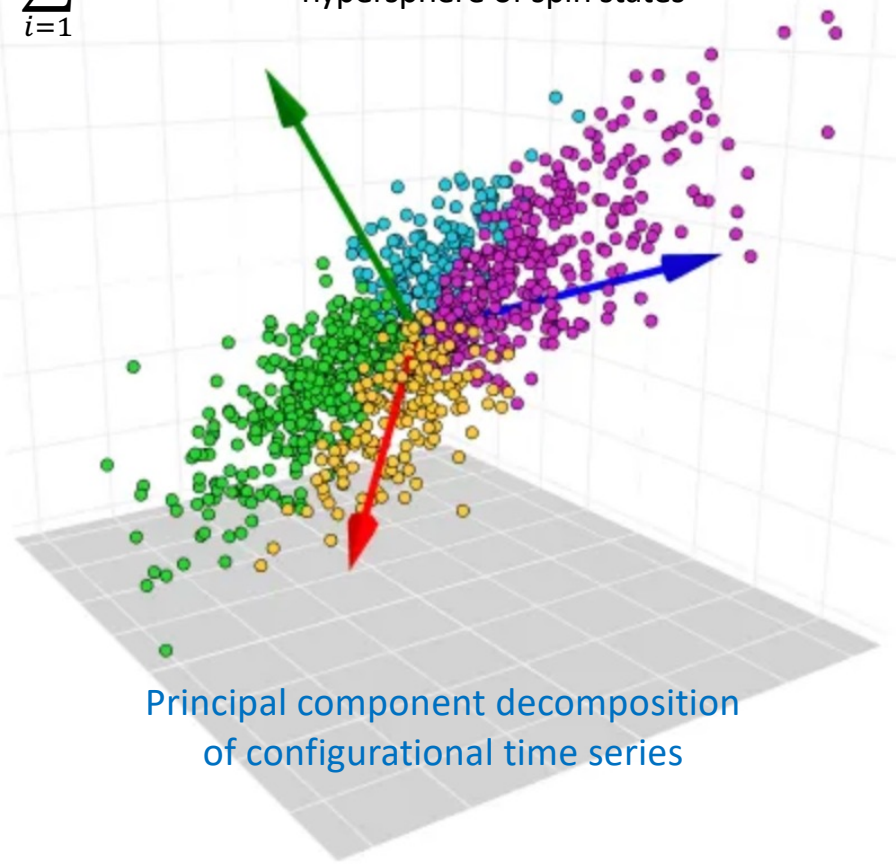
condensation onto "planted state" $\{\sigma_i^0\}$

Random matrix formulation: gap opening and condensation at low temperatures

Laura Foini, Jorge Kurchan, “Annealed averages in spin and matrix models”, *SciPost Phys* **12**, 080 (2022)

$$\sum_{i=1}^{N} S_i^2 = N$$

N-dimensional hypersphere of spin states



Principal component decomposition of configurational time series

https://towardsdatascience.com/principal-component-analysis-pca-explained-visually-with-zero-math-1cbf392b9e7d

Spectral representation

Spectral representation of the coupling matrix:

$$H = -\sum_{1\le i<j\le N} J_{ij}S_iS_j = -\vec{S}\boldsymbol{J}\vec{S}^T = -\sum_{1\le\mu\le N}\lambda_\mu s_\mu^2$$

$s_\mu = \vec{S}\cdot\vec{V_\mu}$ $\quad$ z = Lagrange multiplier

λ_μ the set of eigenvalues

$\vec{V_\mu}$ the corresponding eigenvectors

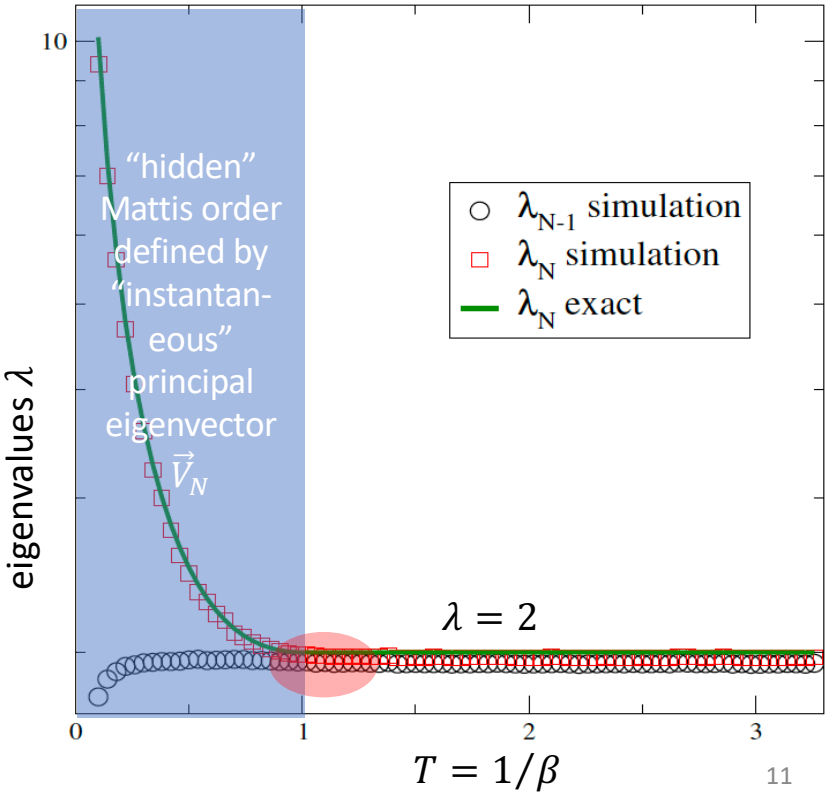
$$Z = \int [dJ][dS]P(\boldsymbol{J})\, e^{-\beta H}\delta\left(\sum_{i=1}^{N} S_i^2 - N\right)$$

$$= \beta^{1-N/2}\int [d\lambda]dz\, e^{-Nf(\lambda_1,\cdots,\lambda_N;z)}$$

$N \longrightarrow \infty$: $\quad z = \beta + \frac{1}{\beta}$

$T > T_c = 1$, unchanged from the infinite T

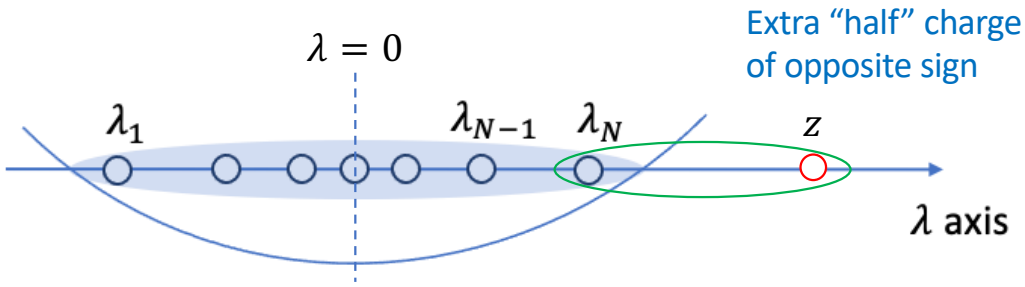
$T < T_c$, $\lambda_N = z$ separates from the rest



Exact finite-size scaling at spectral edge

Coulomb gas on a string

$$f(\lambda_1, \cdots, \lambda_N; z) = \frac{1}{4}\sum_{\mu=1}^{N} \lambda_\mu^2 - \frac{1}{N}\sum_{1\le\mu<\nu\le N} \ln|\lambda_\mu - \lambda_\nu| + \frac{1}{2N}\sum_{\mu=1}^{N} \ln(z-\lambda_\mu) - \frac{\beta}{2} z$$



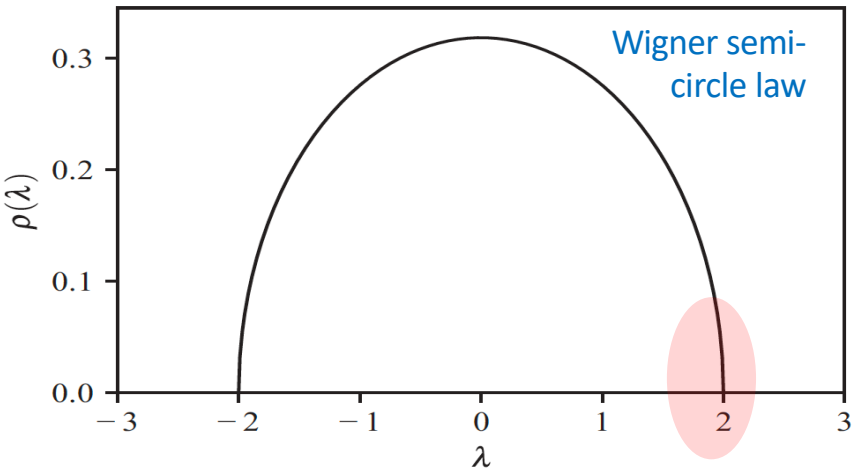
Eigenvalues respond to temperature $T = \beta^{-1}$

Maximum Likelihood Spectrum

$$\frac{\partial f}{\partial \lambda_\mu} = \frac{1}{2}\lambda_\mu - \frac{1}{N}\sum_{\nu,\,\nu\neq\mu}\frac{1}{\lambda_\mu - \lambda_\nu} - \frac{1}{2N}\frac{1}{z-\lambda_\mu} = 0$$

$$\frac{\partial f}{\partial z} = \frac{1}{2N}\sum_{\mu=1}^{N}\frac{1}{z-\lambda_\mu} - \frac{\beta}{2} = 0$$

Zeroth order:



Stieljtes transform: $g_N(x) = \frac{1}{N}\sum_{\mu=1}^{N}\frac{1}{x-\lambda_\mu}$

$$g_N^2(x) - x g_N(x) + 1 = -\epsilon g_N'(x) + \epsilon\,\frac{g_N(x) - g_N(z)}{x-z}$$

Scaling ansatz near $x = 2$:

$$g_N(x) = 1 - \epsilon^{1/3}\varphi\left(\frac{x-2}{\epsilon^{2/3}}\right), \qquad \epsilon = \frac{1}{N}$$

(u is the scaled variable)

$$\varphi'(u) = \varphi^2 - u + \frac{\varphi(u) - \varphi(c)}{u-c}$$

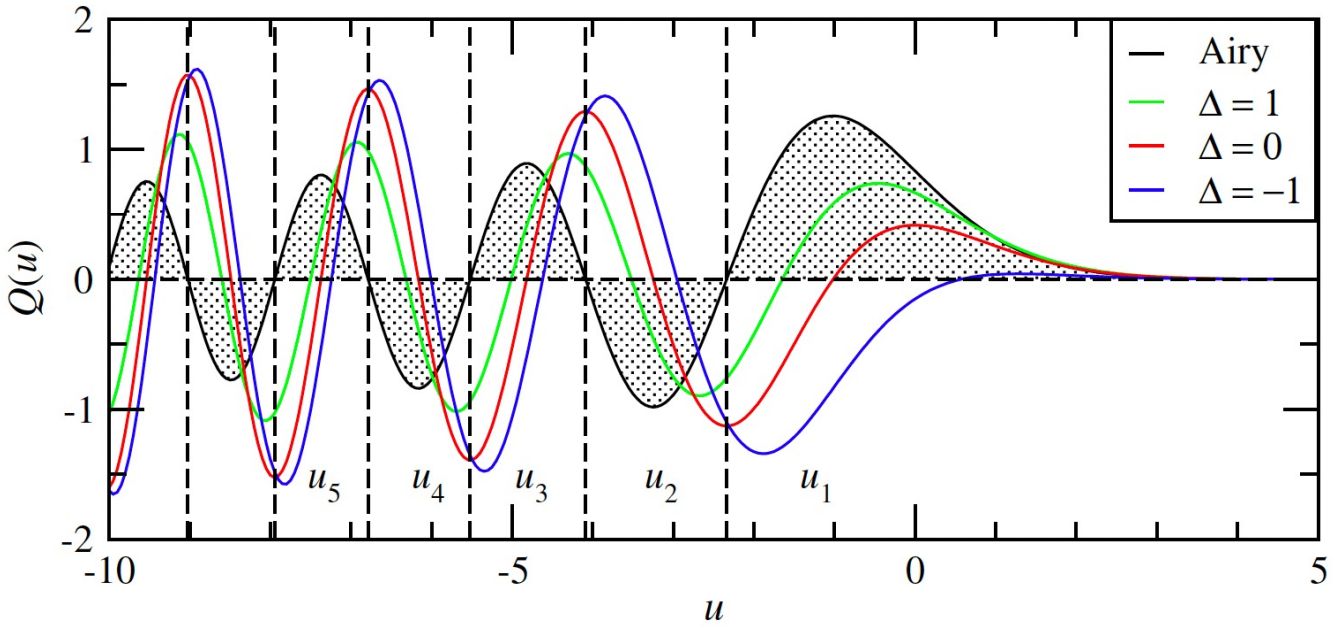
ODE of the Riccati type

$$\varphi(c) = \Delta \equiv \frac{1}{2}N^{1/3}(\beta^{-1} - \beta)$$

$$\frac{Q'}{Q} = -\varphi \quad \Rightarrow \quad Q'' = uQ + \frac{Q' - Q\Delta}{u-c}$$

Ding Wang and LHT, arXiv:2405.14215

Nodal points of $Q(u)$ = location of eigenvalues at the spectral edge



k	1	2	3	4	5
u_k^0	−2.3381074	−4.0879494	−5.5205598	−6.7867080	−7.9441336
u_k^c	−1.0187930	−3.2481977	−4.8200993	−6.1633075	−7.3721773

Airy function nodes

Finite-size scaling of principal components of spin configurations

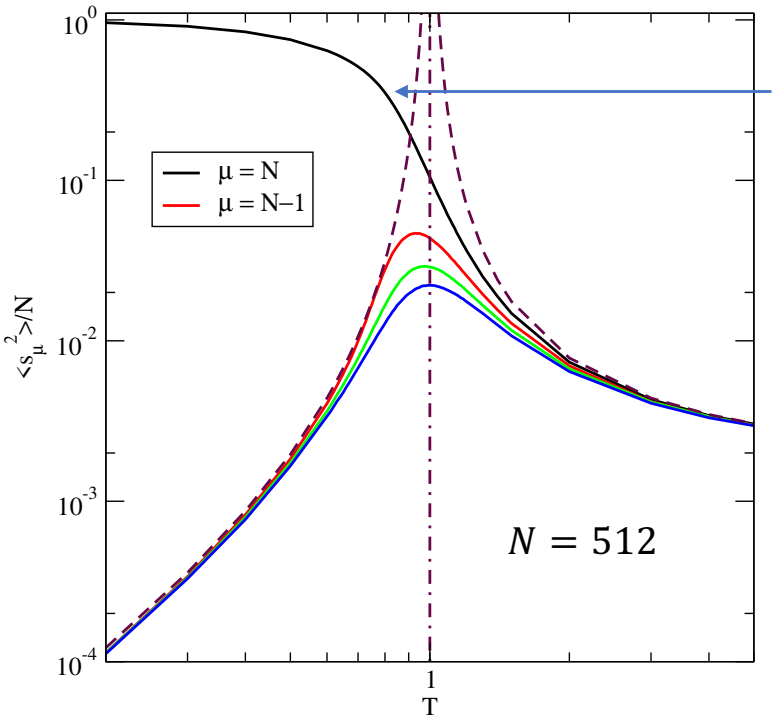
$$\langle s_\mu^2 \rangle = \left\langle \frac{T}{z - \lambda_\mu} \right\rangle , \qquad \sum_{\mu=1}^{N} \langle s_\mu^2 \rangle = N$$

In the critical region, MLE yields

$$\lambda_k = 2 + u_{N-k+1} N^{-2/3}$$

$$z = 2 + \Delta^2 N^{-2/3}$$

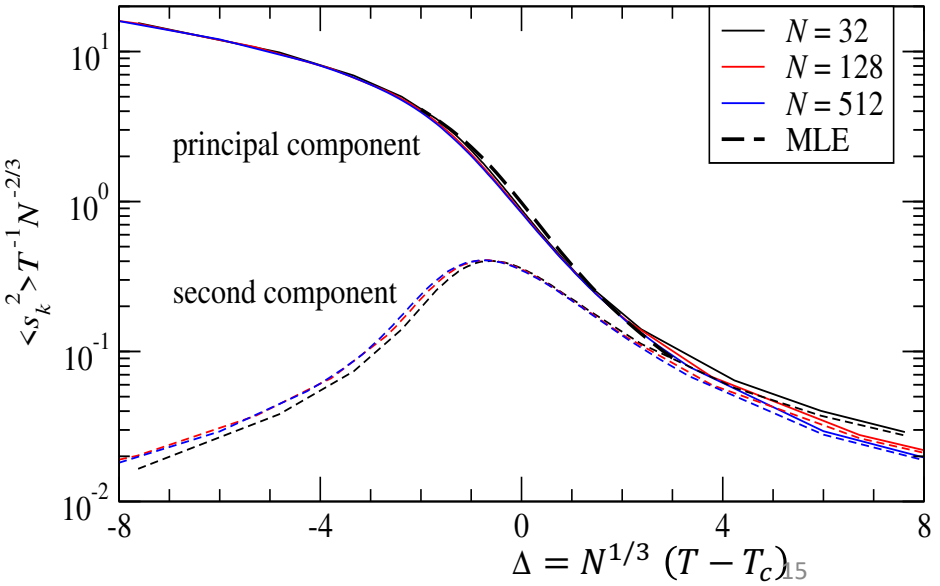
$$\boxed{\langle s_k^2 \rangle = T N^{2/3} \psi_k \left(N^{1/3} (T - 1) \right)}$$



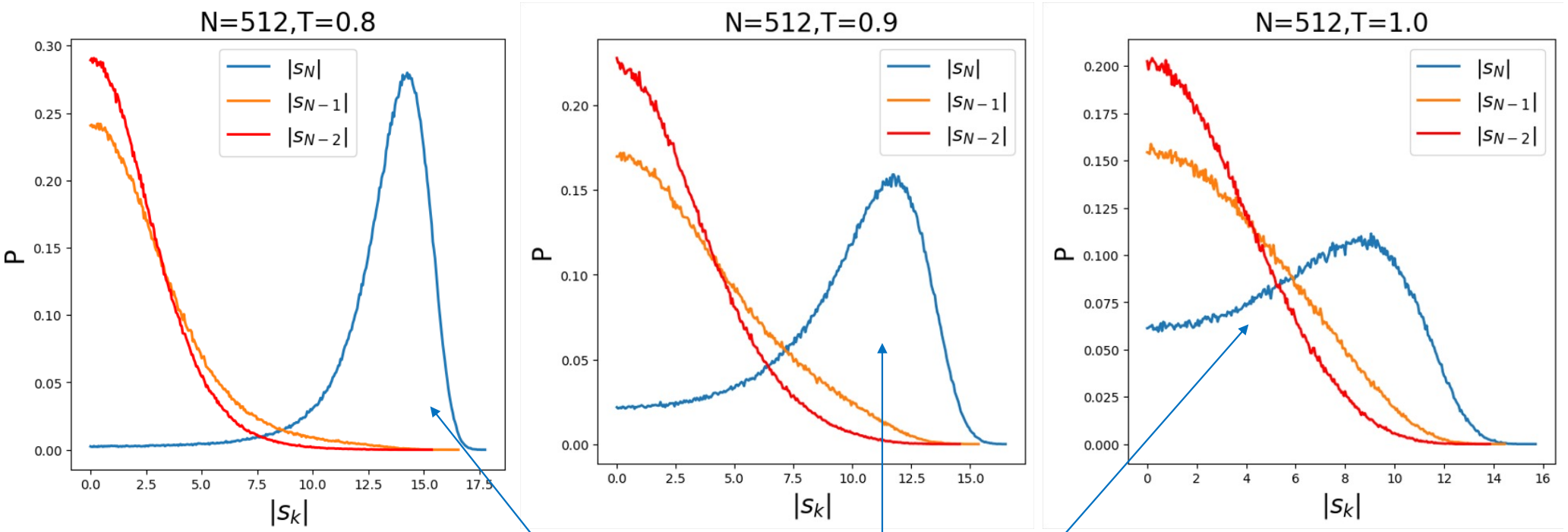
Principal component

$$\frac{\langle s_N^2 \rangle}{N} = 1 - T^2$$

comparison of simulation data with maximum likelihood estimations (MLE)



Distribution of instantaneous spin amplitudes on the first three eigenvectors



broadening due to λ_N fluctuations

Monte Carlo Simulations of the annealed SK model

- Metropolis with **fast spin flips** and **slow update of $J'_{ij}s$**
- Compute instantaneous orthonormal eigenvectors $\vec{V}_\mu(t)$ of the coupling matrix $\mathbf{J}(t)$ and projection

$$s_\mu(t) = \vec{S}(t) \cdot \vec{V}_\mu(t)$$

of the spin configuration $\vec{S}(t)$ on the eigen-directions.

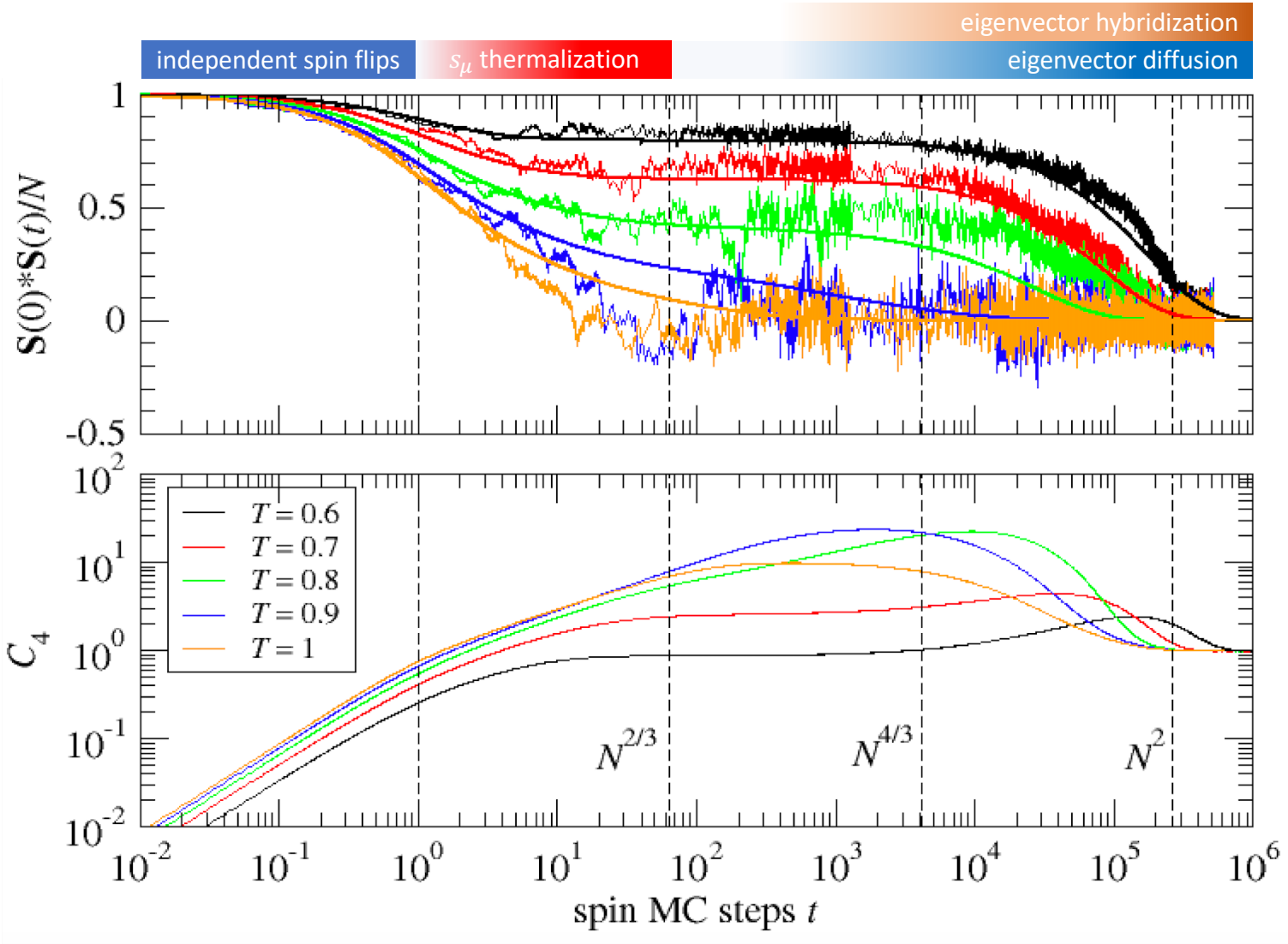
1 spin MC step = *N* attempted spin flips

1 attempted J_{ij} flip = $\frac{1}{2}N(N-1)$ spin MC steps

$N = 512$

auto spin correlation $C_2(t)$

$C_2(t)$ fluctuations (dynamic heterogeneity)



Principal Component Decomposition

$$s_\mu(t) = \vec{S}(t) \cdot \vec{V}_\mu(t)$$

eigenvectors of $\overleftrightarrow{J}(t)$

Separation of timescales and global reorganization near criticality

$\vec{S}(t)$: glass "phenotype", fast

$\overleftrightarrow{J}(t)$: "backbone", slow



Instantaneous eigenvectors in the *N*-dimensional configurational space

Dynamic evolution of the spin condensate driven by

i) slow diffusive motion of $\vec{V}_\mu(t)$

ii) eigenvector hybridization (level crossing) of the coupling matrix

Trajectory of a particular sample at $N = 512$

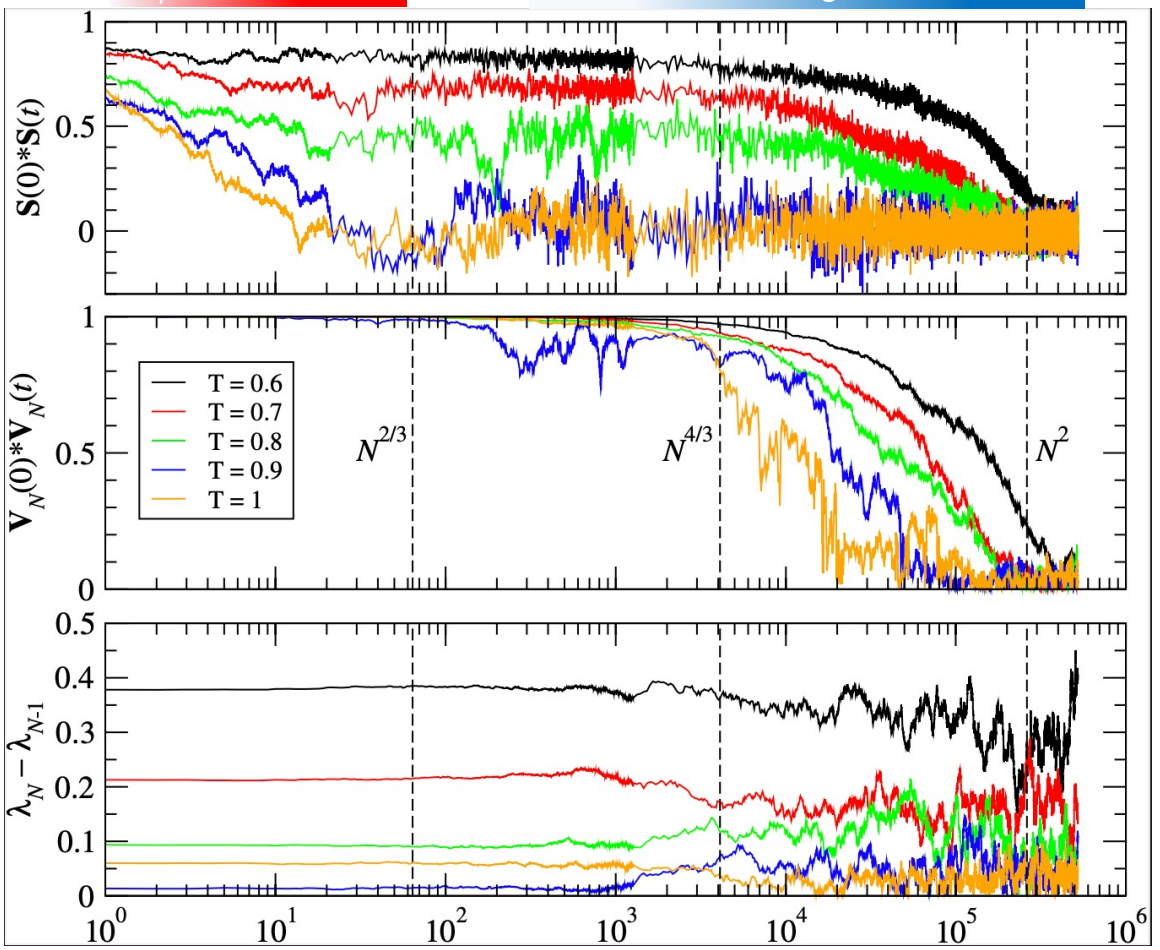
$$s_\mu(t) = \vec{S}(t) \cdot \vec{V}_\mu(t)$$

$\langle s_\mu^2 \rangle \approx 1$ $\langle s_\mu^2 \rangle \approx N^{2/3}$

s_μ thermalization

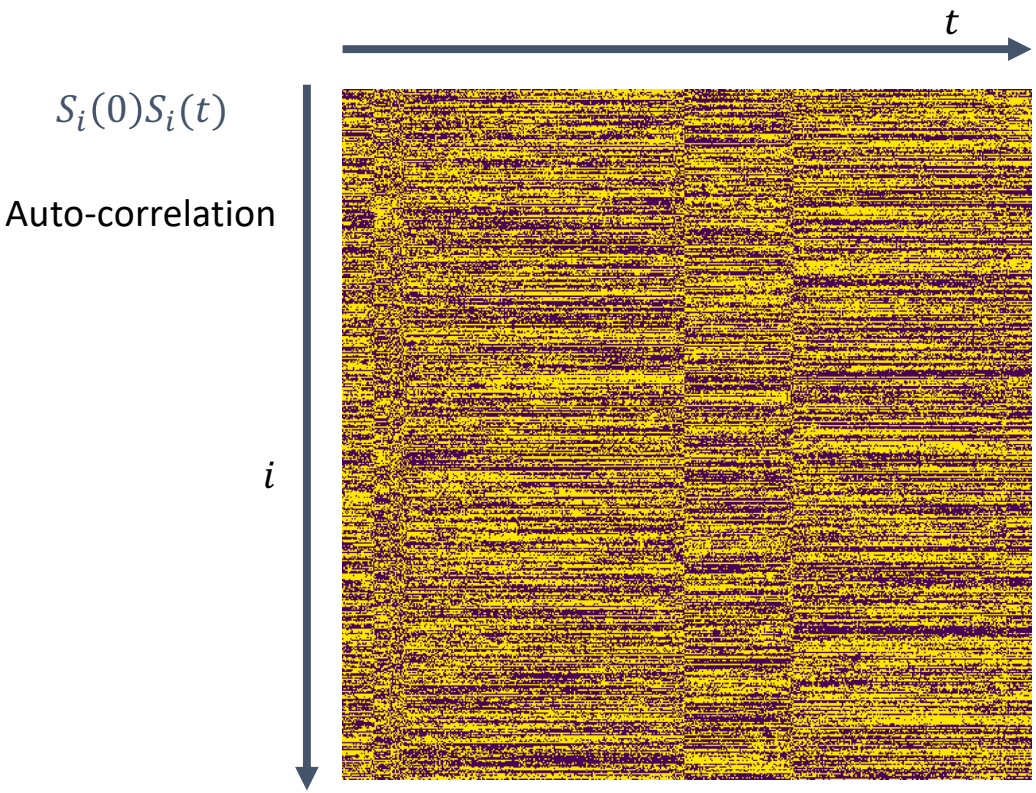
eigenvector hybridization

eigenvector diffusion

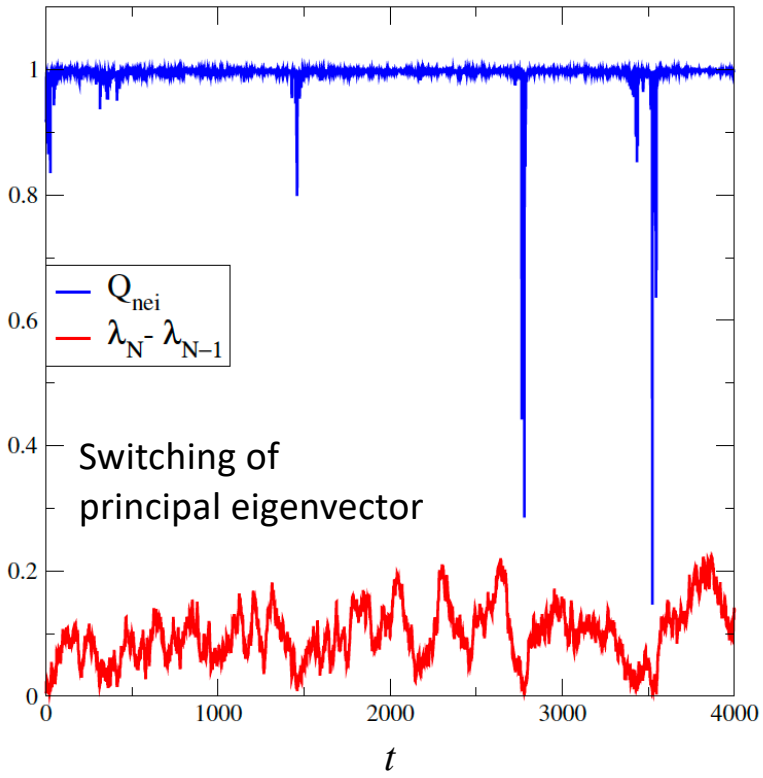


Condensate restructuring/hybridization

Evolution of spin configuration at $N = 512,\ T = 0.8$



$$Q_{nei} = \overrightarrow{V_N}(t) \cdot \overrightarrow{V_N}(t+1)$$



gap closing

Dynamical evolution of the principal eigenvector (Dyson Brownian Motion)

perturbation theory

$$\mathbf{J}(t+\delta t) = \mathbf{J}(t) + \delta\mathbf{J}(t)$$

$$\lambda_\mu(t+\delta t) = \lambda_\mu(t) + \delta\lambda_\mu(t)$$

$$\vec{V}_\mu(t+\delta t) = \vec{V}_\mu(t) + \delta\vec{V}_\mu(t)$$

$$\delta\lambda_\mu(t) = \frac{\vec{V}_\mu(t)\delta\mathbf{J}(t)\vec{V}_\mu(t)}{\left|\vec{V}_\mu(t)\right|^2}$$

Focus on the principal eigenvector

$$\delta\vec{V}_N(t) = \sum_{\mu=1}^{N-1} \delta_\mu(t)\vec{V}_\mu(t)$$

$$\delta_\mu(t) = \frac{1}{\lambda_N(t) - \lambda_\mu(t)}\left(\vec{V}_\mu(t)\delta\mathbf{J}(t)\vec{V}_N(t)\right)$$

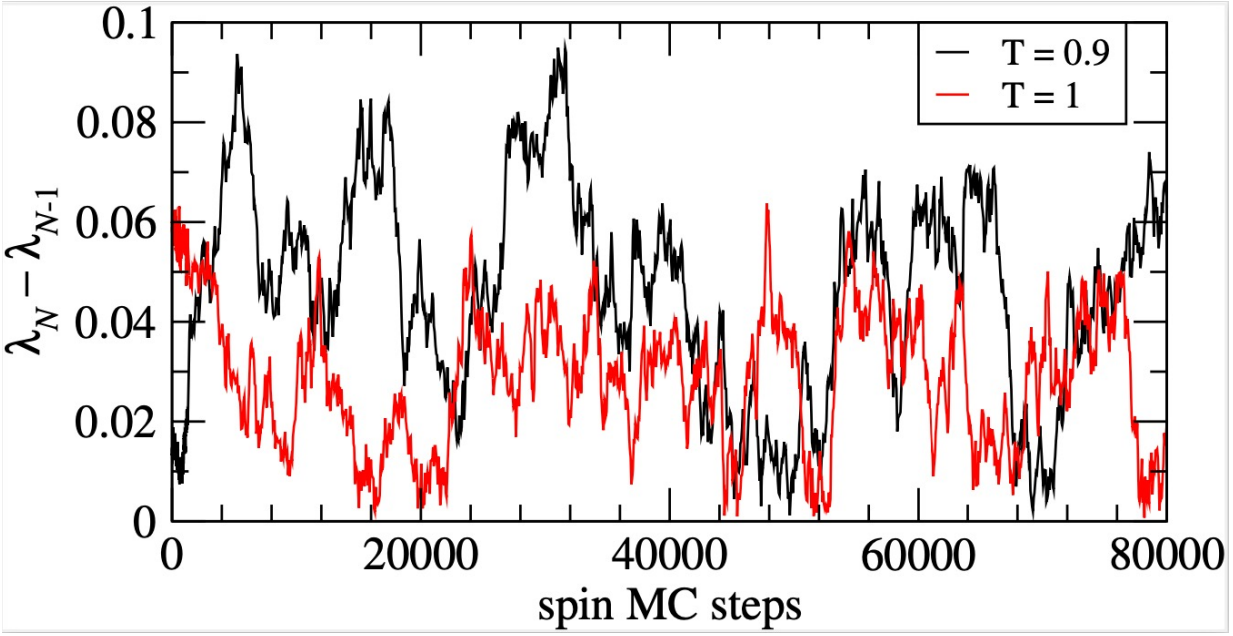
Diffusive motion of $\vec{V}_N(t)$:

$$\left\langle\left|\delta\vec{V}_N(t)\right|^2\right\rangle = \left\langle\sum_{\mu=1}^{N-1}\frac{\left(\vec{V}_\mu(t)\delta\mathbf{J}(t)\vec{V}_N(t)\right)^2}{\left(\lambda_N(t)-\lambda_\mu(t)\right)^2}\right\rangle = 2\alpha\delta t$$

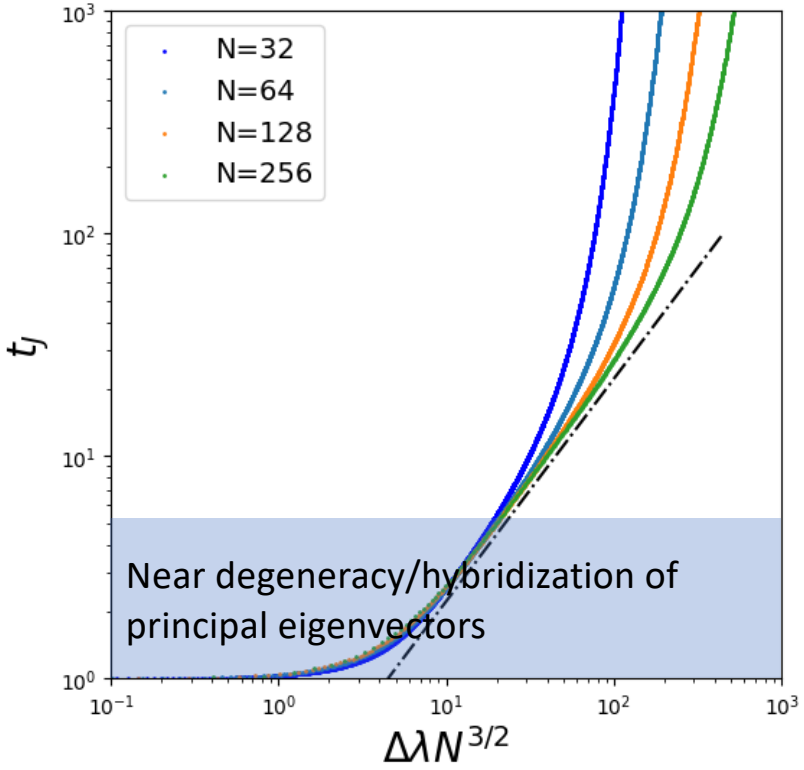
Diffusion constant:

$$\alpha = \frac{4}{N}\left\langle\sum_{\mu=1}^{N-1}\frac{1}{\left(\lambda_N(t)-\lambda_\mu(t)\right)^2}\right\rangle$$

Spectral gap time series



t_J: mean first return time (in J_{ij} flips)



(work in progress)

Summary

- **Condensate formation** in the **annealed SK model** is described by **gap opening** of the coupling matrix $\{J_{ij}\}$ at the spectral edge.
- Finite-size scaling of principal spin components derived from an **exact analysis** of the edge spectrum of the random matrix.
- **Equilibrium dynamics** of the condensate evolution follows "Dyson Brownian motion" of the random matrix $\{J_{ij}\}$:

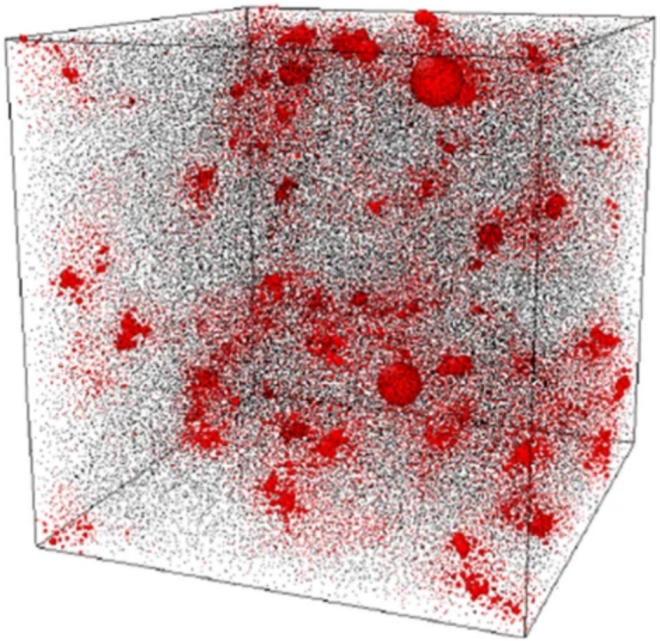
  i) drifting of the principal eigenvector, and

  ii) sudden "restructuring/hybridization".

  Finite-size scaling of relevant timescales in the critical region in progress.
- 4-point correlation function of the toy model behaves similarly to that of a **supercooled liquid** near the **glass transition**

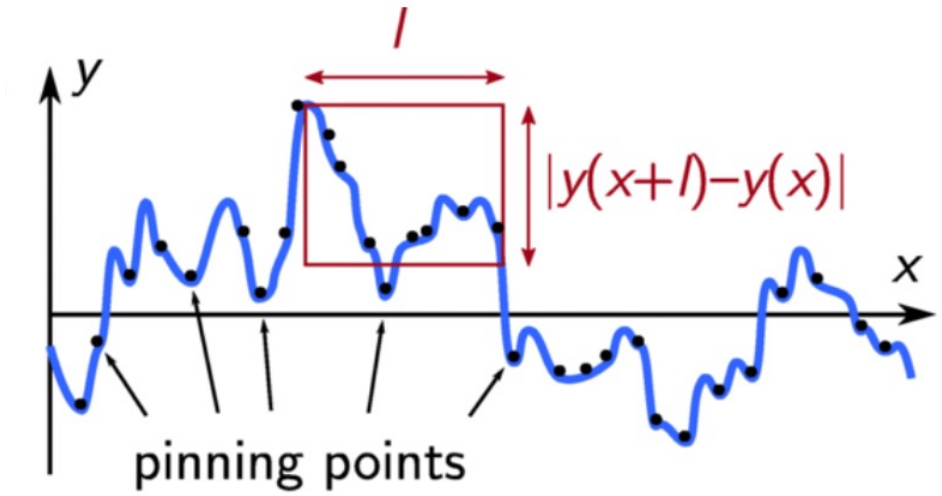
  $\Longrightarrow$ slow evolution of interactions between neighboring grains

A sophisticated **dynamic mean-field theory** for supercooled liquids/glass?



Emergence of hidden order on large spatiotemporal scales

Depinning of domain walls/flux lines



Physics of depinning in a correlated volume

≠

Physics of large-scale ordering and fluctuations


Thank you for your attention!