Istituto Nazionale di Fisica Nucleare

Università di Camerino 1336

Università degli Studi di Napoli Federico II

Neural Quantum Monte Carlo for quantum simulators

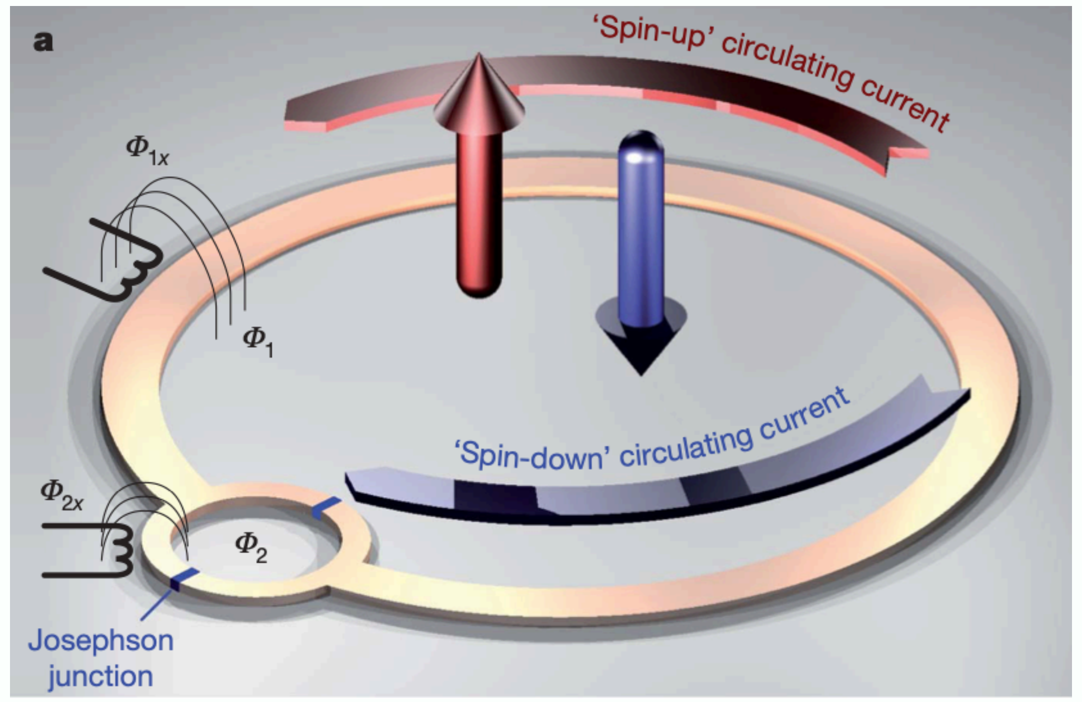
Luca Brodoloni - University of Camerino

Quantum Computing @ INFN - Padova, 28-31 October 2024

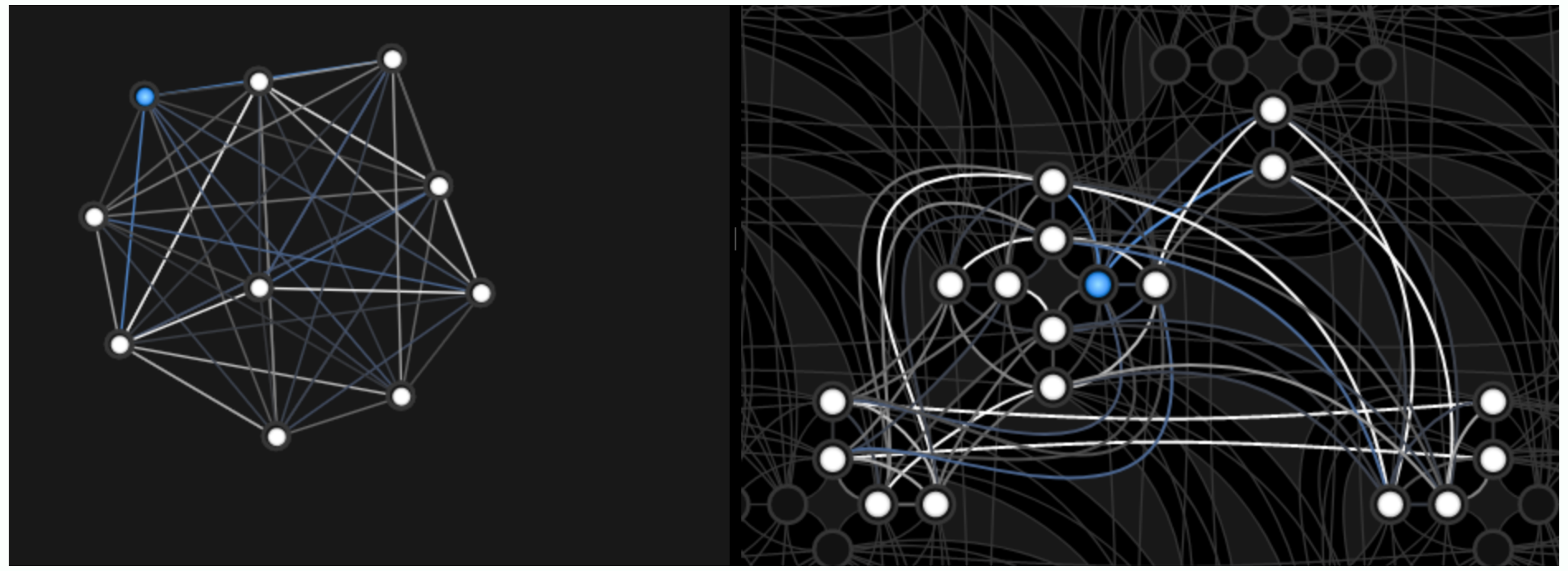
Programmable quantum platforms

$$H = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i\sigma_i^x - h\sum_i \sigma_i^z$$

Quantum annealers

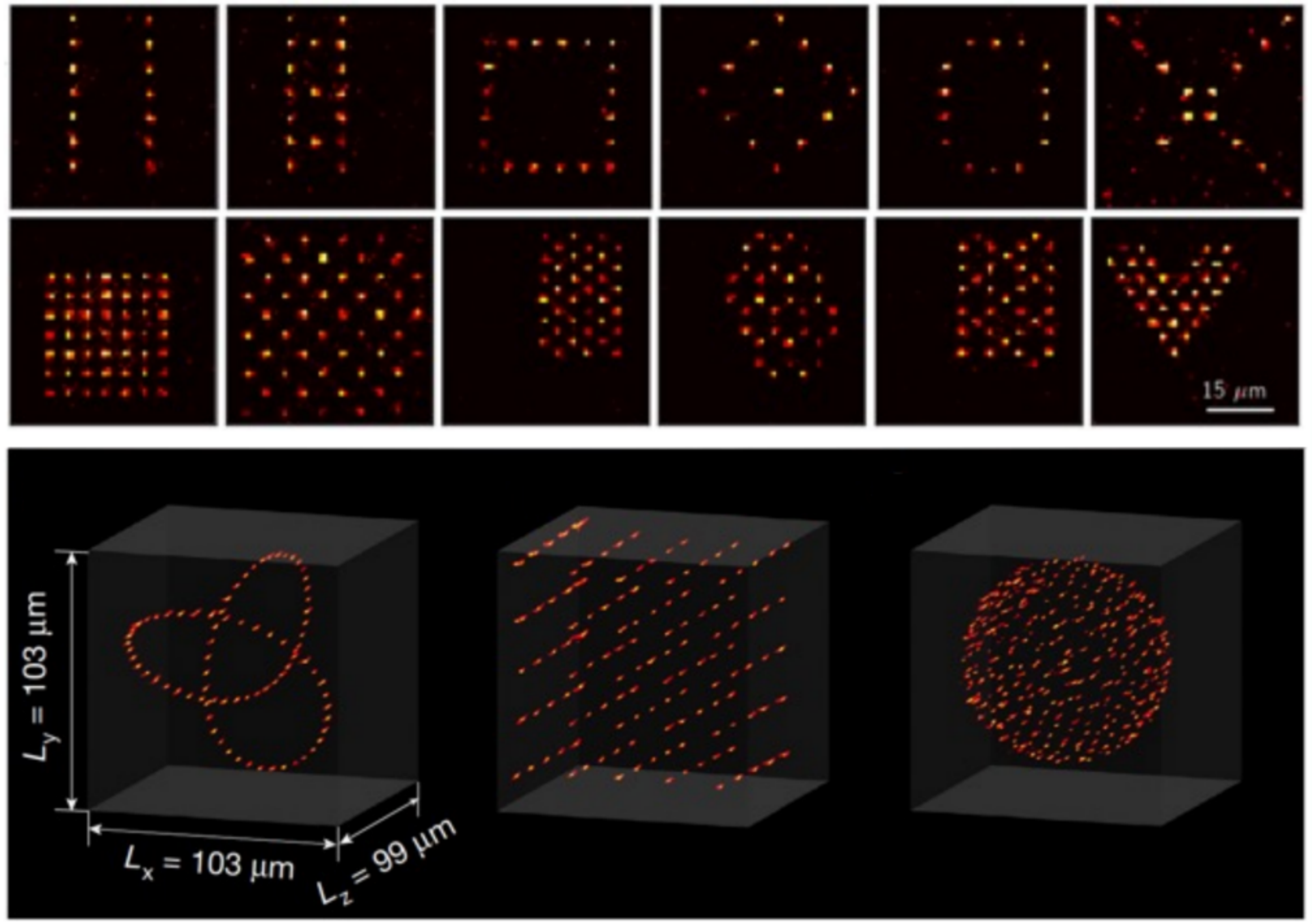


Nature 473, 194–198 (2011)



D-Wave QPU - 10 qubits all-to-all connections

Rydberg atoms in optical tweezers

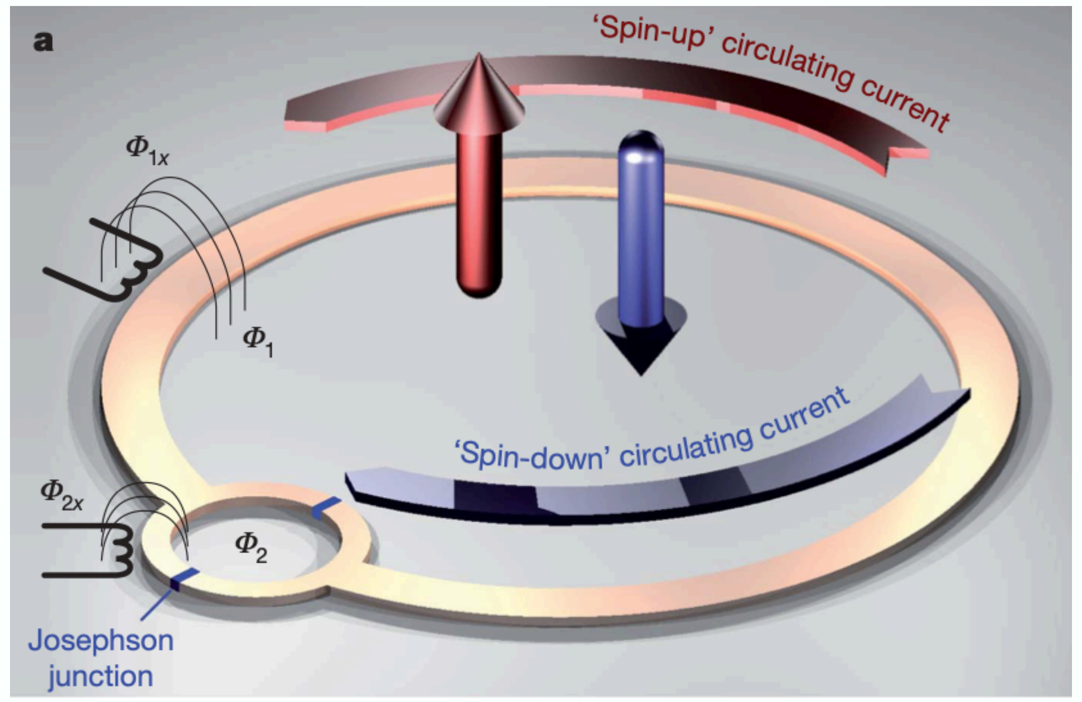


Nature 561, 79-82 (2018)

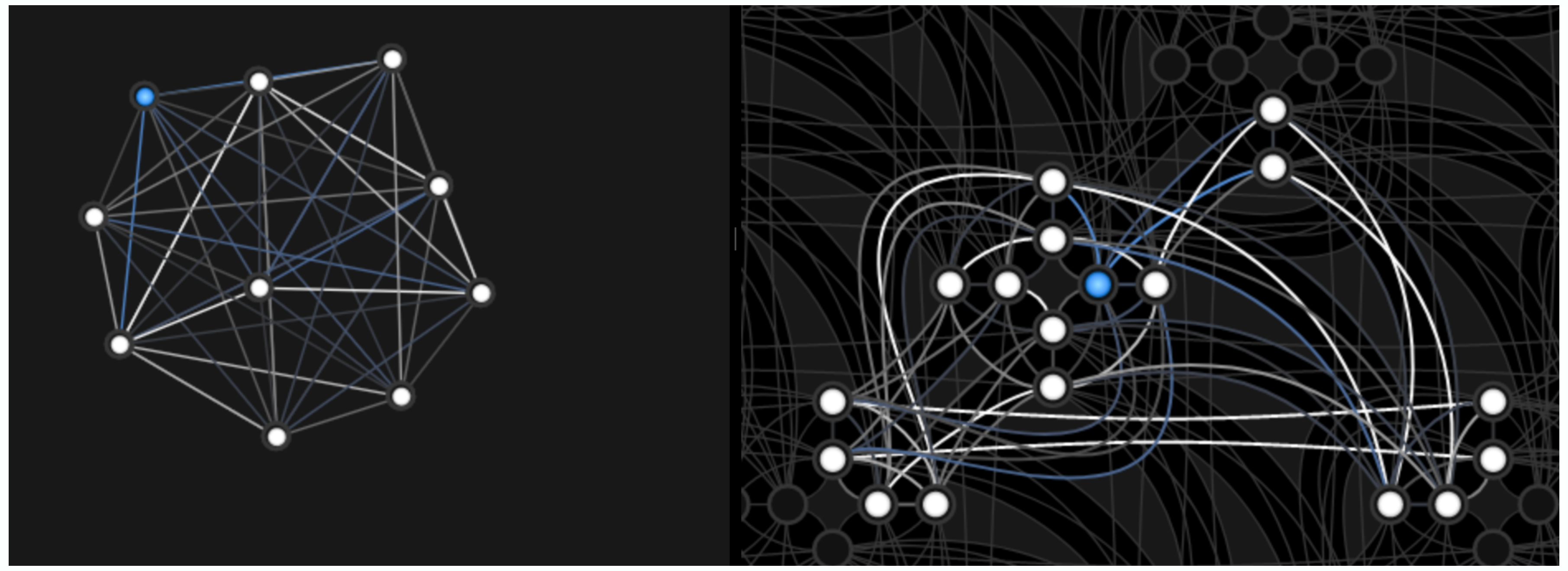
Programmable quantum platforms

$$H = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i \sigma_i^x - h\sum_i \sigma_i^z$$

Quantum annealers



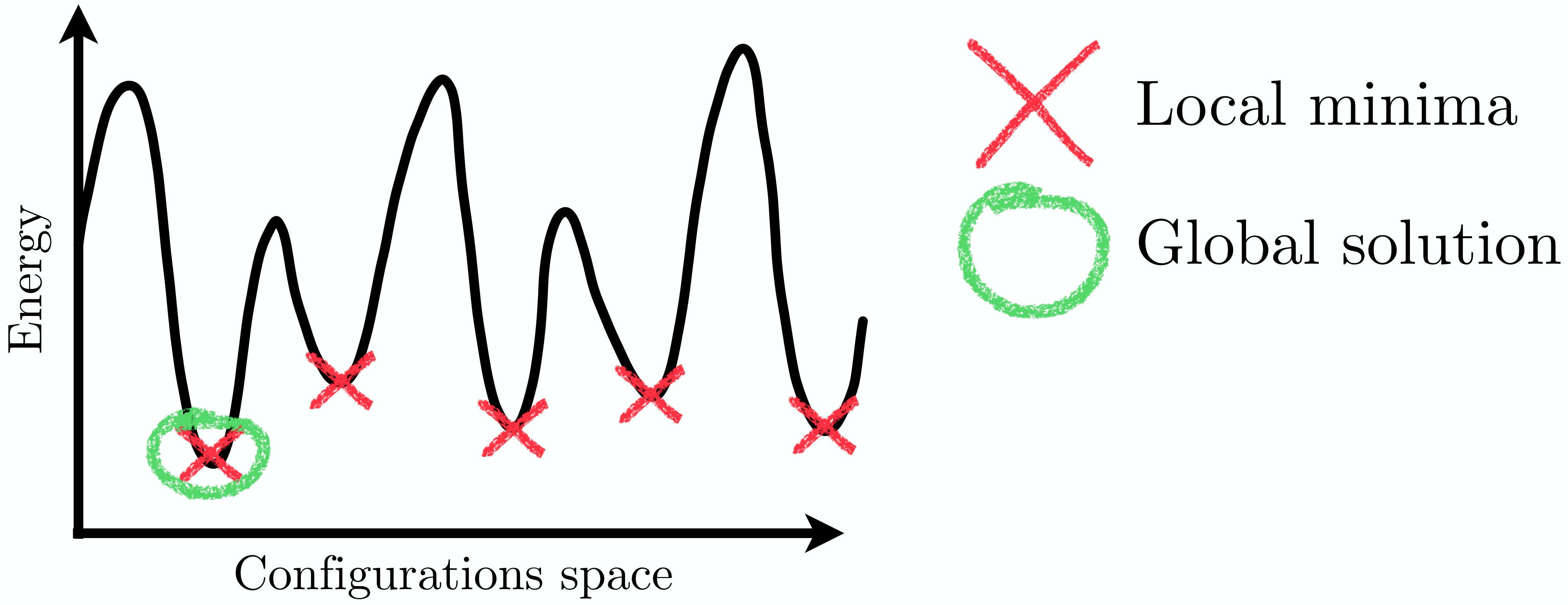
Nature 473, 194–198 (2011)



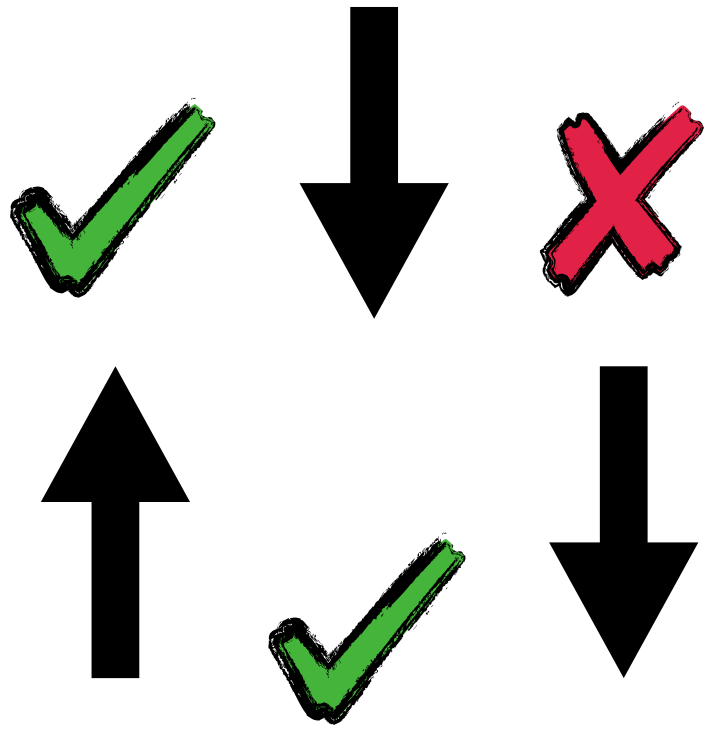
D-Wave QPU - 10 qubits all-to-all connections

Problems:

- Optimization (energy minimization)
- Sampling (from many low energy states)



Quantum spin glasses



$$H = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i\sigma_i^x$$

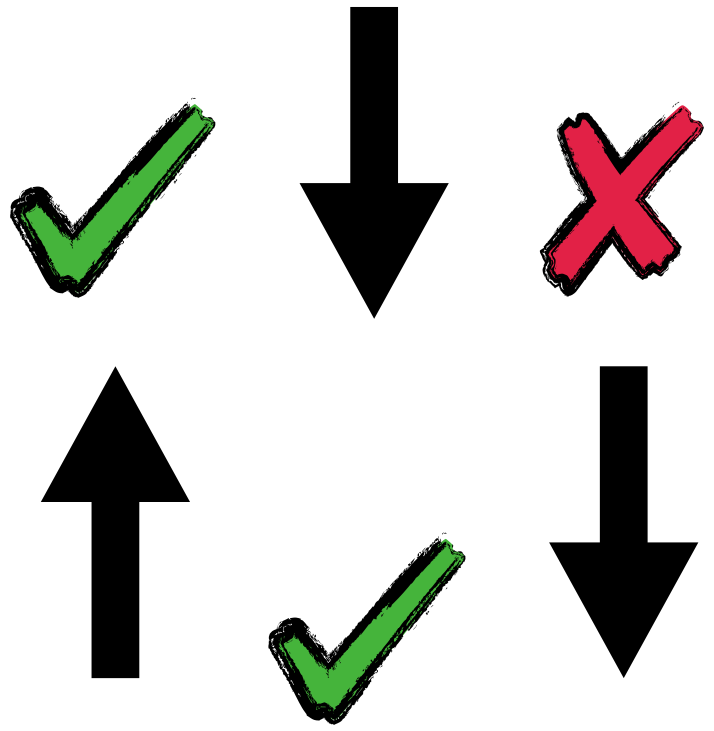
Frustration in triangular lattice with anti-ferromagnetic interactions.

Frustration arises from:

- Geometry of the lattice
- Nature of the couplings J_{ij}

Quantum spin glasses

$$H = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i \sigma_i^x$$



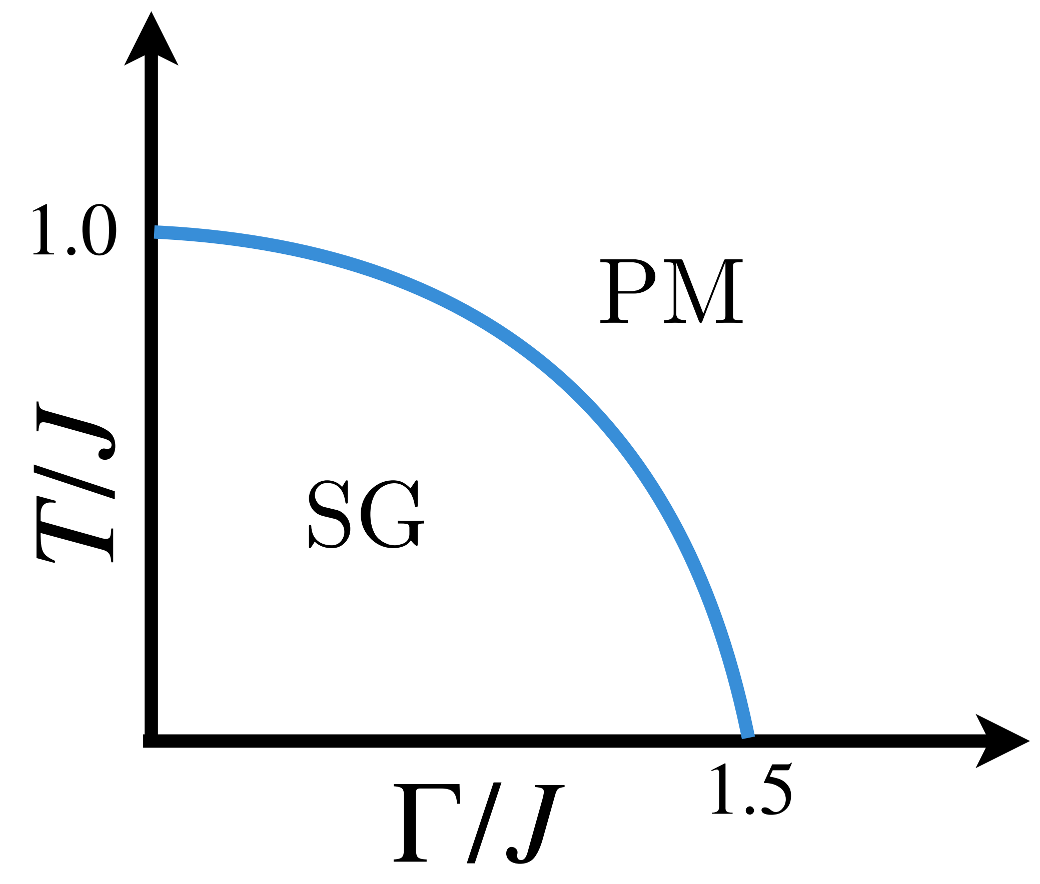
Frustration in triangular lattice with anti-ferromagnetic interactions.

Frustration arises from:

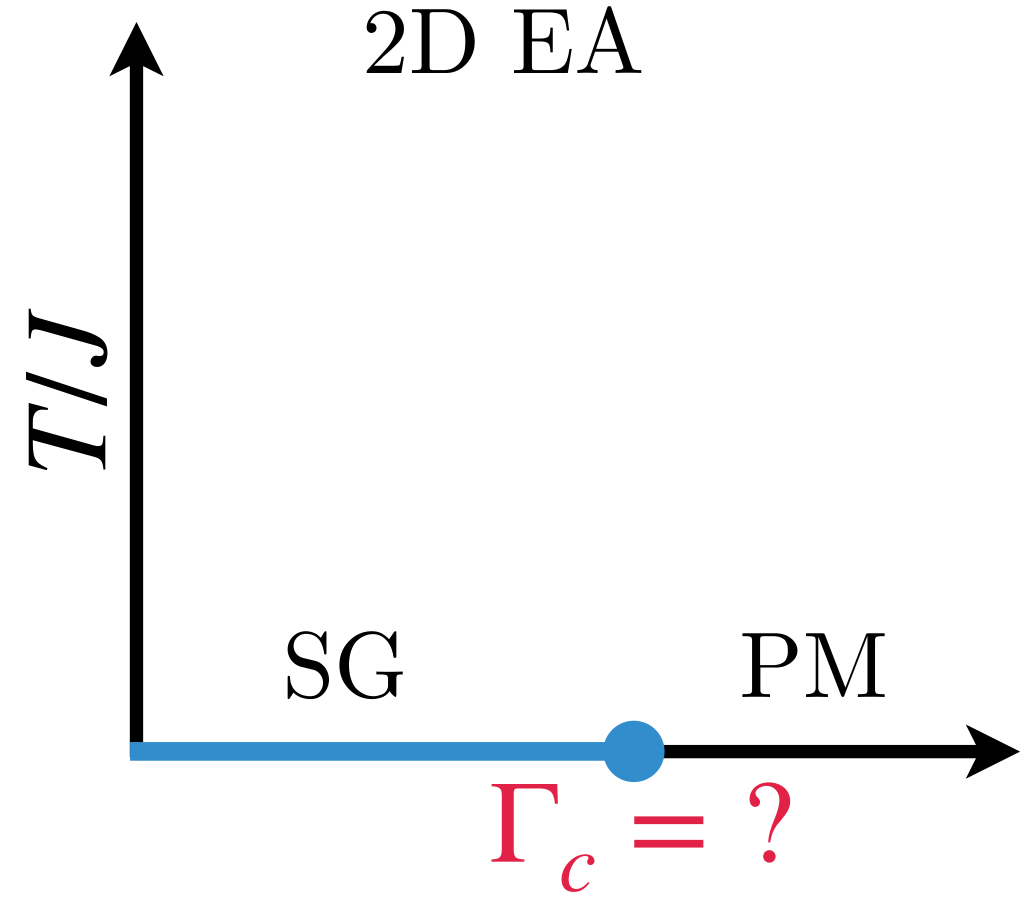
- Geometry of the lattice
- Nature of the couplings J_{ij}

- 1D, NN interactions → No frustration, no spin glass
- Finite D (e.g. 2D or 3D) → Spin glass, RSB or Droplet?
- D=∞ (Sherrington-Kirkpatrick) → Exact MF solution, RSB

SK model



2D EA



Projective Quantum Monte Carlo for random Ising Model

Imaginary-time evolution: $\psi(\mathbf{x},\tau) = \exp(-\tau H)\psi(\mathbf{x},\mathbf{0}) \underset{\tau\to\infty}{=} \psi_{\mathrm{GS}}(\mathbf{x})$

Stochastic process: $\psi(\mathbf{x},\tau+\Delta\tau) = \sum_{\mathbf{x}'} G(\mathbf{x},\mathbf{x}',\Delta\tau)\psi(\mathbf{x}',\tau)$

Green's function: $G(\mathbf{x},\mathbf{x}',\Delta\tau) = \left\langle \mathbf{x} \middle| \exp\left(-\tau\left(H - E_{\mathrm{ref}}\right)\right) \middle| \mathbf{x}' \right\rangle$

Not a stochastic matrix!

- In general $G(\mathbf{x},\mathbf{x}',\Delta\tau)$ can be $< 0 \implies$ sign problem! NOT OUR CASE
- $\sum_{\mathbf{x}} G(\mathbf{x},\mathbf{x}',\Delta\tau) \neq 1 \implies$ Transition probability not normalized

Projective Quantum Monte Carlo for random Ising Model

Imaginary-time evolution: $\psi(\mathbf{x},\tau) = \exp(-\tau H)\psi(\mathbf{x},\mathbf{0}) \underset{\tau\to\infty}{=} \psi_{\mathrm{GS}}(\mathbf{x})$

Stochastic process: $\psi(\mathbf{x},\tau+\Delta\tau) = \sum_{\mathbf{x}'} G(\mathbf{x},\mathbf{x}',\Delta\tau)\psi(\mathbf{x}',\tau)$

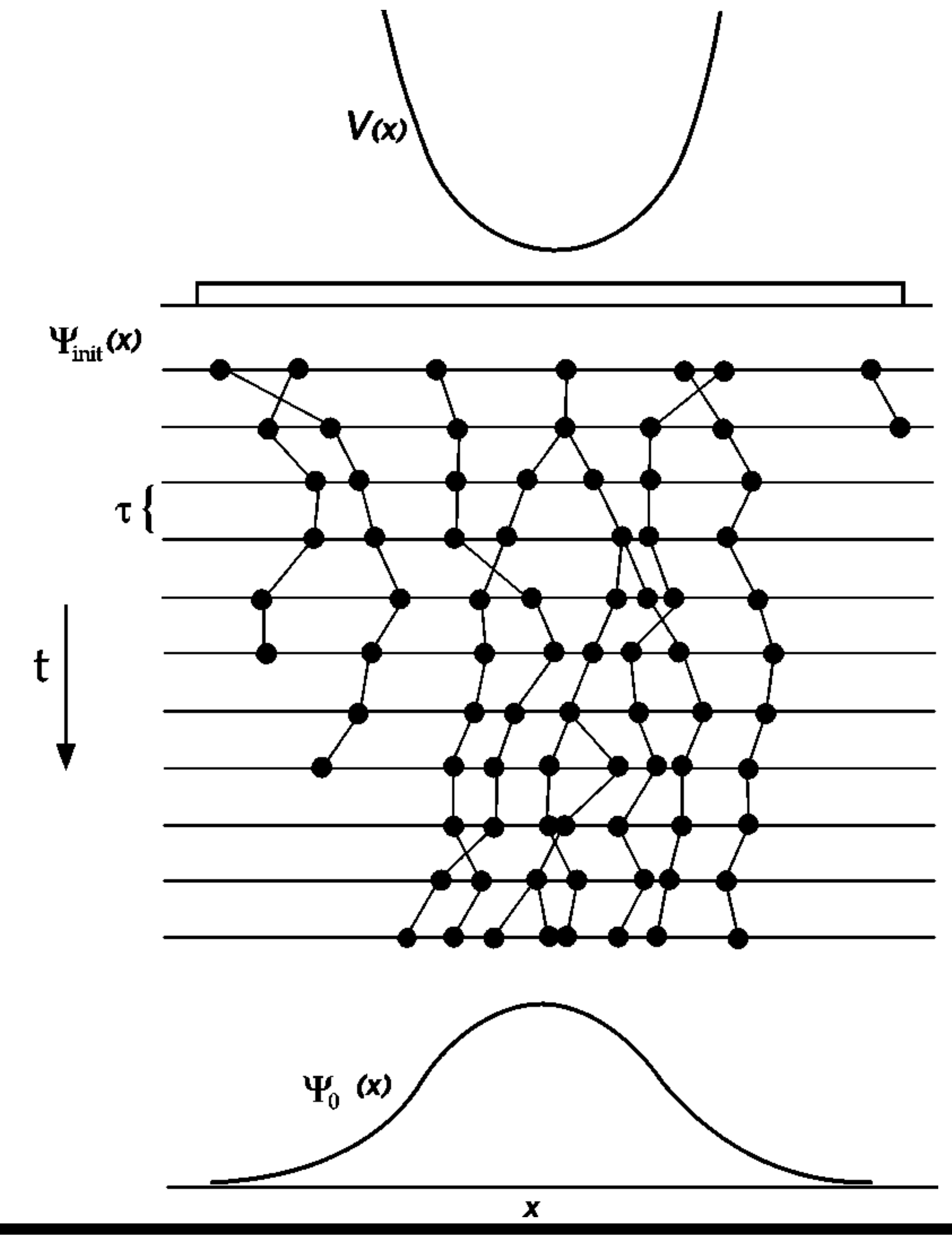
Green's function: $G(\mathbf{x},\mathbf{x}',\Delta\tau) = \left\langle \mathbf{x} \middle| \exp\left(-\tau\left(H - E_{\mathrm{ref}}\right)\right) \middle| \mathbf{x}' \right\rangle$

Not a stochastic matrix!

- In general $G(\mathbf{x},\mathbf{x}',\Delta\tau)$ can be $< 0 \implies$ sign problem! NOT OUR CASE
- $\sum_{\mathbf{x}} G(\mathbf{x},\mathbf{x}',\Delta\tau) \neq 1 \implies$ Transition probability not normalized

Stochastic evolution of walker population

branching process: kill or replicate



W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal
Rev. Mod. Phys. 73, 33

Projective Quantum Monte Carlo for random Ising Model

Importance sampling with a neural guiding wave-function

Imaginary-time evolution: $\psi(\mathbf{x},\tau)\psi_g(\mathbf{x}) = \exp(-\tau H)\psi(\mathbf{x},\mathbf{0})\psi_g(\mathbf{x}) \underset{\tau\to\infty}{=} \psi_{\mathrm{GS}}(\mathbf{x})\psi_g(\mathbf{x})$

Stochastic process: $\psi(\mathbf{x},\tau+\Delta\tau)\psi_g(\mathbf{x}) = \sum_{\mathbf{x}'} \tilde{G}(\mathbf{x},\mathbf{x}',\Delta\tau)\psi(\mathbf{x}',\tau)\psi_g(\mathbf{x}')$

Modified Green's function: $\tilde{G}(\mathbf{x},\mathbf{x}',\Delta\tau) = \left\langle \mathbf{x} \middle| \exp\left(-\tau\left(H - E_{\mathrm{ref}}\right)\right) \middle| \mathbf{x}' \right\rangle \frac{\psi_g(\mathbf{x})}{\psi_g(\mathbf{x}')}$

Common choices for $\psi_g(\mathbf{x})$:

- Jastrow WF;
- Hartree-Fock WF;
- Variational ansatz;

Projective Quantum Monte Carlo for random Ising Model

Importance sampling with a neural guiding wave-function

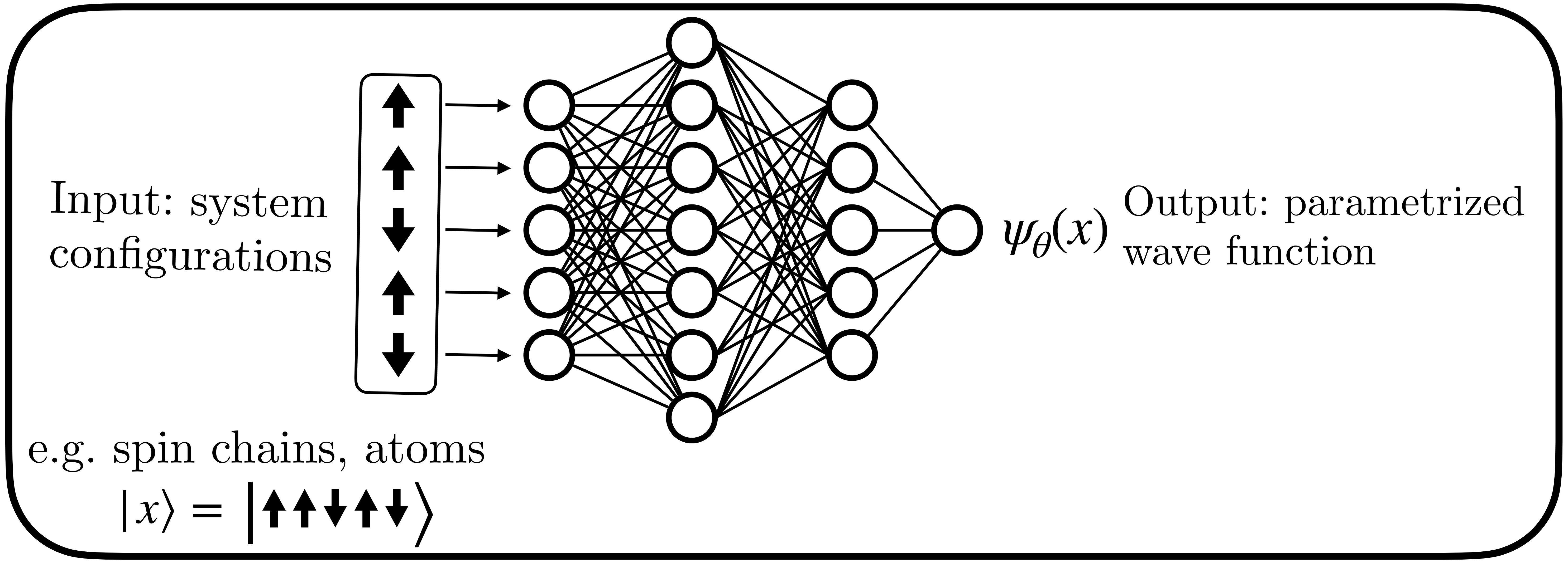
Imaginary-time evolution: $\psi(\mathbf{x},\tau)\psi_g(\mathbf{x}) = \exp(-\tau H)\psi(\mathbf{x},\mathbf{0})\psi_g(\mathbf{x}) \underset{\tau\to\infty}{=} \psi_{\mathrm{GS}}(\mathbf{x})\psi_g(\mathbf{x})$

Stochastic process: $\psi(\mathbf{x},\tau+\Delta\tau)\psi_g(\mathbf{x}) = \sum_{\mathbf{x}'} \tilde{G}(\mathbf{x},\mathbf{x}',\Delta\tau)\psi(\mathbf{x}',\tau)\psi_g(\mathbf{x}')$

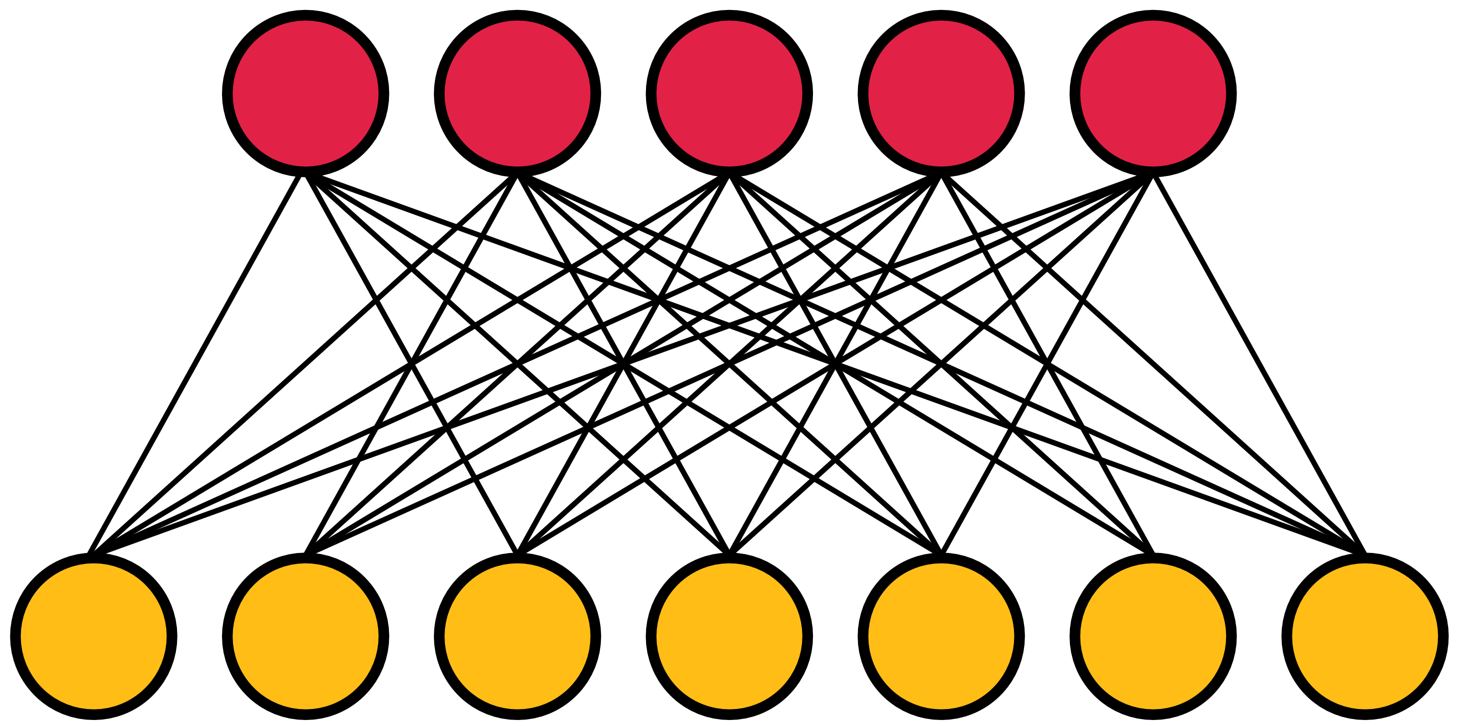
Modified Green's function: $\tilde{G}(\mathbf{x},\mathbf{x}',\Delta\tau) = \left\langle \mathbf{x} \middle| \exp\left(-\tau\left(H - E_{\mathrm{ref}}\right)\right) \middle| \mathbf{x}' \right\rangle \frac{\psi_g(\mathbf{x})}{\psi_g(\mathbf{x}')}$

Common choices for $\psi_g(\mathbf{x})$:

- Jastrow WF;
- Hartree-Fock WF;
- Variational ansatz;
- Neural Quantum States



Neural guiding function - Restricted Boltzmann Machine



$\mathbf{h} = \{h_j\}_{N_h}$

$\mathbf{v} = \{v_i\}_N$

RBM learns marginal distribution of visible variables

$$P_{RBM}(\mathbf{v}) = \sum_{\mathbf{h}} P(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} \sum_{\mathbf{h}} \exp\left(-E_{RBM}(\mathbf{v}, \mathbf{h})\right)$$

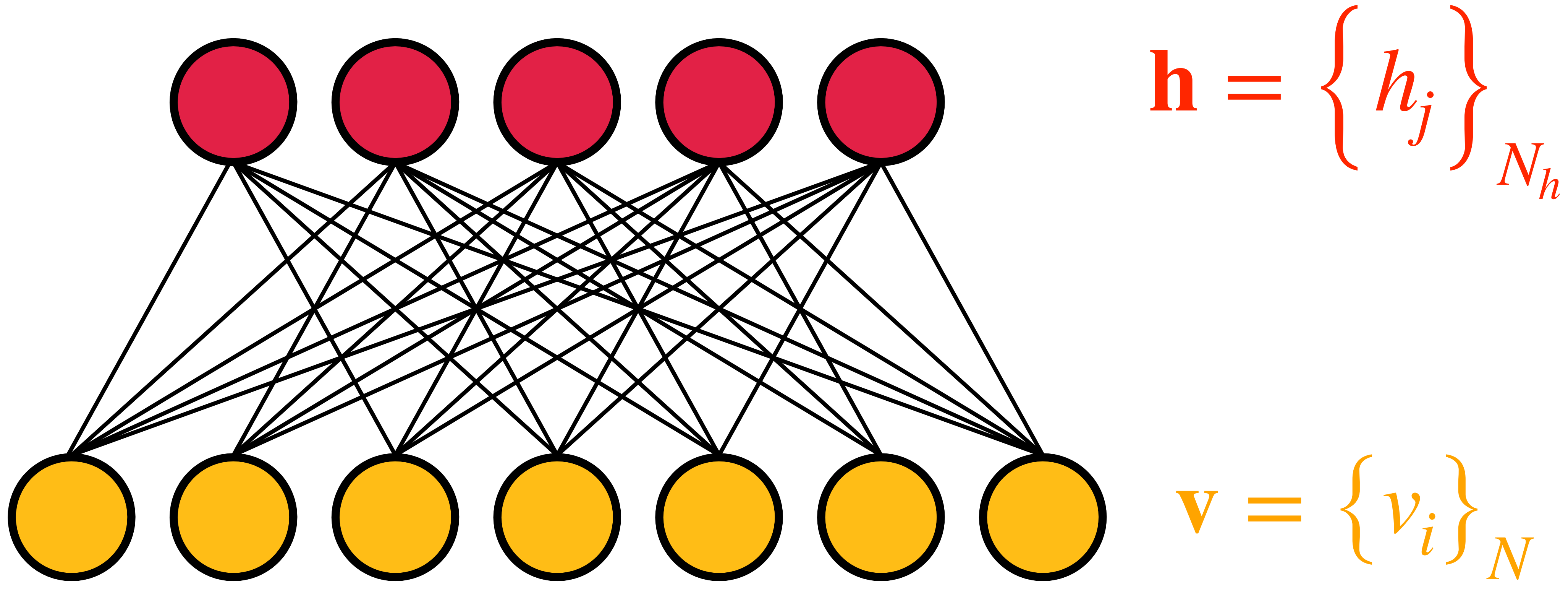
$$\psi_g = \psi_{RBM} \propto \sqrt{P_{RBM}}$$

Energy-based model

$$E_{RBM}(\mathbf{v}, \mathbf{h}) = -\sum_{j=1}^{N_h} \sum_{i=1}^{N} w_{ij} v_i h_j - \sum_{i=1}^{N} v_i b_i - \sum_{j=1}^{N_h} h_j c_j$$

w_{ij} : weights $\quad$ b_i, c_j : biases

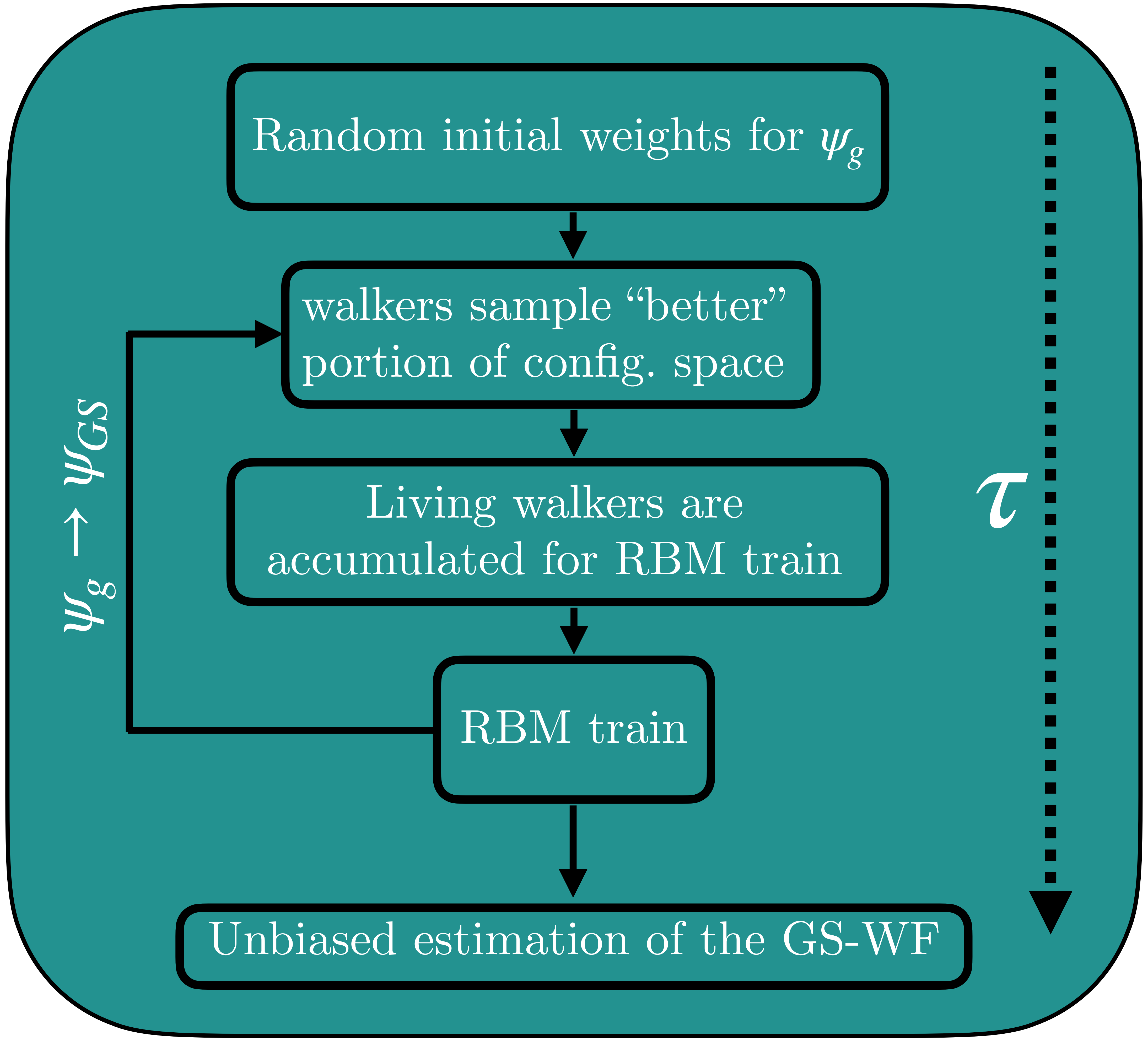
Neural guiding function - Restricted Boltzmann Machine



$$P_{RBM}(\mathbf{v}) = \sum_{\mathbf{h}} P(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} \sum_{\mathbf{h}} \exp\left(-E_{RBM}(\mathbf{v}, \mathbf{h})\right)$$

$$\psi_g = \psi_{RBM} \propto \sqrt{P_{RBM}}$$

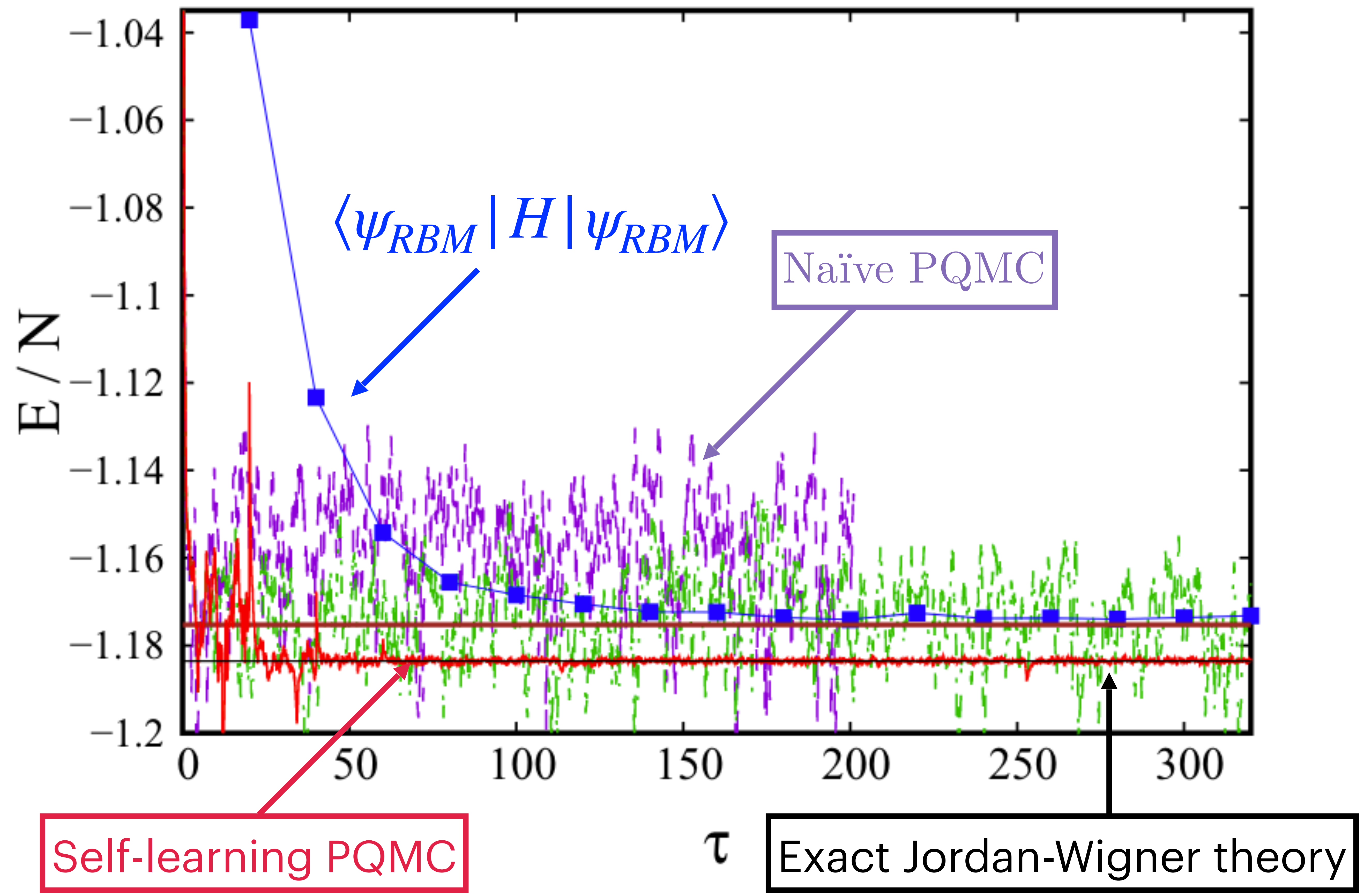
Self-learning PQMC



S. Pilati, E. M. Inack, and P. Pieri Phys. Rev. E 100, 043301

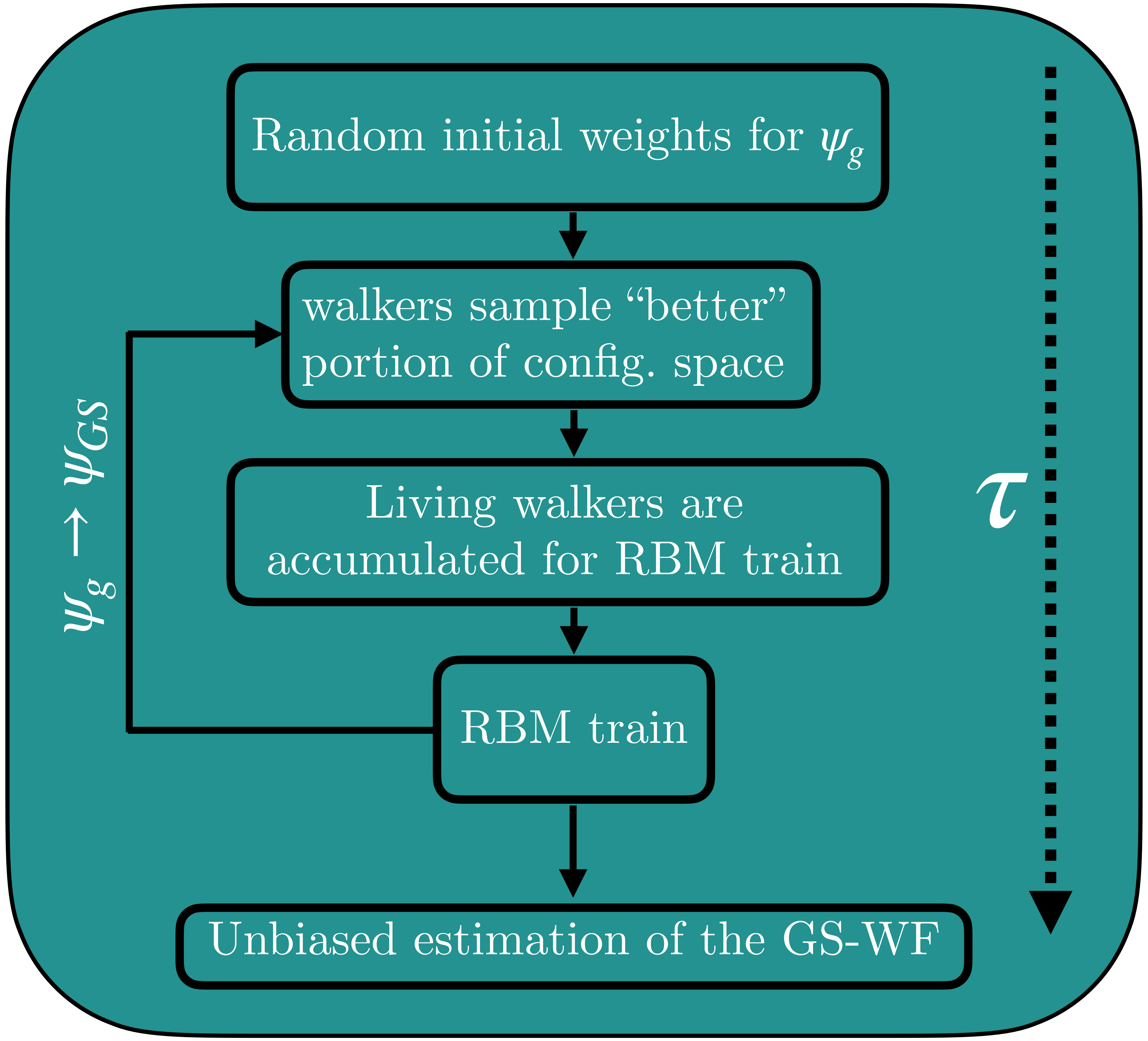
Neural guiding function - Restricted Boltzmann Machine

Ferrom. 1D, N=80



- No population control bias!
- Exact variational ansatz not needed!

Self-learning PQMC



S. Pilati, E. M. Inack, and P. Pieri Phys. Rev. E 100, 043301

2D Edwards-Anderson model

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i \sigma_i^x \quad J_{ij} \sim \text{Norm}[\mu = 0, \sigma = 1]$$

Two copies of the system are needed

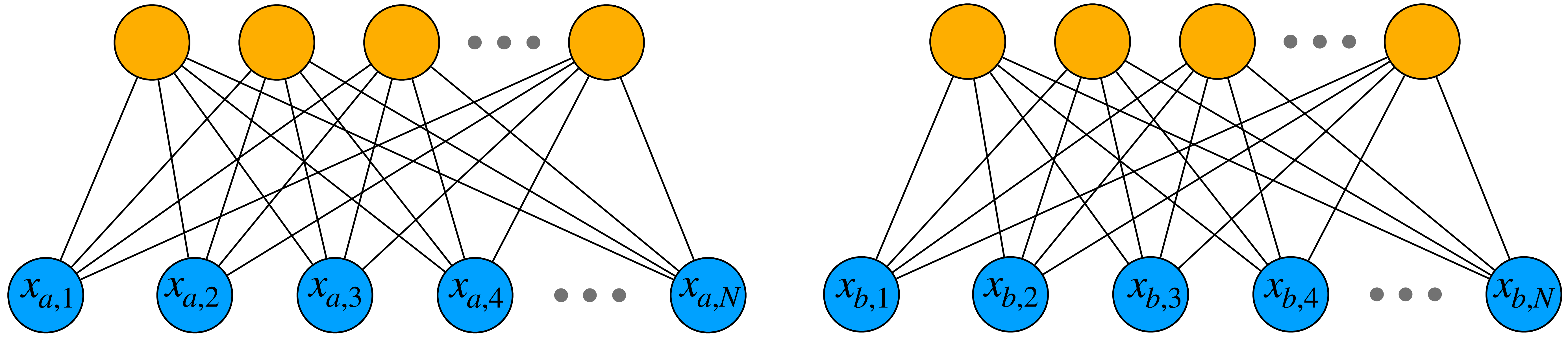
EA order parameter: $q_{EA} = \frac{1}{N}\sum_{i=1}^{N}\langle \sigma_i^z \rangle^2$

Spin overlap: $\hat{q} = \frac{1}{N}\sum_{i=1}^{N} \sigma_{iA}^z \sigma_{iB}^z$

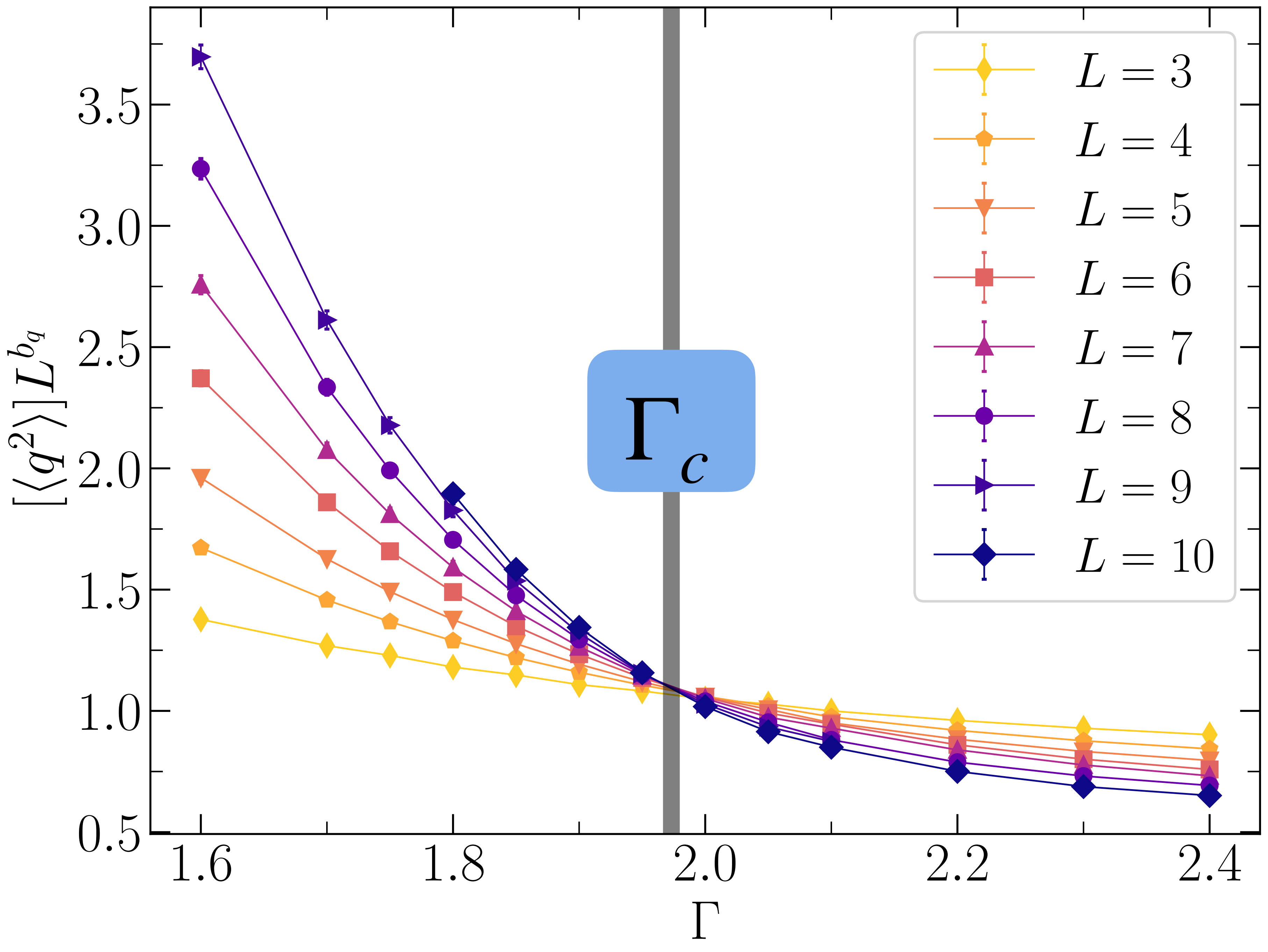
Spin glass susceptibility: $\frac{\chi_{SG}}{N} = \left[\langle \hat{q}^2 \rangle\right]$

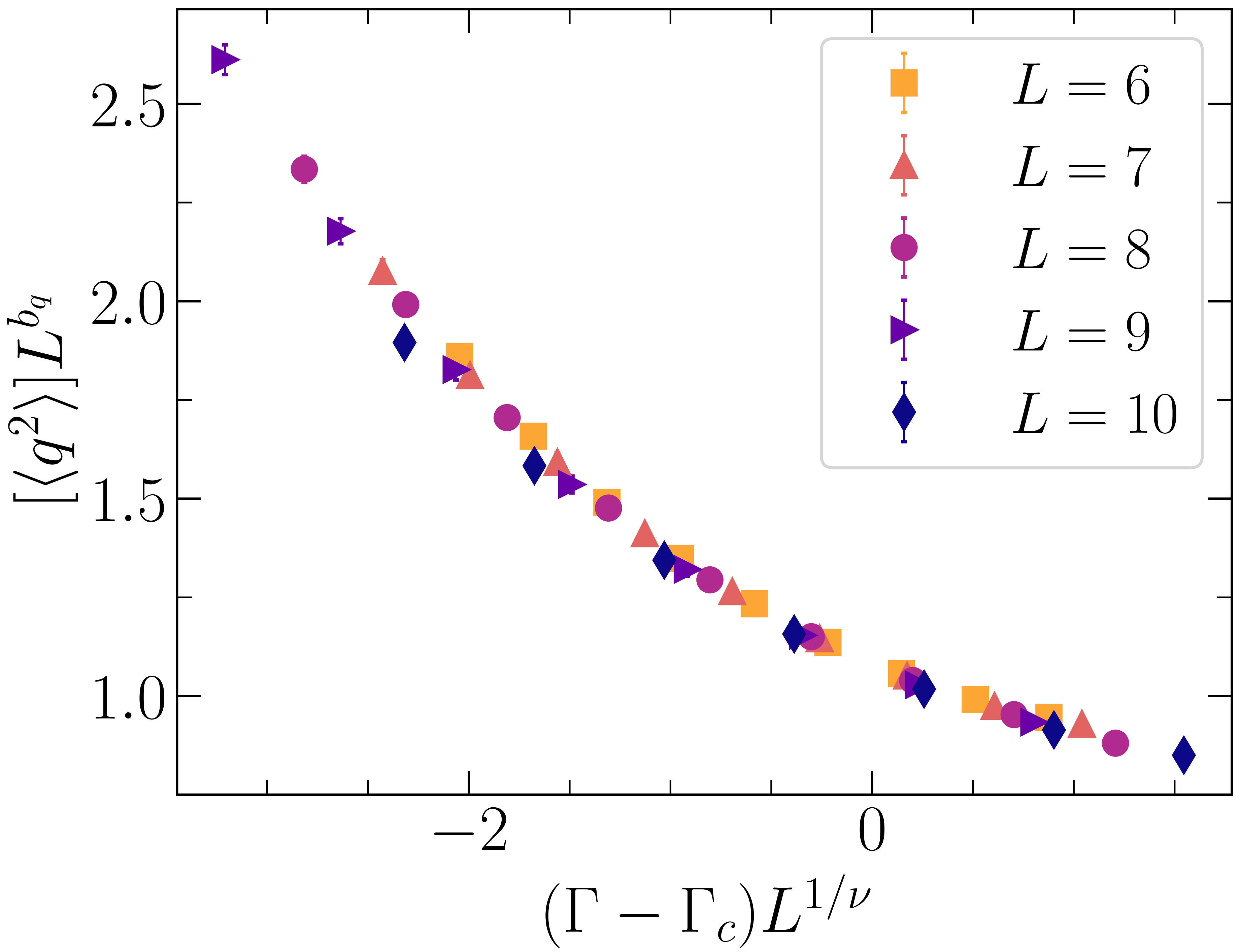
$H_{TOT} = H_A + H_B$

separable RBM



2D Edwards-Anderson model





Scaling ansatz:

$$\left[\langle \hat{q}^2 \rangle\right] L^{b_q} = f\left(\left(\Gamma - \Gamma_c\right) L^{1/\nu}\right)$$

Couplings	$1/\nu$	b_q	Γ_c	Ref.
50%. ±1	1.02(16)	1.76(3)	2.11(1)	A.D. King *et al.*, Nature (2023)
50% ±1	0.71(24)(9)	1.73(8)(8)	2.18(1)	M. Bernaschi *et al.*, Nature (2024)
$\mathcal{N}(0,1)$	1.11(22)	1.68(8)	1.98(7)	This work

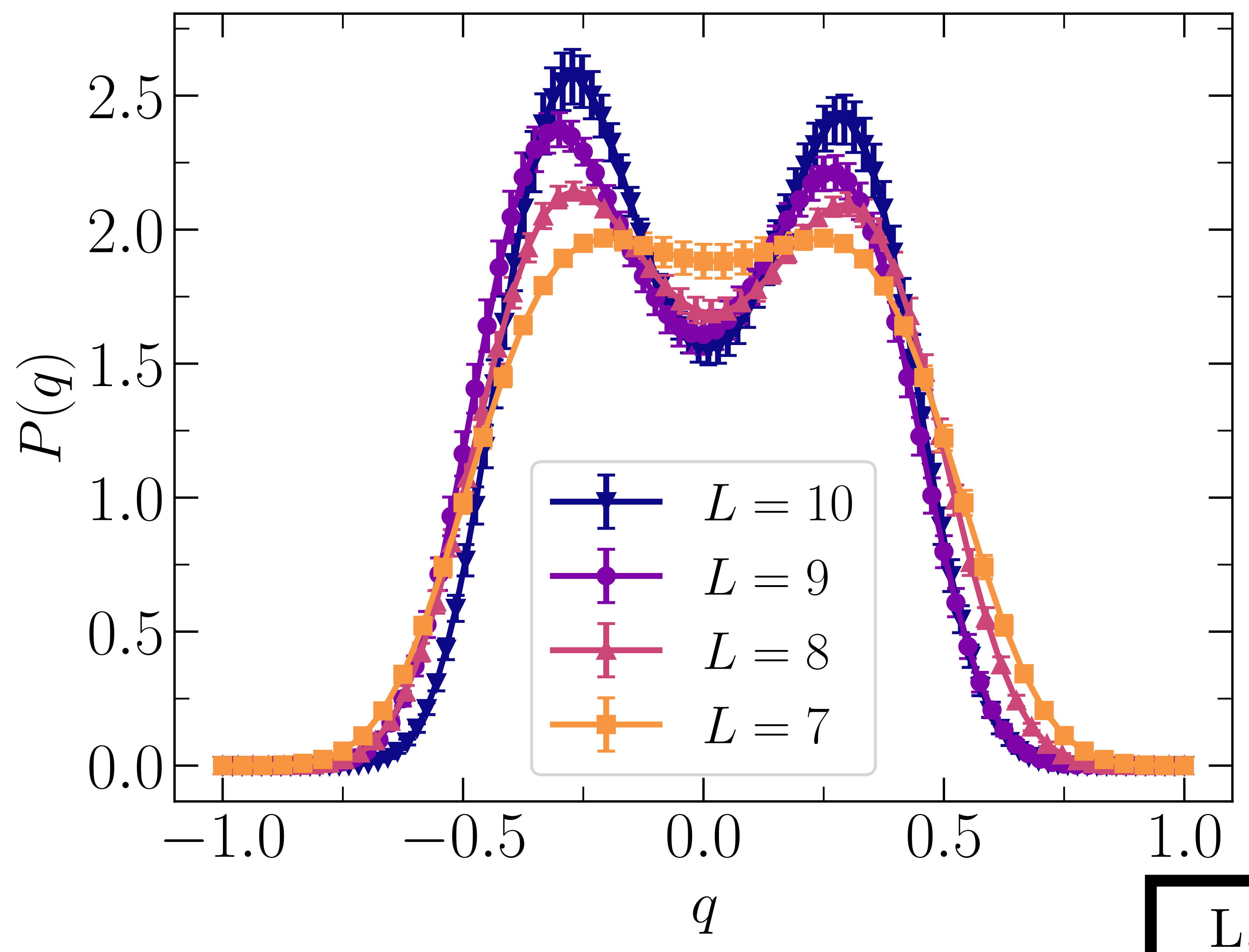
L.Brodoloni, S.Pilati arXiv:2407.05978(2024)

2D Edwards-Anderson model

Replica symmetry breaking

$$\hat{q} = \frac{1}{N}\sum_{i=1}^{N} \sigma_{iA}^{z}\sigma_{iB}^{z}$$

Overlap distribution: $P(q) = \left\langle \delta\left(q - \hat{q}\right)\right\rangle$



Droplet picture

$$P(q) = \frac{1}{2}(\delta(q - q_{EA}) + \frac{1}{2}(\delta(q + q_{EA})$$

Replica Symmetry Breaking

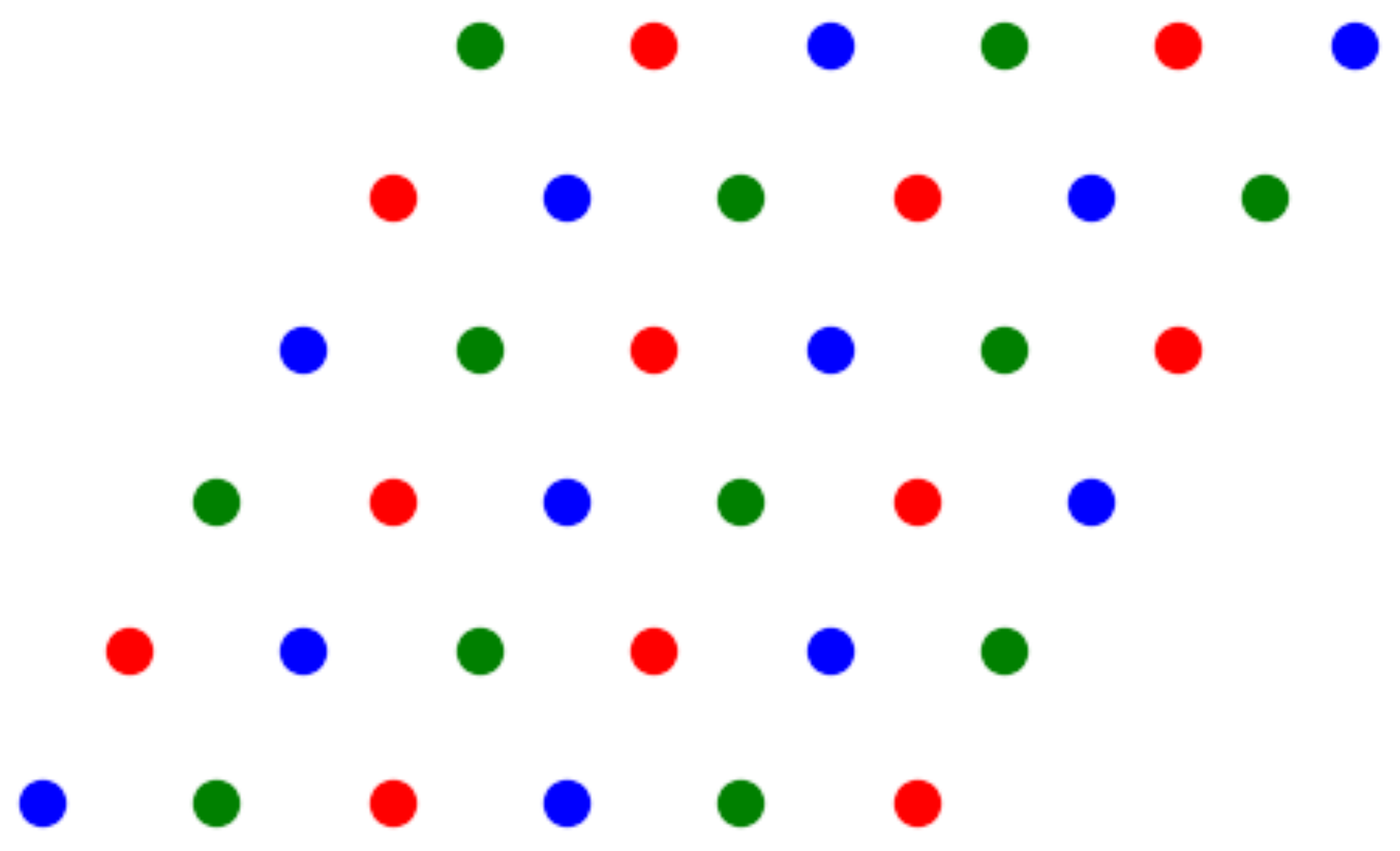
$$P(q = 0) > 0$$

- Non-trivial distribution of feasible sizes, hints to RSB
- Larger sizes needed to take $L \to \infty$ limit

L.Brodoloni, S.Pilati arXiv:2407.05978(2024)

Preliminary results on triangular lattices

$J_{ij} < 0$ (antiferrom.) → Intrinsic geometric frustration



3 sublattices (blue, red, green)

"Order by disorder" mechanism:

Small quantum fluctuations: Clock phase

High quantum fluctuations: PM phase

Ordered phase: spins in the sublattices assumes 6 discrete preferred orientations

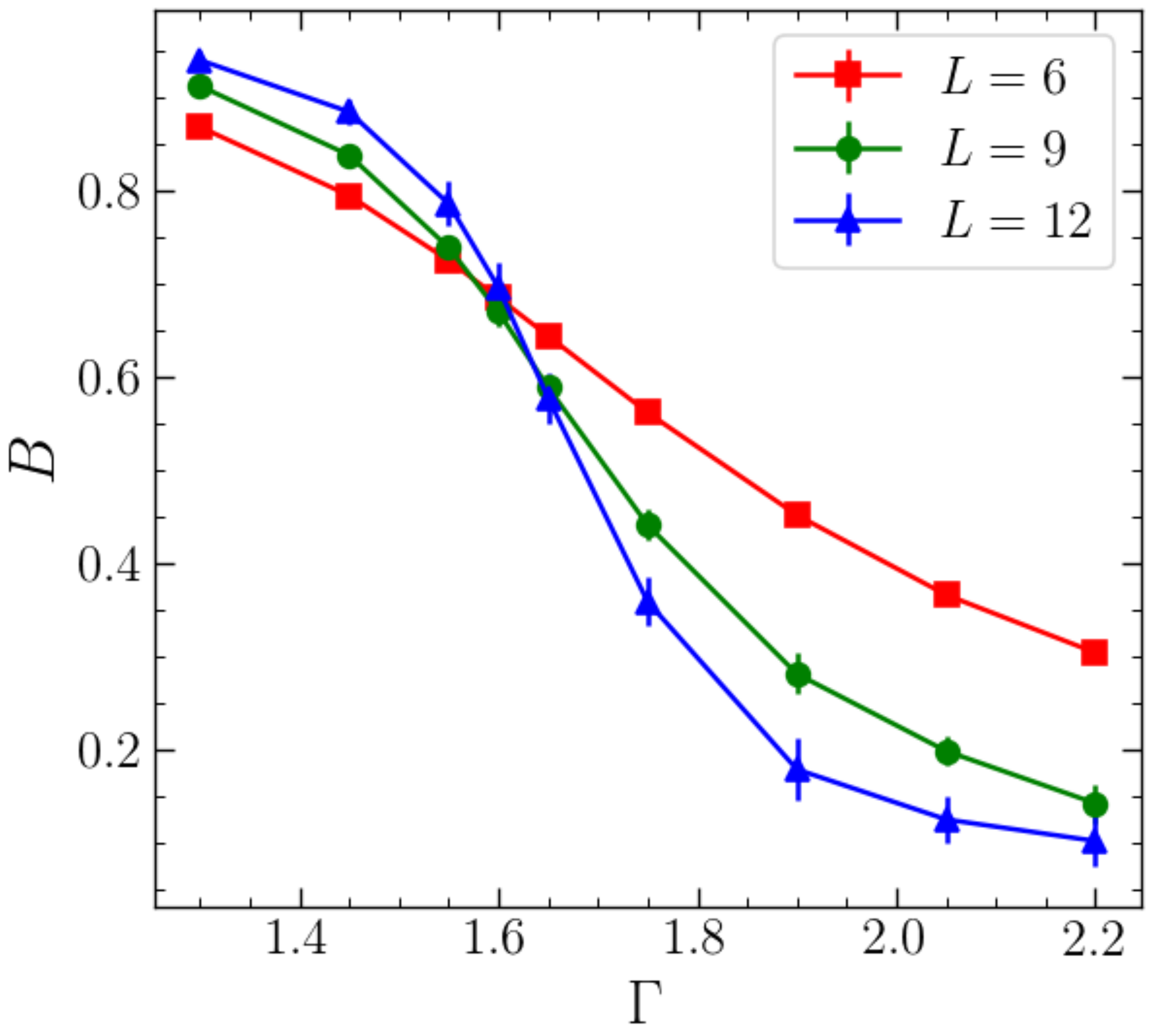
XY complex magnetization:

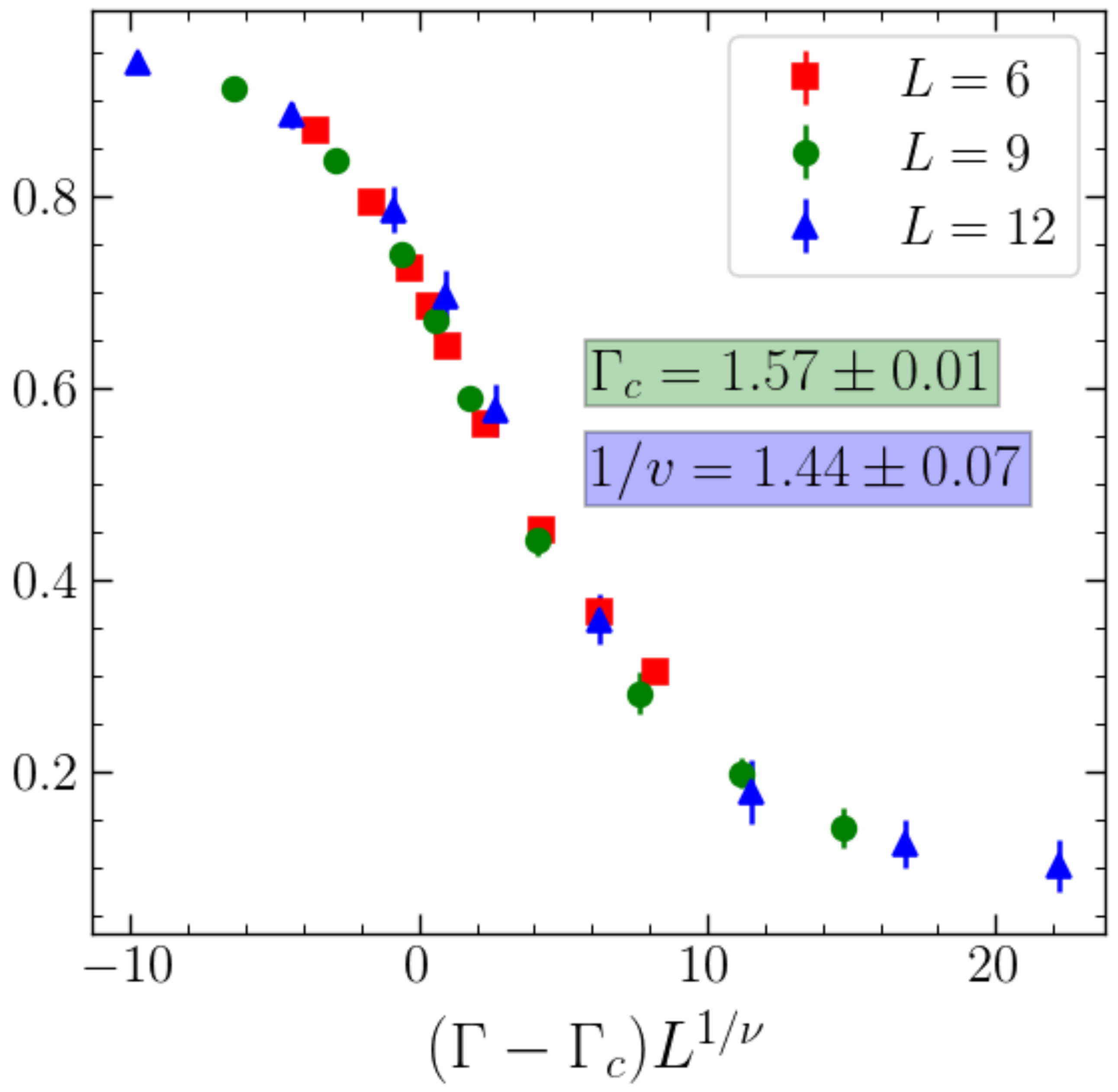
$$me^{i\theta} = m_1 + m_2 e^{i(4\pi/3)} + m_3 e^{i(-4\pi/3)} / \sqrt{3}$$

Preliminary results on triangular lattices

NN Model

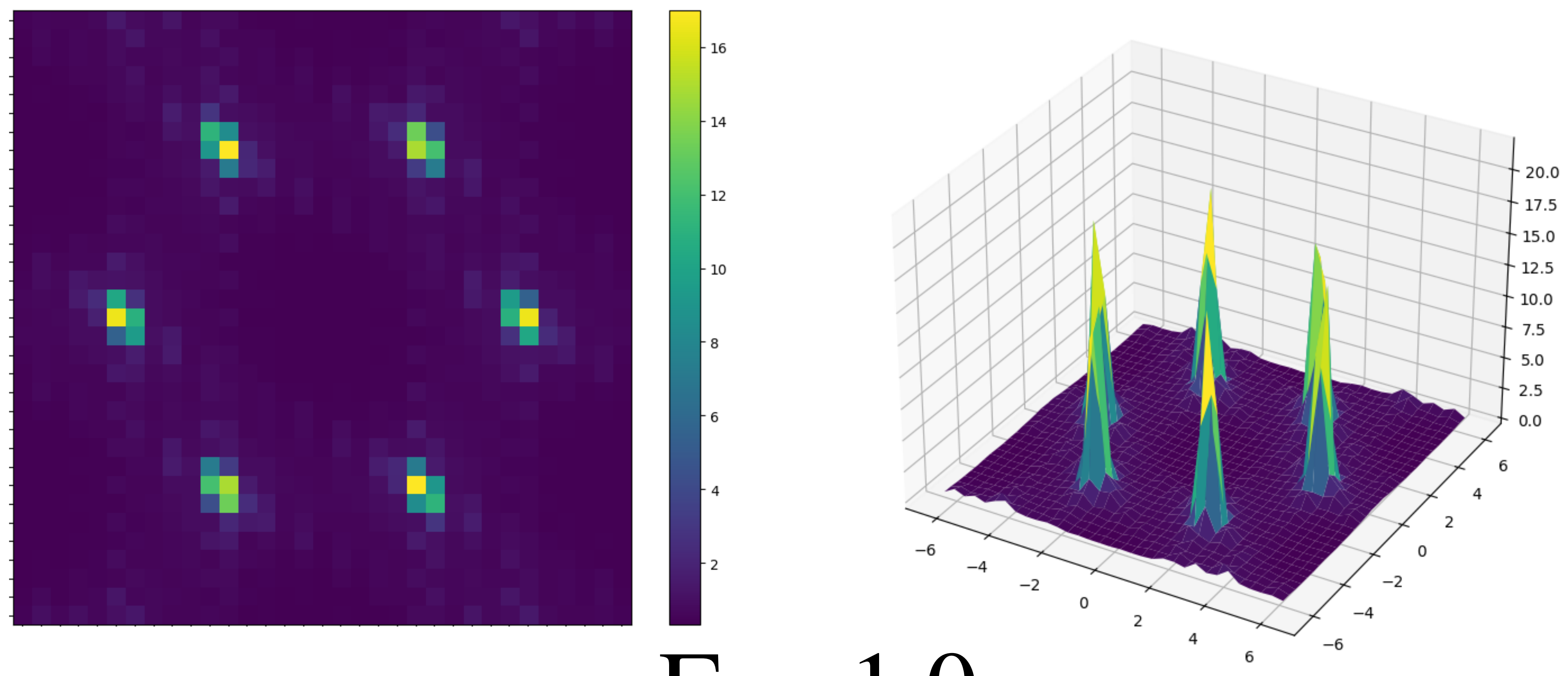
Binder cumulant: $B = 2\left(1 - \frac{\langle m^4 \rangle}{2\langle m^2 \rangle^2}\right)$



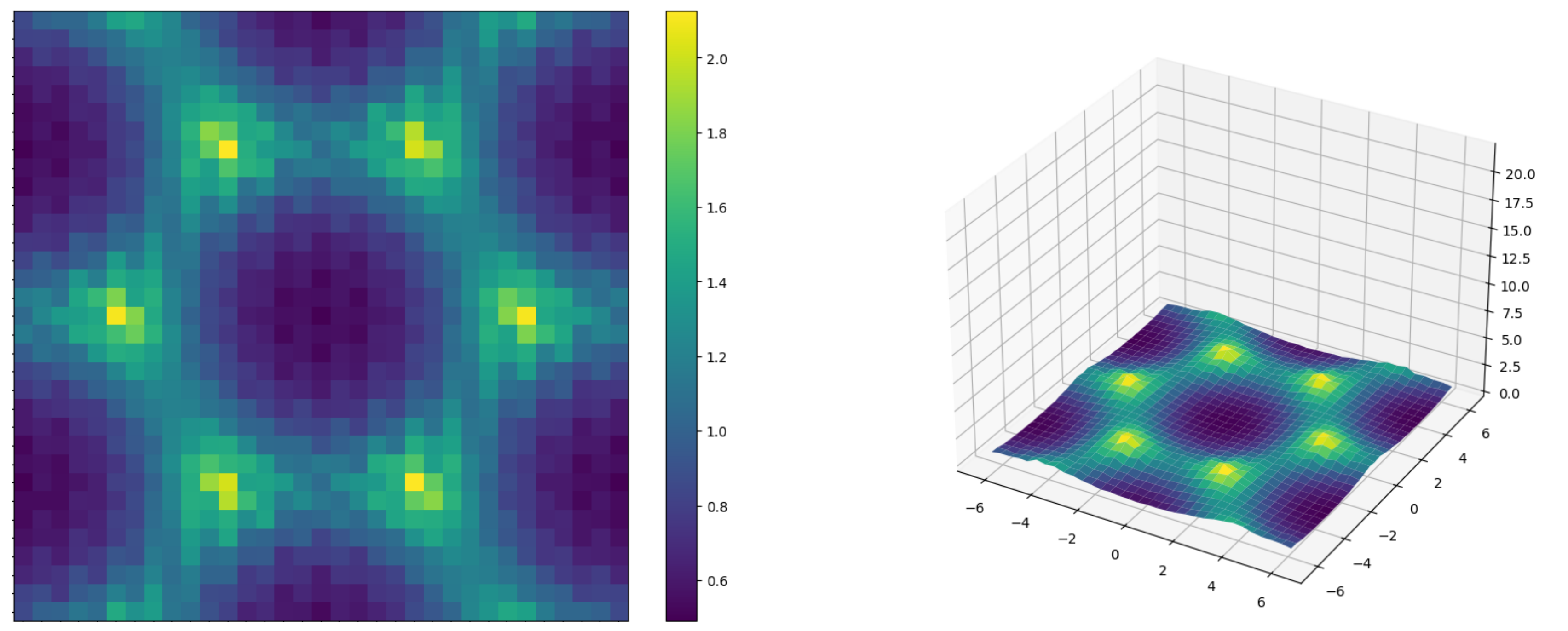


Spin structure factor:

$$S(\mathbf{q}) = \langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}} \rangle = \frac{1}{N} \sum_{ij} \langle S^z_i S^z_j \rangle e^{i\mathbf{q}\cdot(\mathbf{x}_i - \mathbf{x}_j)}$$



$\Gamma = 1.0$



$\Gamma = 2.0$

Conclusions

- Our Neural PQMC technique allow us to investigate the spin glass phase of the 2D EA model
- We determine the critical transverse field as well as the critical exponents in good agreement with state-of-the-art works
- Large scale PQMC simulation allow us to compute $P(q)$: hints to RSB

L.Brodoloni, S.Pilati arXiv:2407.05978(2024)

- Preliminar results on "order-by-disorder" phenomena enlight a promising route to explore different kinds of interactions (Rydberg)

Complex Quantum Matter @ UNICAM

Left to right: Giovanni Midei, Victor Velasco, Luis Ardila, Sebastiano Pilati, Andrea Perali, Nicola Pinto, Simone Cantori, Luca Brodoloni, Andrea Della Valle and Verdiana Piselli. CQM-Unicam, May 30 2024.
Not Included: Carlo Lucheroni, Filippo Pascucci, Meenakshi Sharma and Gabriele Spada.

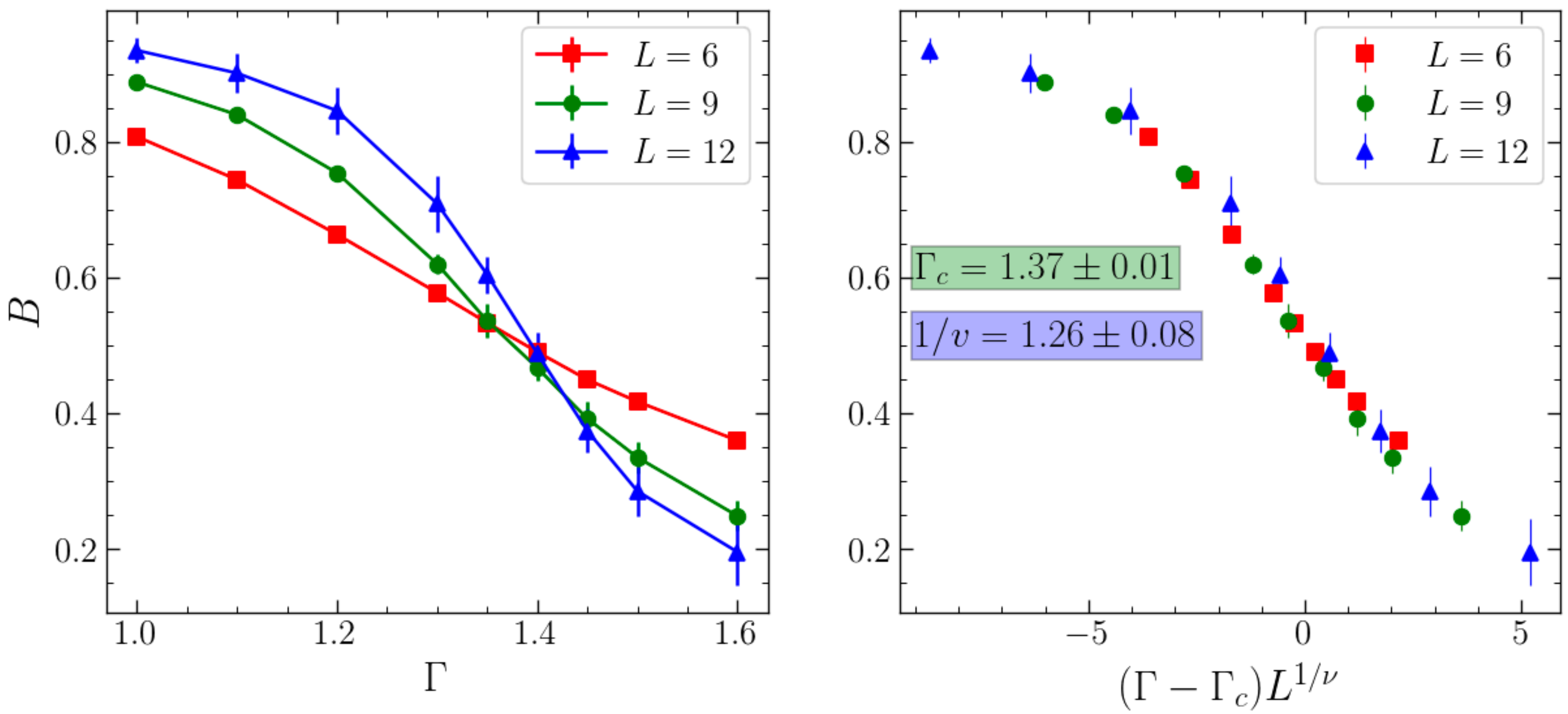
Long range interactions model

$$H = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i\sigma_i^x$$

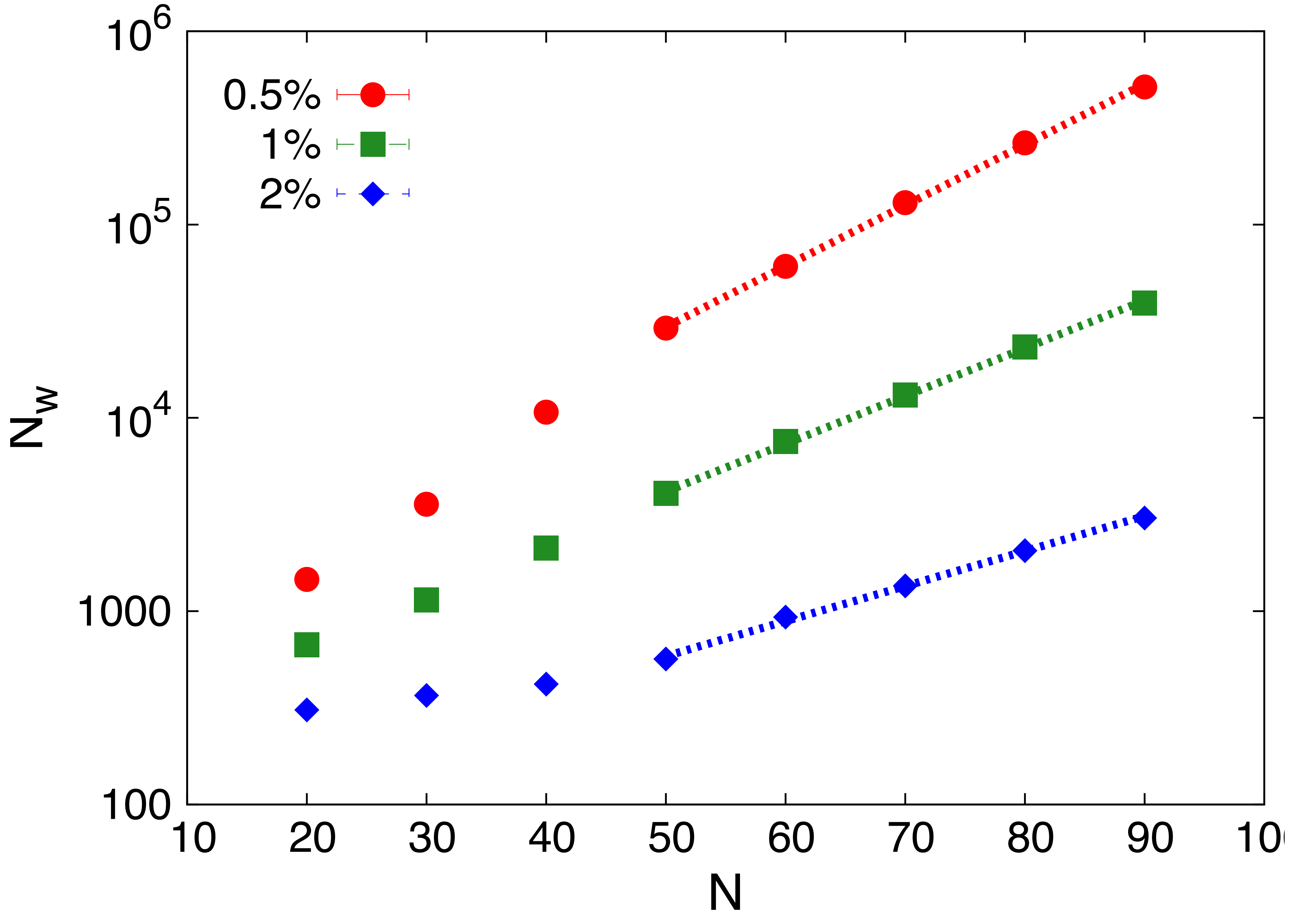
$$J_{ij} \propto \frac{1}{r_{ij}^6}$$

Rydberg interactions Ising model

$\alpha = 6$ Model



# of walkers required to keep relative err. fixed



System size

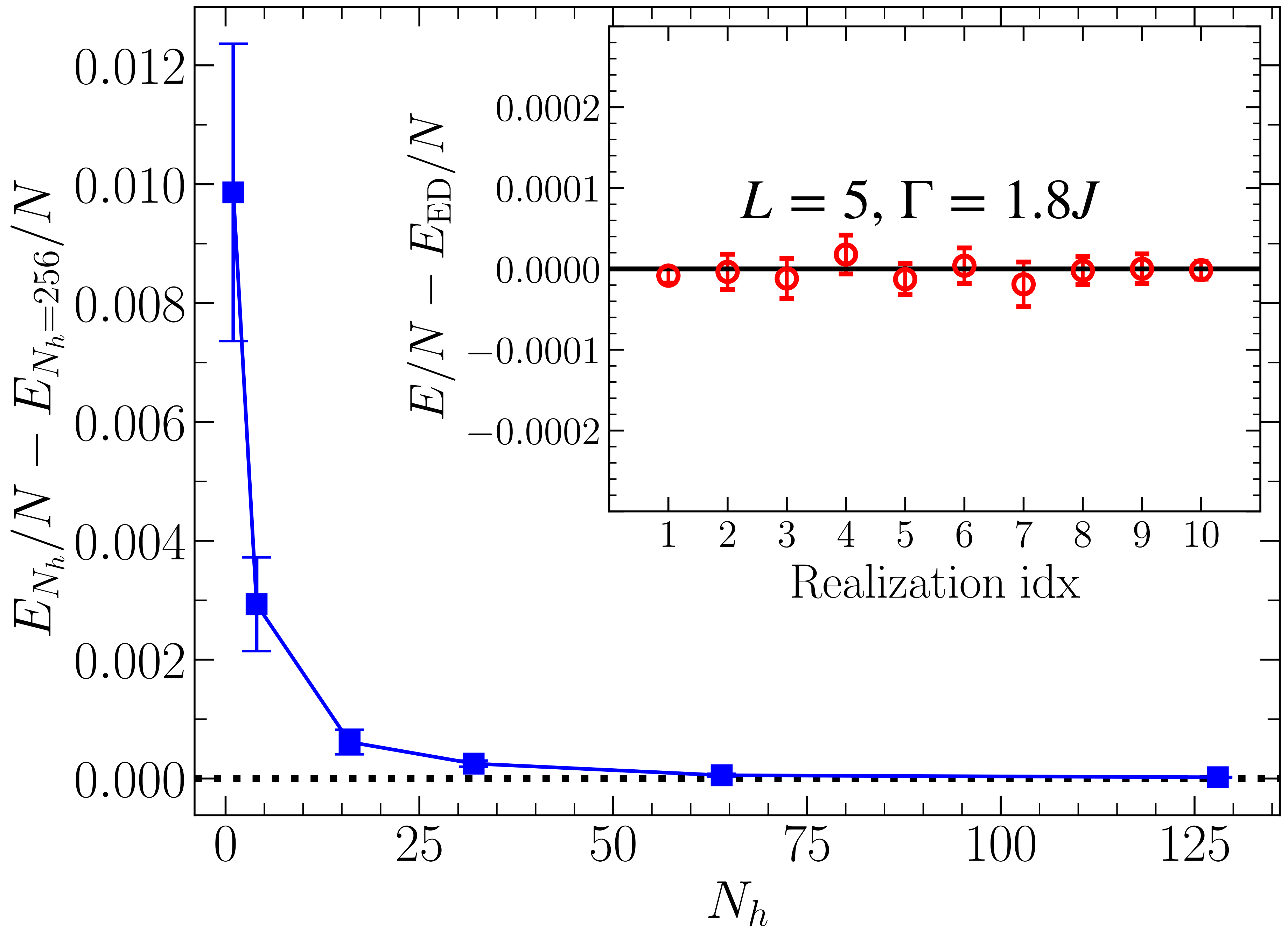
Exponential growth with the system size

No guiding wf

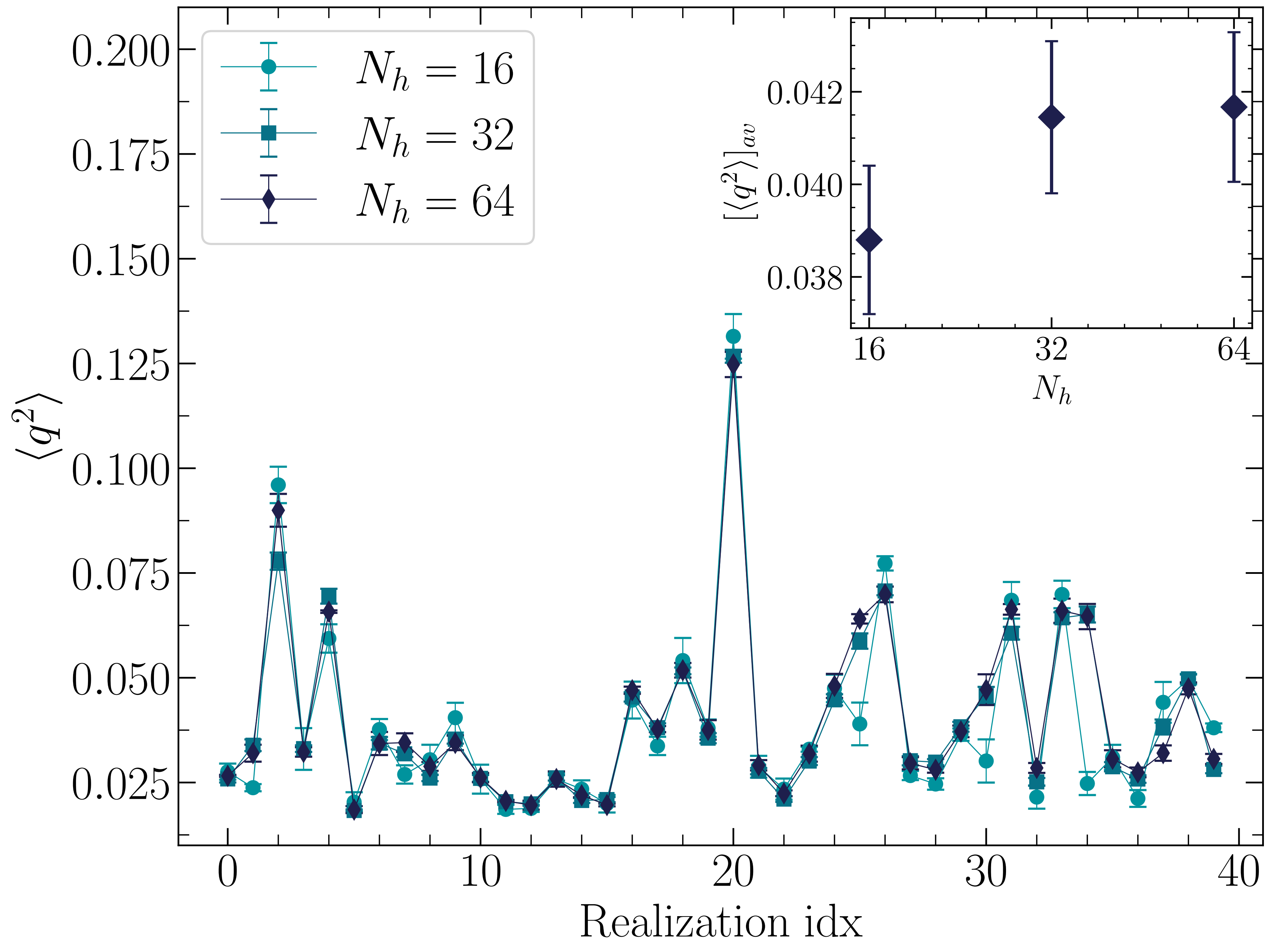
2D Edwards-Anderson model

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma_i \sigma_i^x \quad J_{ij} \sim \mathrm{Norm}[\mu = 0, \sigma = 1]$$

Unbiased estimations of GS properties



$L = 10, \Gamma = 1.8J, N_{\mathrm{w}} = 4000$



L.Brodoloni, S.Pilati arXiv:2407.05978(2024)