Self-learning projective quantum Monte Carlo simulations guided by neural network states

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Workshop "*Many-Body quantum physics with machine learning*"
ECT*, Trento, 7 Sept. 2023

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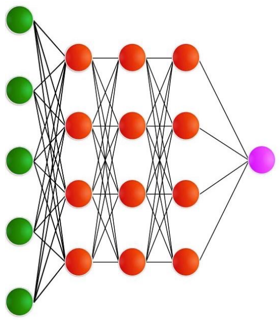
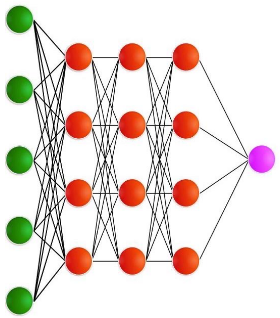
NQSTI QST

ISCRA CINECA

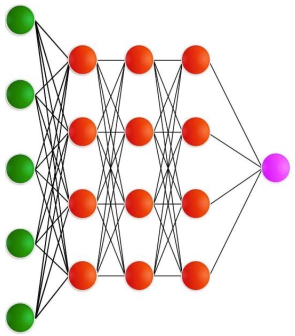
Deep learning for the quantum many body problem

Neural network states: $\boldsymbol{R}$ →  $\psi(\boldsymbol{R})$

$$E_0 = \min\left\{\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right\}$$

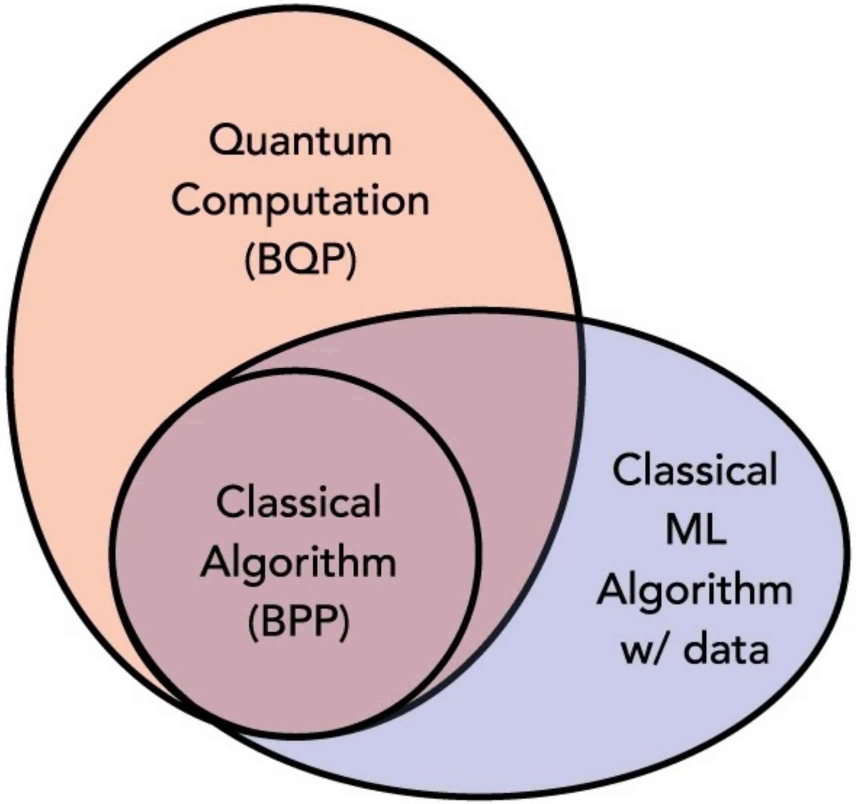
Density functional theory (needs data!) $n(\boldsymbol{R})$ →  $E[n(\boldsymbol{R})]$

$$E_0 \leq E[n(\boldsymbol{R})]$$
$$E_0 = \min\{E[n(\boldsymbol{R})]\}$$

Supervised learning (needs data!) $\hat{H}$ →  E_0

Data might come from:

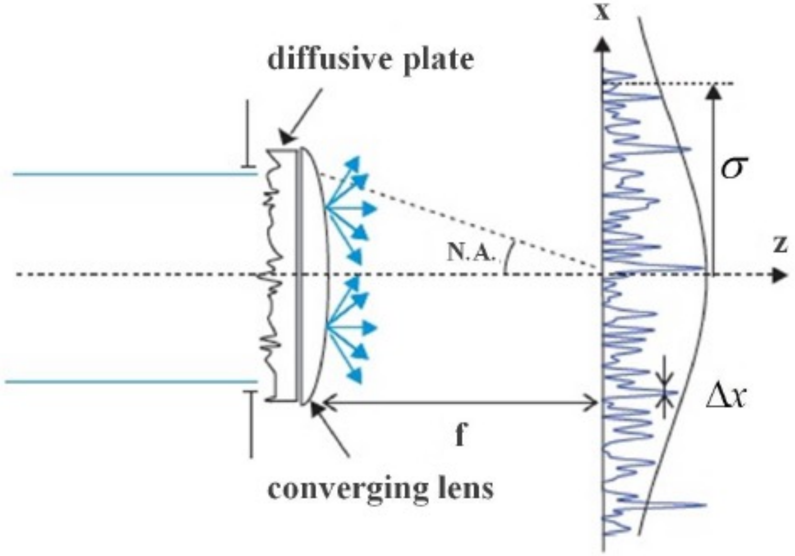
- More ab-initio method (NQS): computational cost
- Smaller systems: scalability
- Quantum device: noise & errors



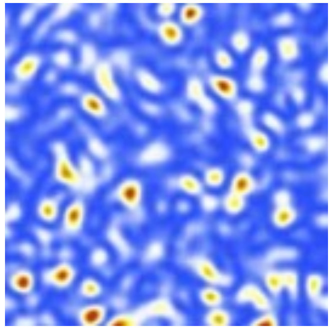
Classical machine learning algorithm trained on (quantum) data can solve otherwise classically intractable problems.

H.-Y. Huang et al, *Power of data in quantum machine learning,* Nat. Commun. **12**, 2631 (2021).
H.-Y. Huang et al., *Provably efficient machine learning for quantum many-body problems,* Science (2022)

Supervised learning: cold-atoms in optical speckle patterns

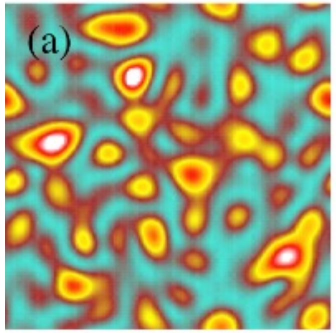


experiment @ LENS



Semeghini et al. Nat. Phys. 2015

num. simulation

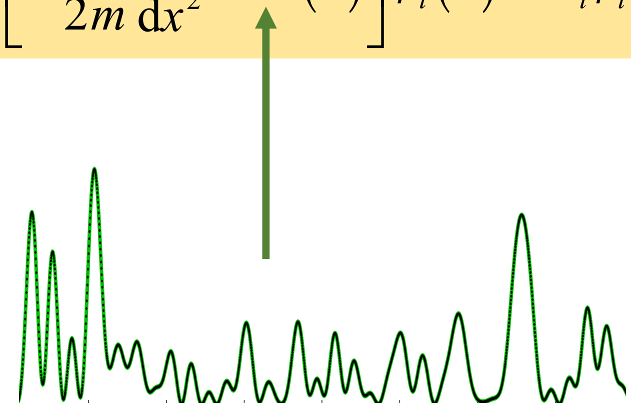


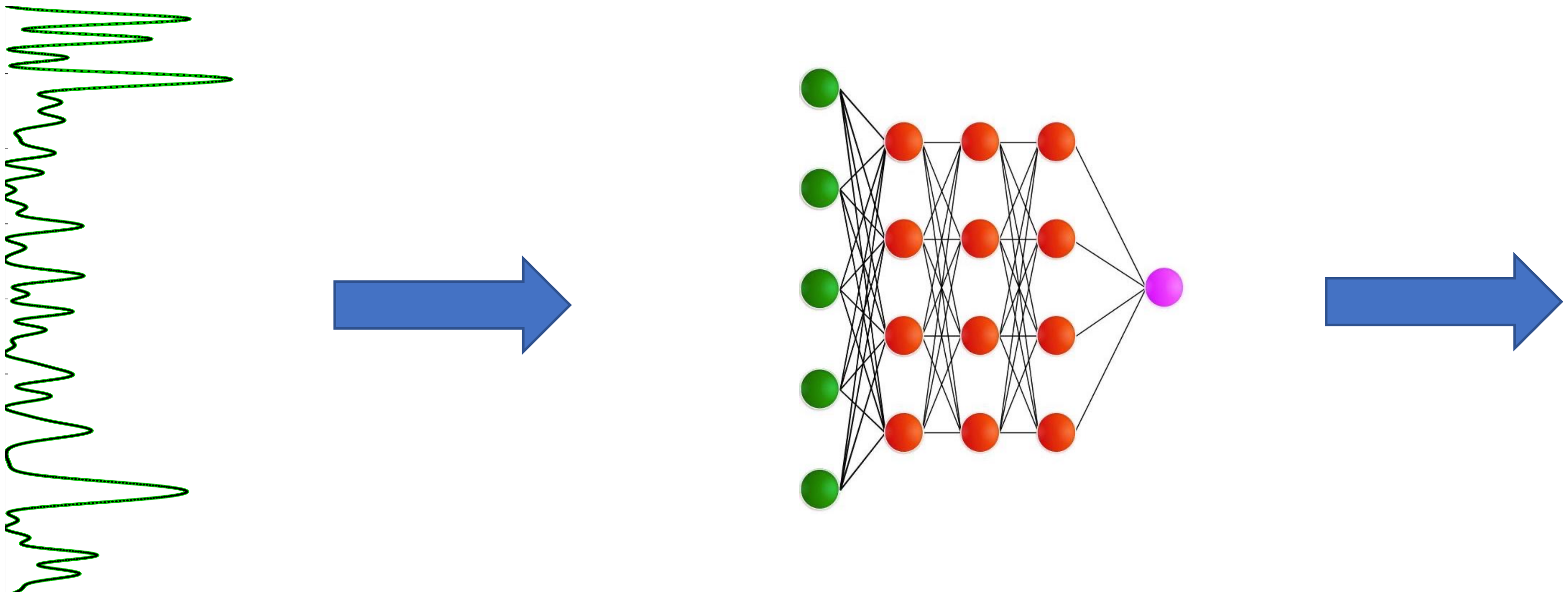
SP, Fratini PRA (2015)

EXP @ LENS, Palaiseau

1D single-particle SE:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V\left(x\right)\right]\varphi_i\left(x\right)=E_i\varphi_i\left(x\right)$$

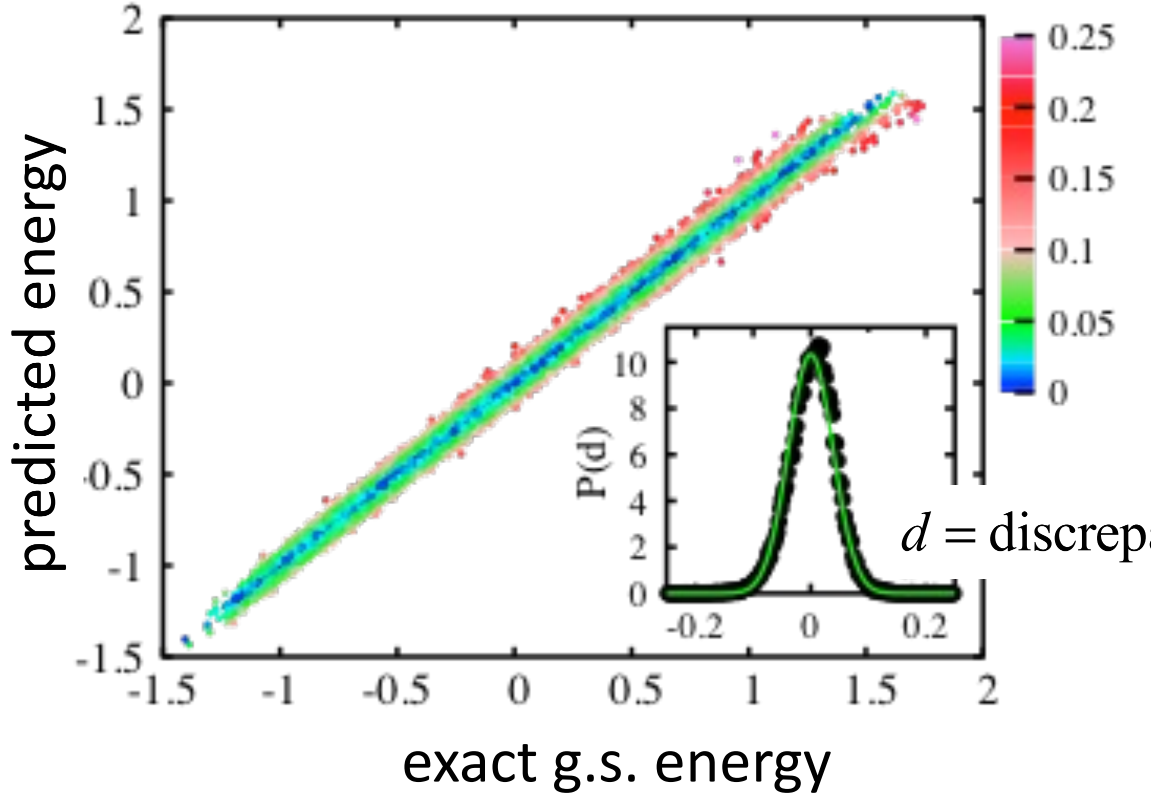




$$E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$

Neural net. predictions vs. exact g.s. energy

SP, Pieri, Sci. Rep. **9**, 5613 (2019)



$N_{\text{train}} = 8\times10^4$

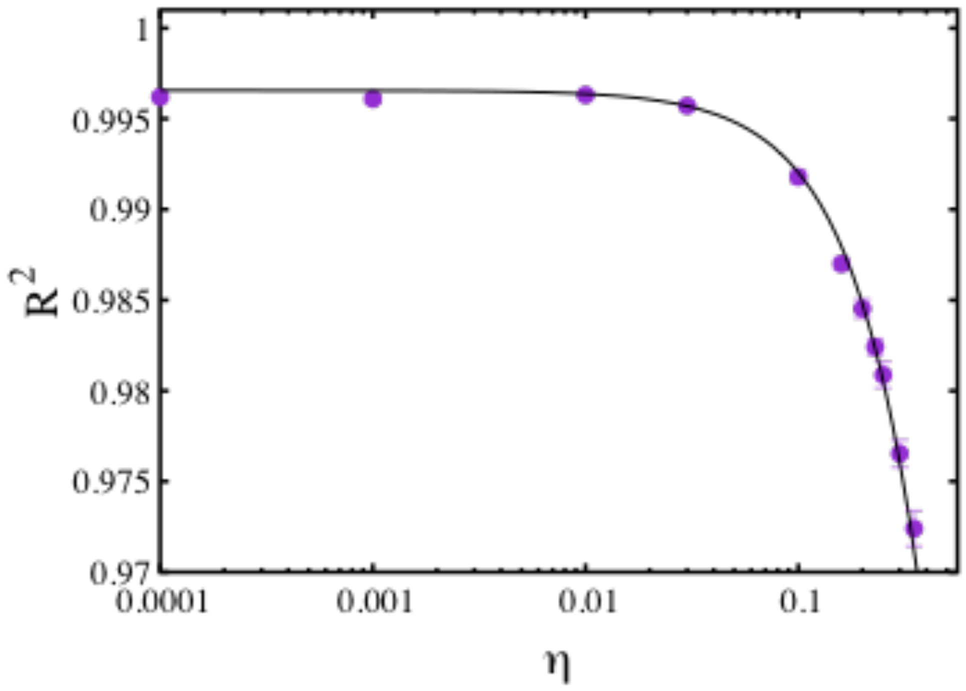
$$d = \text{discrepancy} \equiv \varepsilon^{\text{pred}} - \varepsilon_0$$

Resilinece to noise: cold-atom quantum simulators?

SP, Pieri, Sci. Rep. **9**, 5613 (2019)

Q: could we use QS to train NN to solve computationally intractable problem?

ANALYSIS OF NOISE SENSITIVITY: Training on synthetic data with added noise



added noise

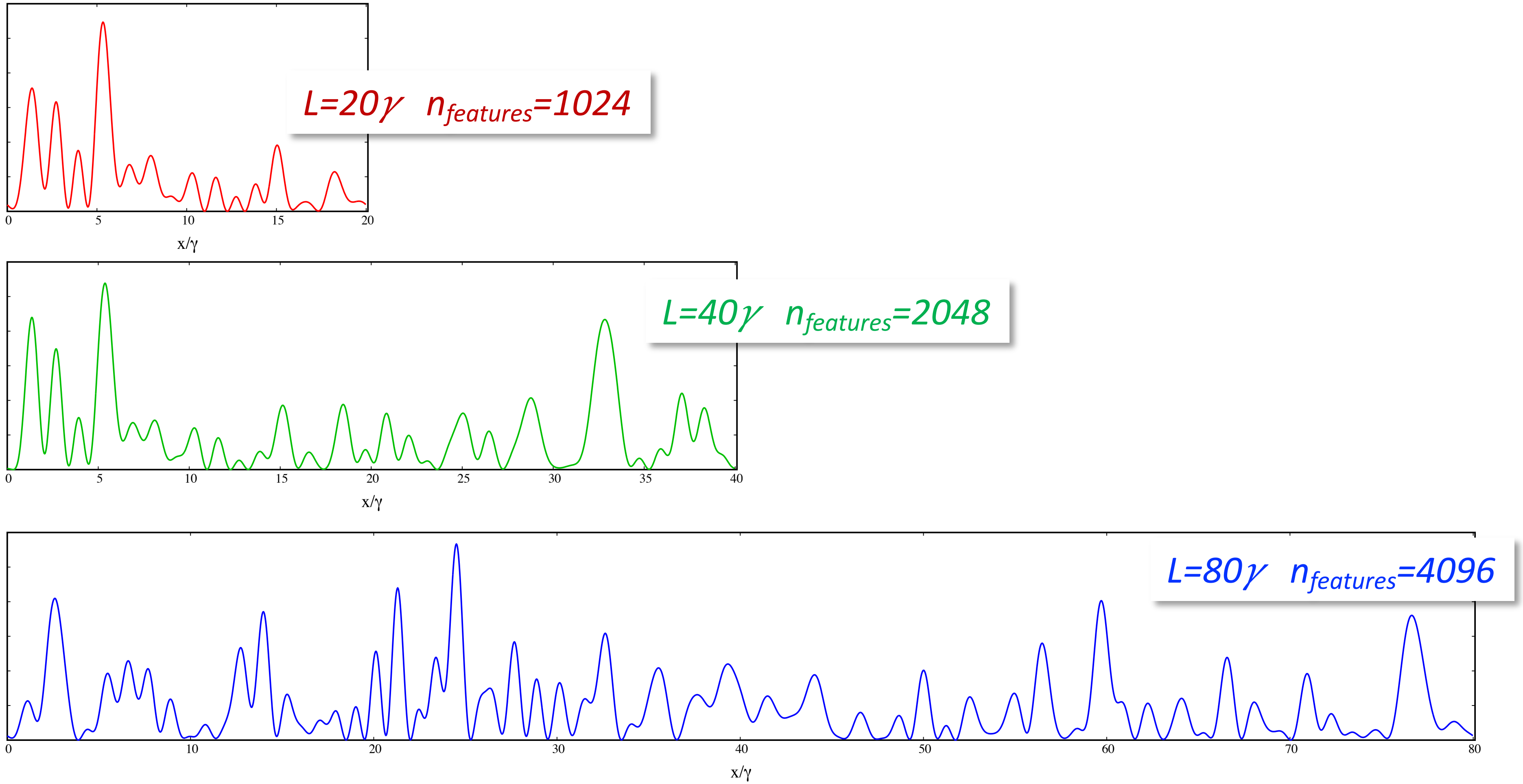
The NN is remarkably resilient, it can filter signal from noise

$$\sigma_{\text{noise}} = \eta\sigma_{data}$$

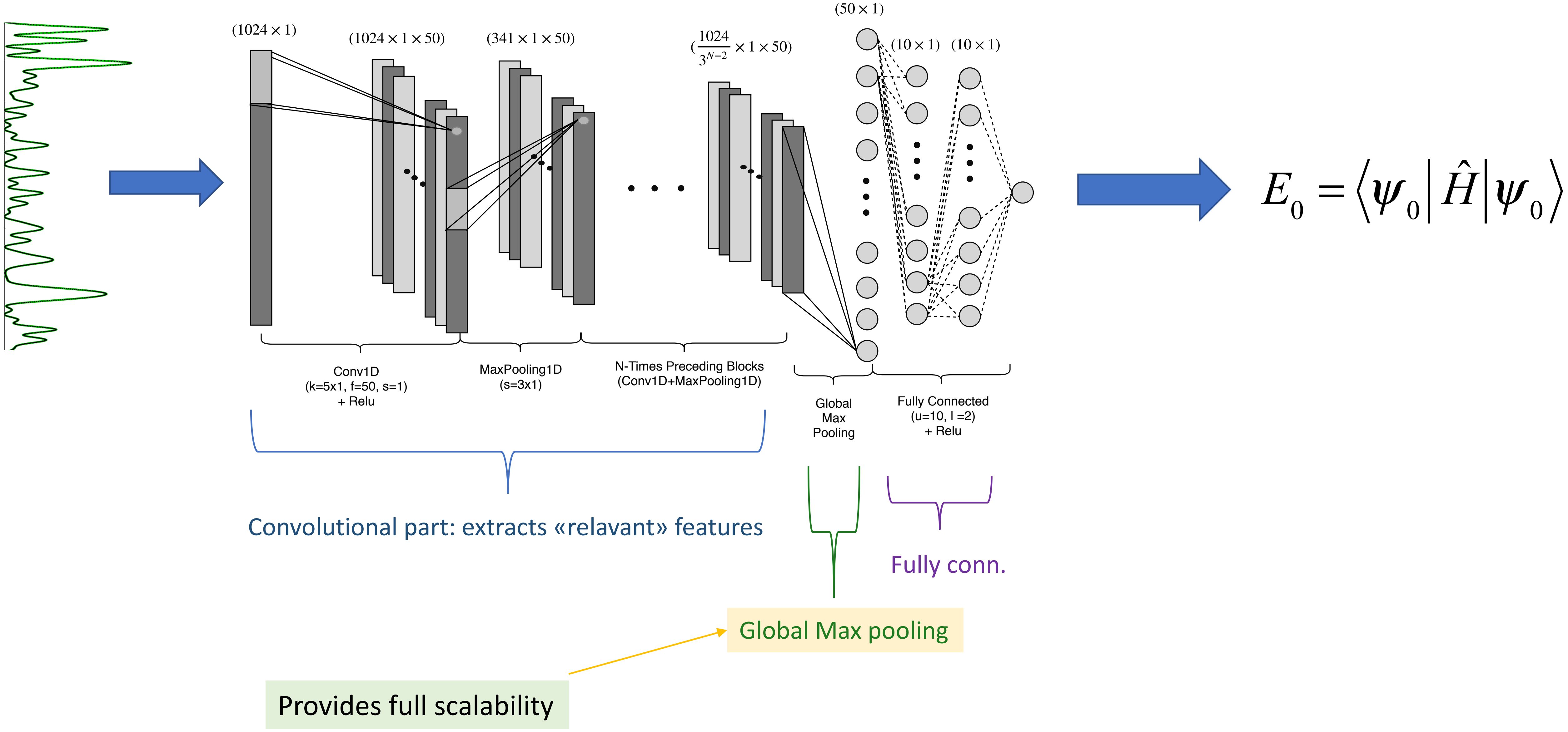
Gaussian noise with stand. dev. proportional to intrinsic data stand. dev.

Scalabale neural networks

- Scalable NN that can address different system sizes
- Heterogeneous training
- Extrapolation: making prediction for larger system sizes

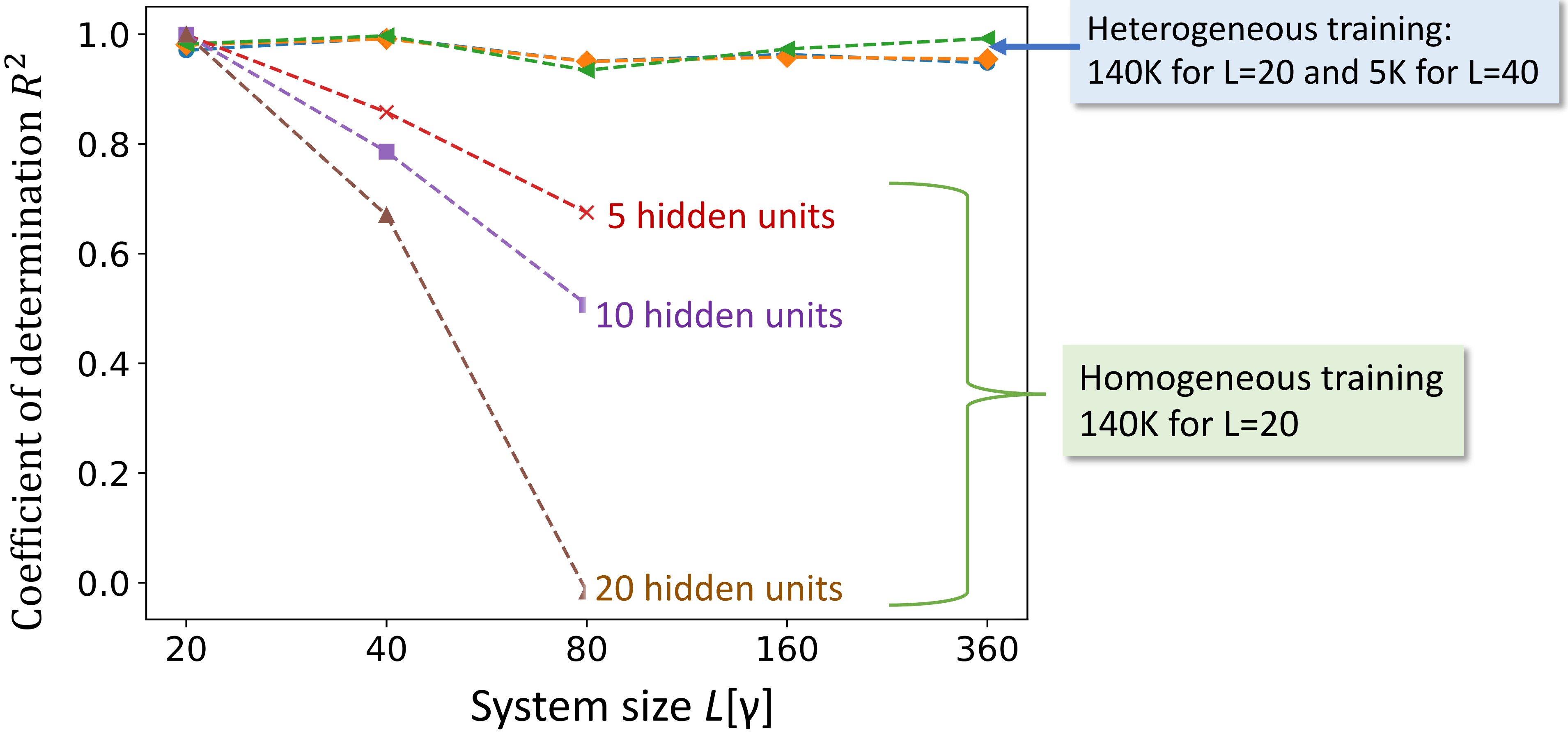


A fully-scalable convolutional neural network



Extrapolation: making predictions for larger systems

Coefficient of determination: $R^2 = 1 - \frac{\text{MSE}}{\text{VAR}}$



Saraceni, Cantori, SP, PRE **102**, 033301 (2020)

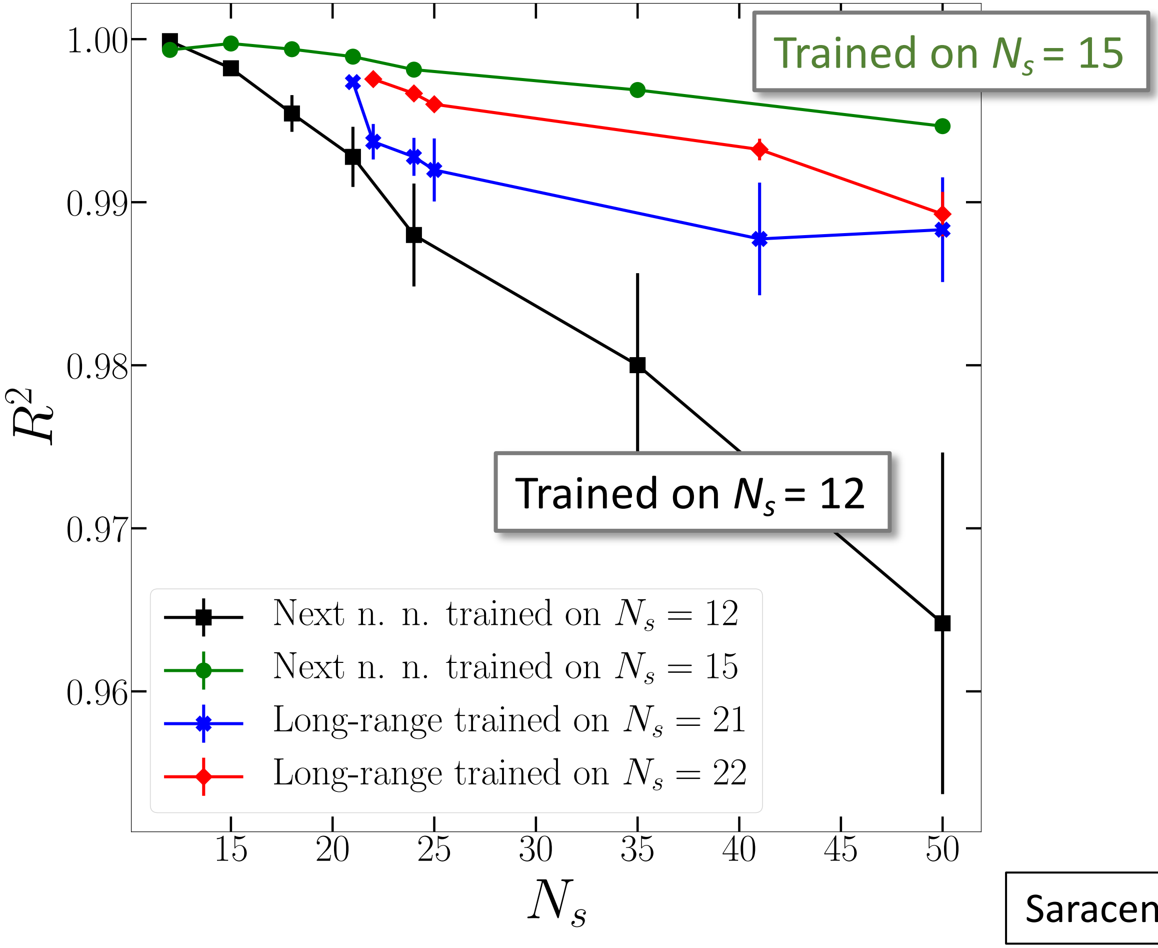
Disordered quantum Ising model in 1D

$$H = -\sum_i \left[J_{i,i+1}\sigma_i^x\sigma_{i+1}^x + J_{i,i+d}\sigma_i^x\sigma_{i+d}^x\right] - \Gamma\sum_i \sigma_i^z$$

$$J_{i,i+1}, J_{i,i+d} \sim \mathrm{Unif}[0,1]$$

Descriptors: $J_{i,i+1}, J_{i,i+d}$

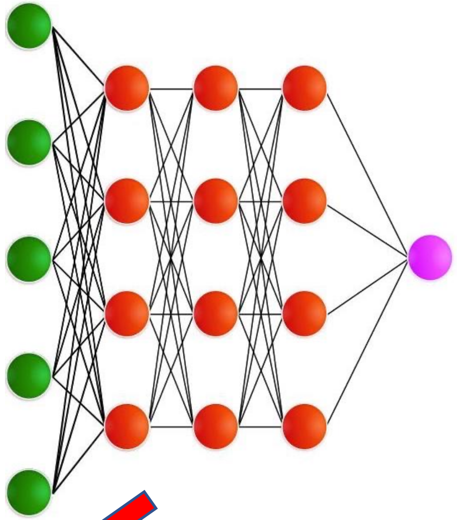
N_{train}: 3×10^4



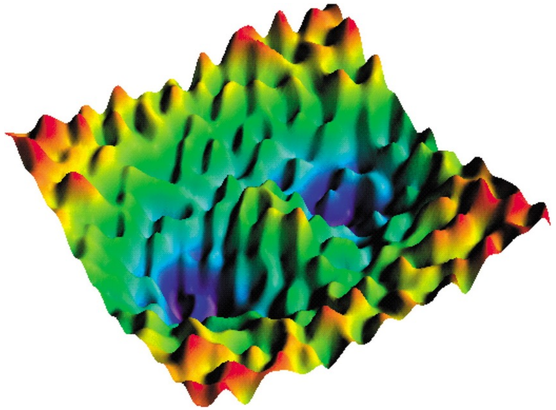
Saraceni, Cantori, SP, PRE **102**, 033301 (2020)

Quantum annealers

Classical deep learning

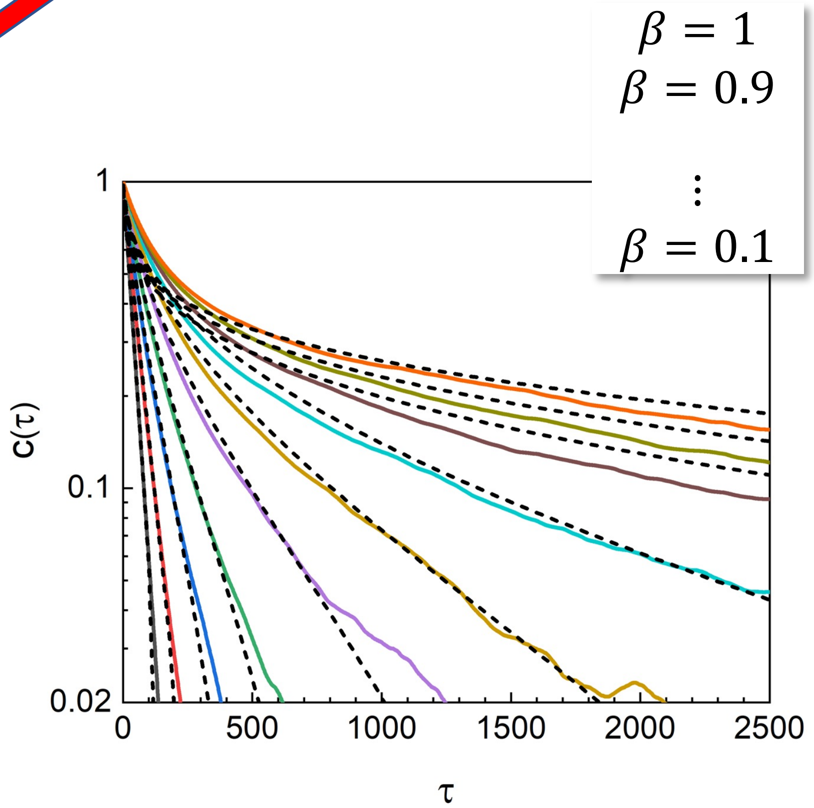


Energy landscape



Low-T equilibrium properties of classical spin glasses

$$H = \sum_{ij} J_{ij} x_i x_j$$



NEURAL CLASSICAL MONTE CARLO SIMULATIONS

McNaughton, Milošević, Perali, SP, PRE (2020)

Proposal matrix in Metropolis-Hastings algorithm: $w_{\mathbf{x}'\mathbf{x}} = p_{\mathrm{NETWORK}}(\mathbf{x}')$ (use ancestral sampling)

Acceptance probability: $A_{\mathbf{x}'\mathbf{x}} = \min\left(1, \frac{p_{\mathrm{BOLTZ}}(\mathbf{x}')w_{\mathbf{x}\mathbf{x}'}}{p_{\mathrm{BOLTZ}}(\mathbf{x})w_{\mathbf{x}'\mathbf{x}}}\right)$

We need: $p_{\mathrm{BOLTZ}}(\mathbf{x}) > 0 \implies p_{\mathrm{NETWORK}}(\mathbf{x}) > 0$

if: $p_{\mathrm{NETWORK}}(\mathbf{x}) \cong p_{\mathrm{BOLTZ}}(\mathbf{x}) \longrightarrow A_{\mathbf{x}'\mathbf{x}} \cong 1$ → efficient simulation!

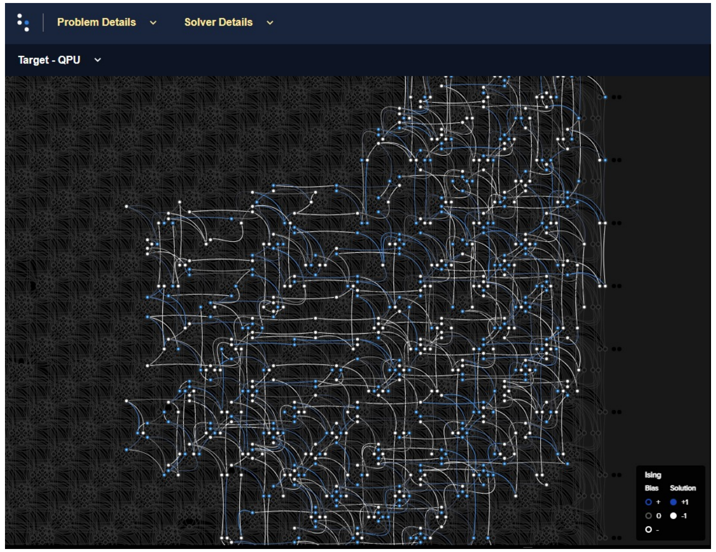
if: $p_{\mathrm{NETWORK}}(\mathbf{x}) \cong 0 \quad \text{where} \quad p_{\mathrm{BOLTZ}}(\mathbf{x}) \approx 1$ → ergodicity problem!

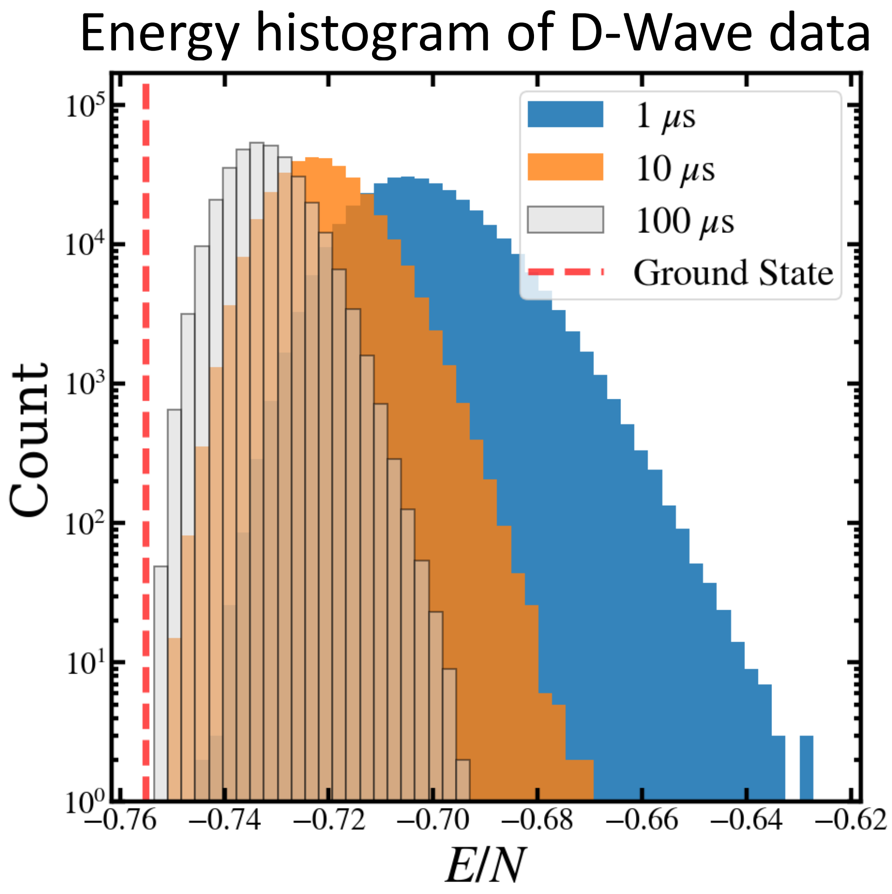
Related work:

- K. A. Nicoli et al., PRE 101, 023304 (2020): MCMC+autoregressive n. for ferromagnetic models.
- F. Noè et al., Science 365, 1147 (2019): normalizing flows for complex-molecule simulations.
- X. Ding et al., J. Phys. Chem. B, 124, 10166 (2020): normalizing flows for free-energy computations.
- M. Gabrié et al., arXiv:2105.12603 (2021): adaptive MCMC via normalizing flows.
- G. S. Hartnett, M. Mohseni,arXiv:2001.00585v2 (2020): spin-glass simulations via normalizing flows.

Neural MC with NN trained on D-WAVE data

Access to D-Wave QPU time via CINECA ISCRA Project





2D square lattice N=484
Nearest and next-nearest neighbor interaction
Uniform random couplings

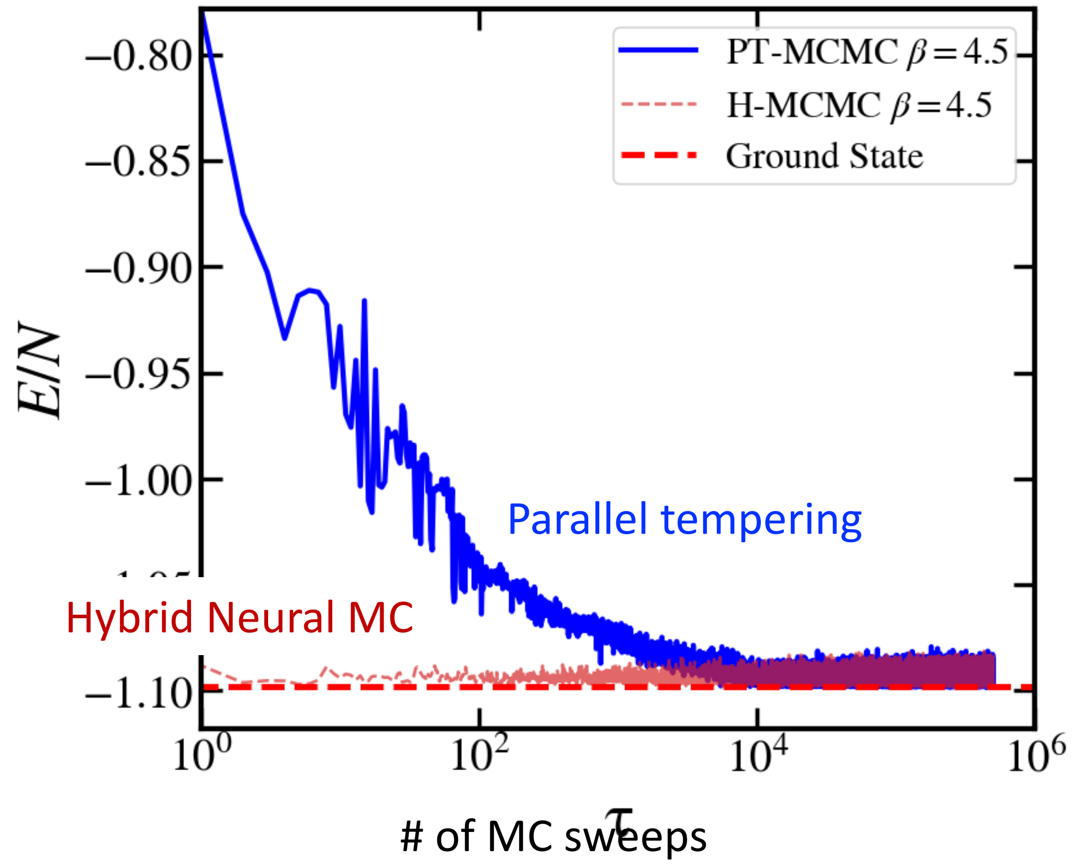
Hybrid neural simulation of a spin glass at low T

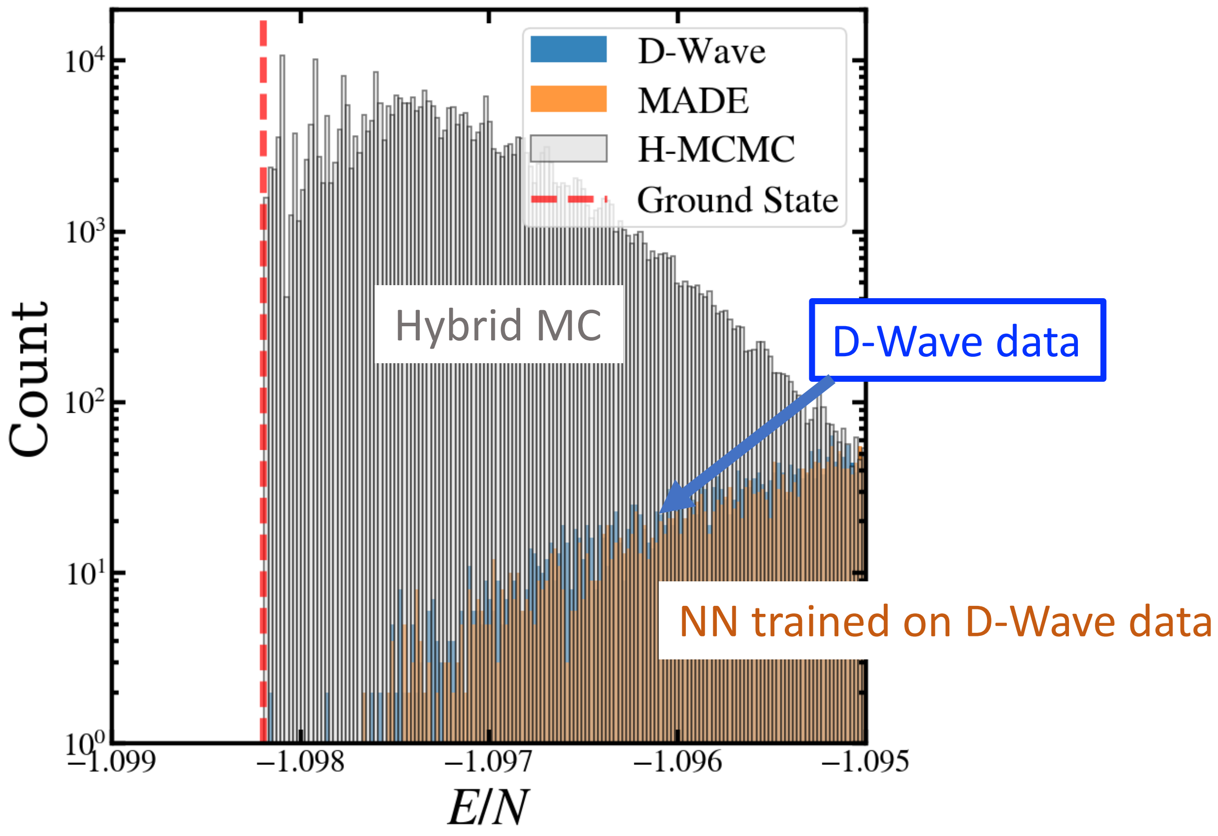
G. Scriva, E. Costa, B. McNaughton, SP, SciPost Physics 15, 018 (2023)

NN trained on D-WAVE data

Annealing time: $100\mu s$

β/J = 4.5
2D square lattice N=484
Nearest and next-nearest neighbor interaction
Uniform random couplings in (-1,1)





DFT for random quantum Ising models via scalable neural networks

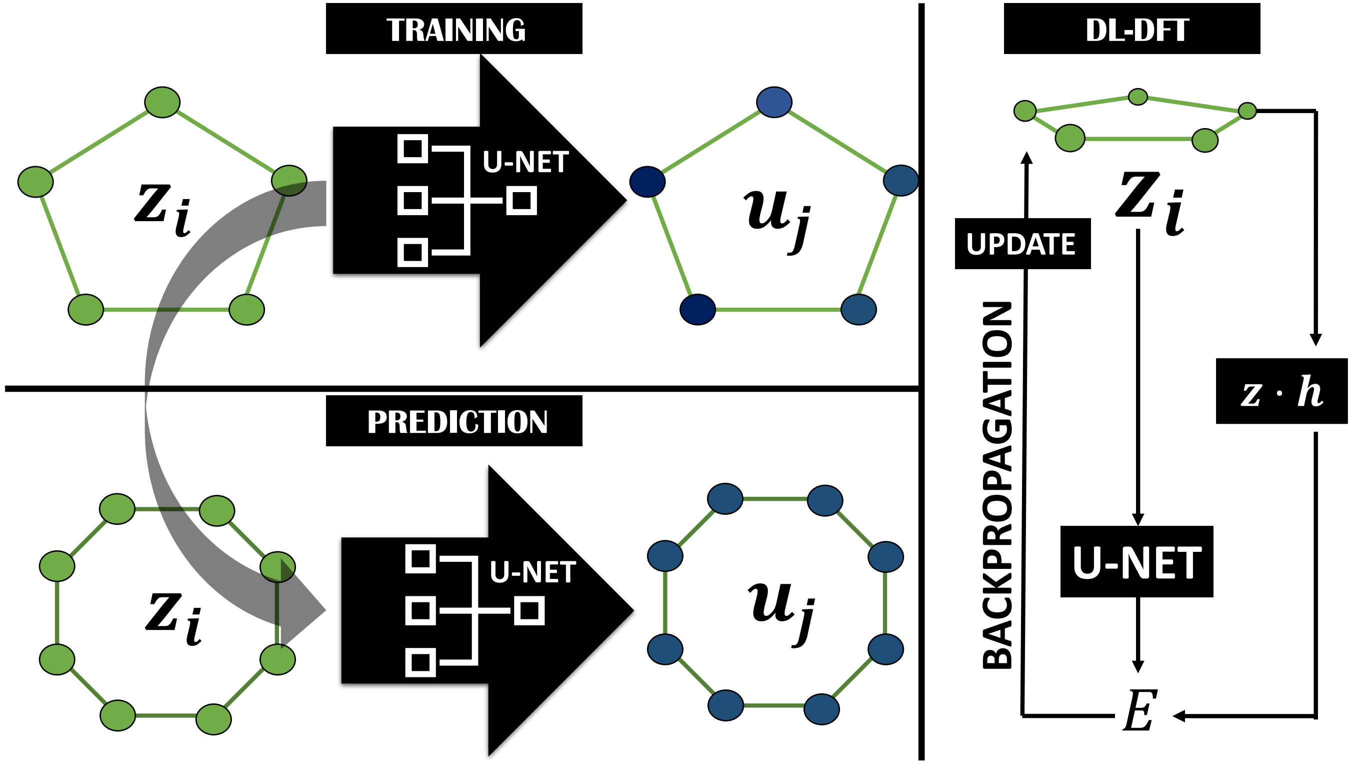
Hamiltonian: $H = -J[\sum_i \sigma_i^x \sigma_{i+1}^x + \sum_i \sigma_i^x \sigma_{i+2}^x] + \sum_i h_i \sigma_i^z$

Universal　　　Random

Functional: $E = E[\boldsymbol{z}] = \sum_j u_j + \boldsymbol{h} \cdot \boldsymbol{z}$

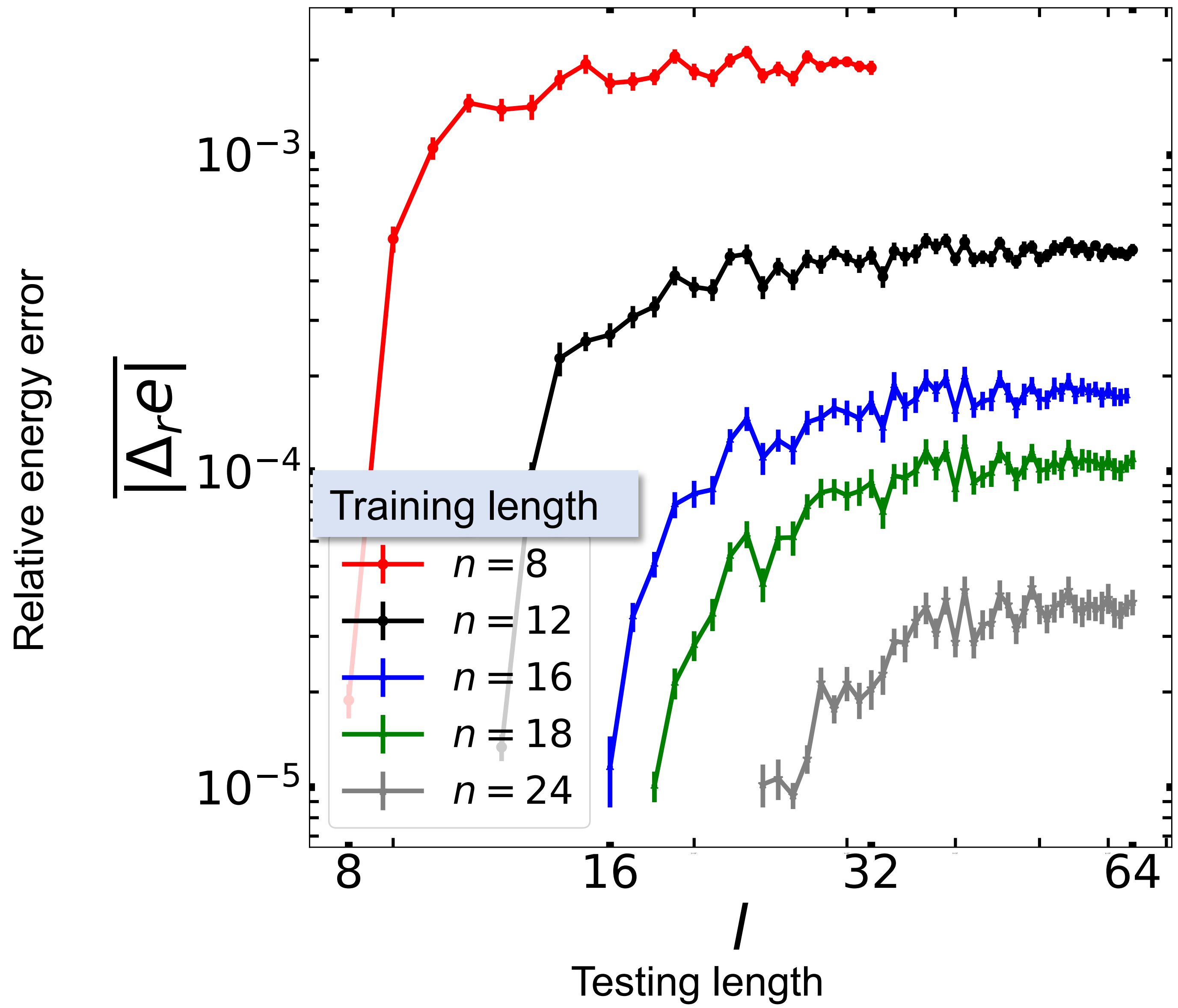
$z_i = \langle \sigma_j^z \rangle$

$u_j = -J \left\langle \left[\sum_i \sigma_i^x \sigma_{i+1}^x + \sum_i \sigma_i^x \sigma_{i+2}^x \right] \right\rangle$



Predicting energies for larger systems than those used for training

E. Costa, R. Fazio, SP, PRB (2023)



Future goal:
dynamics via time-dependent DFT

Projective QMC for Quantum Ising models

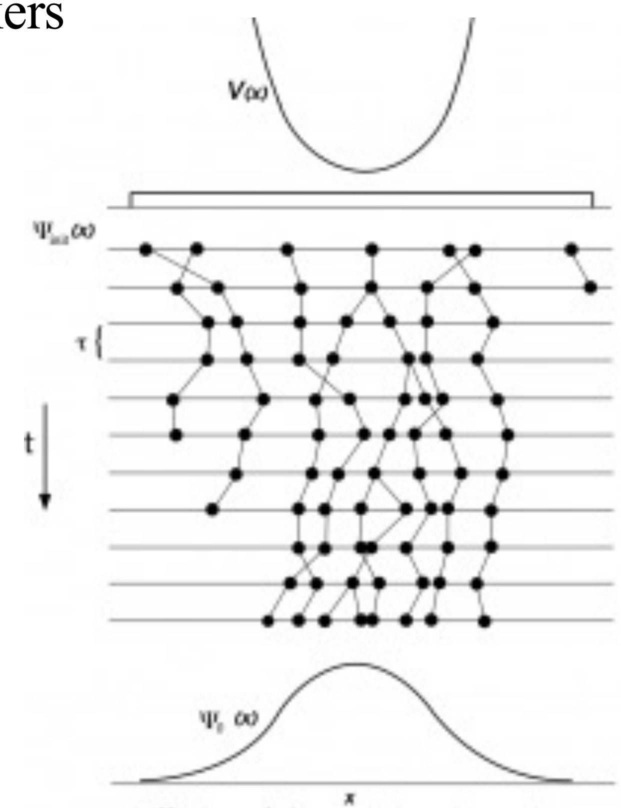
$$H = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x$$

$$\psi(\mathbf{S},\tau) = \exp(-\tau H)\psi(\mathbf{S},0) \underset{\tau\to\infty}{\approx} \psi_0(\mathbf{S},0)$$ Schrödinger eq. in imaginary time

$$\psi(\mathbf{S},\tau+\Delta\tau) = \sum_{\mathbf{S}'} G(\mathbf{S}',\mathbf{S},\Delta\tau)\psi(\mathbf{S}',\tau)$$ defines a Markov process

$G(\mathbf{S}',\mathbf{S},\Delta\tau) \geq 0 \;\Rightarrow$ no sign problem (stoquastic Hamiltonian)

$\sum_{\mathbf{S}'} G(\mathbf{S}',\mathbf{S},\Delta\tau) \neq 1 \Rightarrow$ not a standard Markov process $\Rightarrow$ kill or clone random walkers



Imaginary-time Green's function
$G(\mathbf{S}',\mathbf{S},\Delta\tau) = \langle \mathbf{S}' | \exp(-\Delta\tau(H - E_{ref})) | \mathbf{S} \rangle$

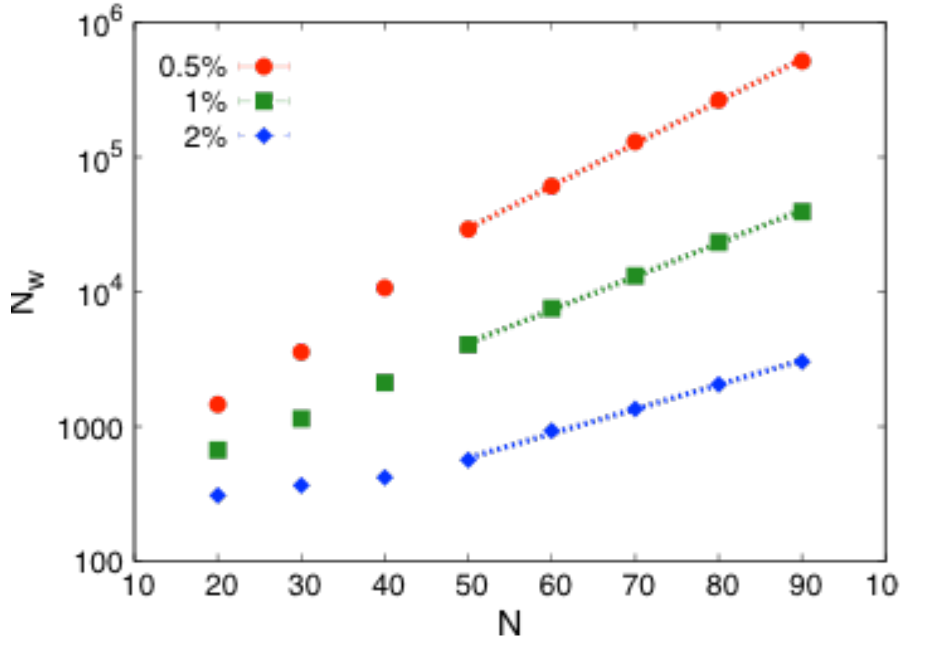
Image from: W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal Rev. Mod. Phys. 73, 33 (2001)

Computational cost of projective QMC simulations

Inack, Giudici, Parolini, Santoro, SP, PRA (2018)

Notice: any diagonal Hamiltonian is stoquastic (sign-problem free).
Finding its ground state encompasses hard classical optimization problems such as k-SAT or MAX-CUT.
Bravyi, Quant. Inf. Comp., Vol. 15, No. 13/14, pp. 1122-1140 (2015)

# of walkers required to keep relative err. fixed



System size

SEE ALSO:
N. Nemec, Phys. Rev. B 81, 035119 (2010).
M. Boninsegni and S. Moroni, Phys. Rev. E 86, 056712 (2012).
K. Ghanem, N. Liebermann, A. Alavi, Phys. Rev. B 103, 155135 (2021)
J. Brand, M. Yang, E, Pahl, Phys. Rev. B 105, 235144 (2022)

Exponentially growing computational cost, even without sign problem

Note: here we use "simple" PQMC algorithm: no guiding wave function.

IMPORTANCE SAMPLING WITH VARIATIONAL ANSATZ

Introduce guiding wave function $\equiv \psi_G(\mathbf{x})$

Modified master eq.: $\Psi(\mathbf{x}, \tau + \Delta\tau)\psi_G(\mathbf{x}) = \sum_{\mathbf{x}'} \tilde{G}(\mathbf{x}, \mathbf{x}', \Delta\tau)\Psi(\mathbf{x}', \tau)\psi_G(\mathbf{x}')$

Modified Green's function: $\tilde{G}(\mathbf{x}, \mathbf{x}', \Delta\tau) = \langle \mathbf{x} | \exp(-\Delta\tau \hat{H} - E_{\mathrm{REF}}) | \mathbf{x}' \rangle \frac{\psi_G(\mathbf{x})}{\psi_G(\mathbf{x}')}$

The guiding wf reduces statistical fluctuations and bias.
Here, we adopt neural network states.

Self-learning projective QMC simulation

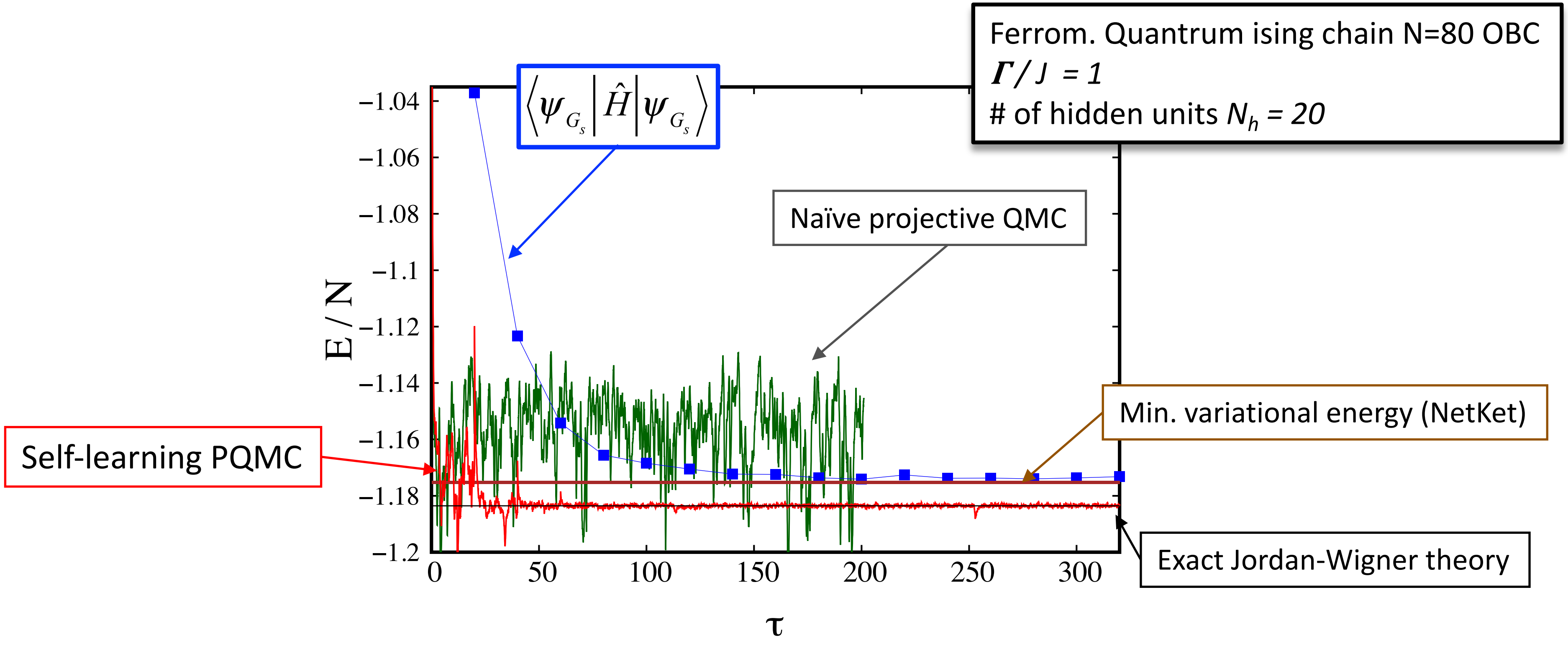
SP, Inack, Pieri, Phys. Rev. E 100, 043301 (2019)

- RBM learns the random-walker distribution: $P(\mathbf{x}) \propto \psi_G(\mathbf{x})\psi_0(\mathbf{x})$
- Guiding wf for the next stint: $\psi_G(\mathbf{x}) = \sqrt{P(\mathbf{x})}$

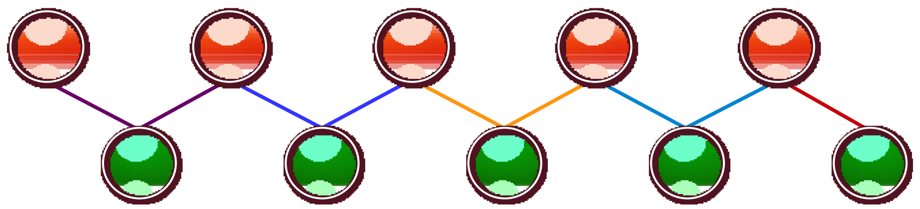
stoquastic model $\Rightarrow \psi_0(\mathbf{x}) \geq 0$

$\psi_{G_0}(\mathbf{x})\psi_0(\mathbf{x})$ $\quad \sqrt{\psi_{G_0}(\mathbf{x})\psi_0(\mathbf{x})}\psi_0(\mathbf{x})$ $\quad$ … $\quad$ … $\quad \psi_{G_0}^{1/2^2}(\mathbf{x})\psi_0^{2-1/2^n}(\mathbf{x})$ $\quad$ …

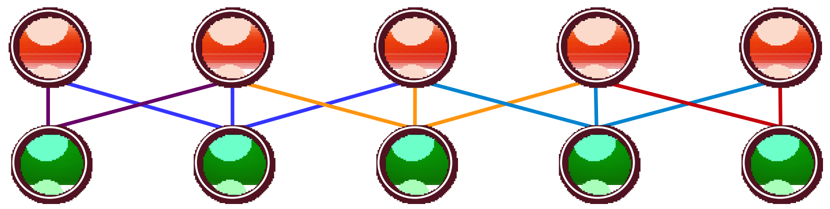
imaginary time



Sparse RBM, connectivity 2

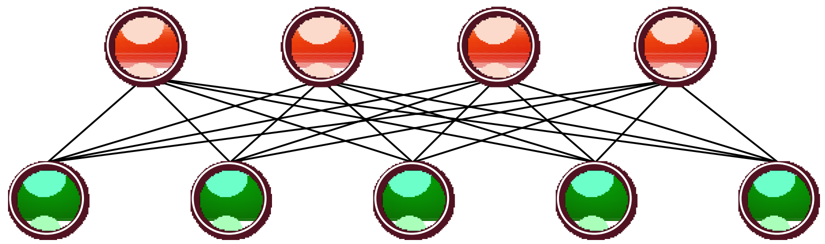


Sparse RBM, connectivity 3



Dense restricted Boltzmann machine

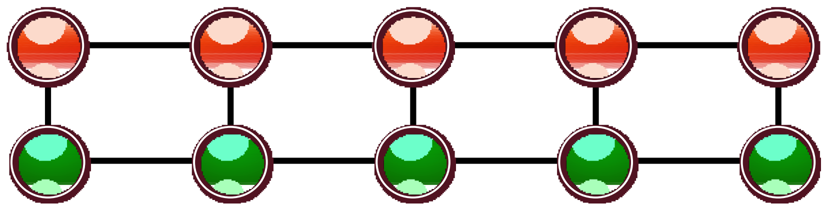
Carleo, Troyer, Science (2017)



Shadow-wave function

Reatto, Masserini, PRB (1988)

Vitiello, Runge, Kalos, PRL (1988)



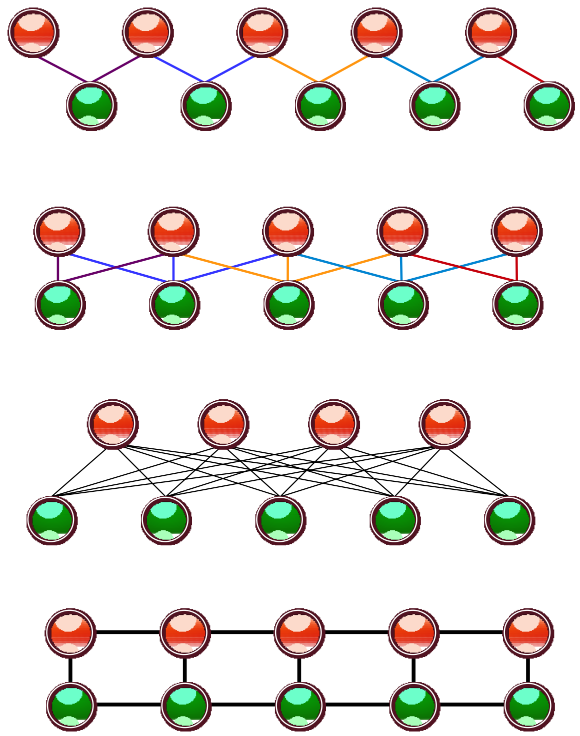
Random 1D quantum Ising chain: sparse neural networks

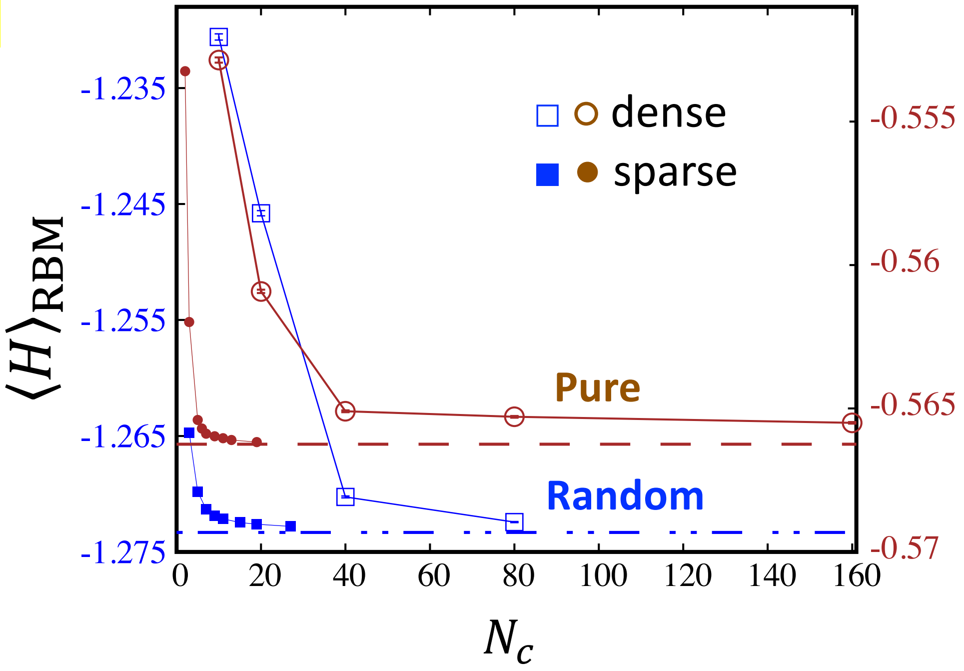
Connectivity $N_c = 2$

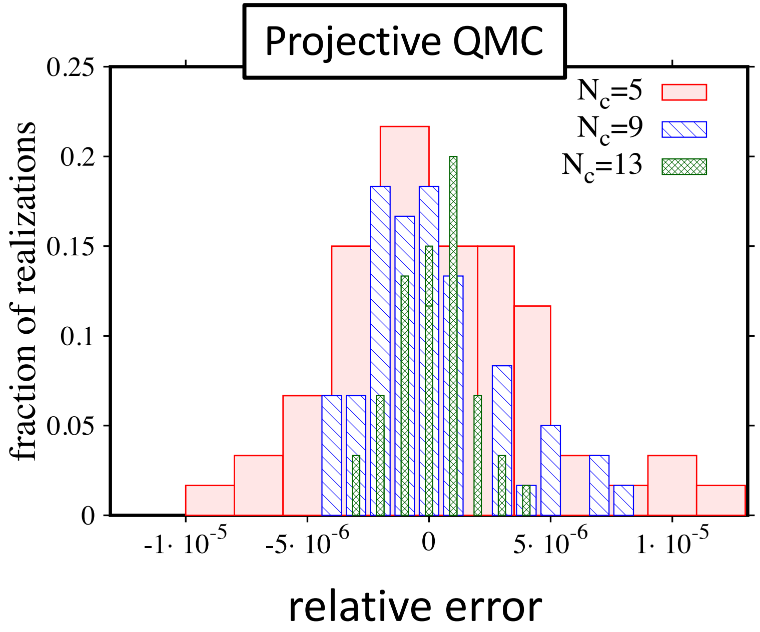
Connectivity $N_c = 3$

Dense

Shadow wf







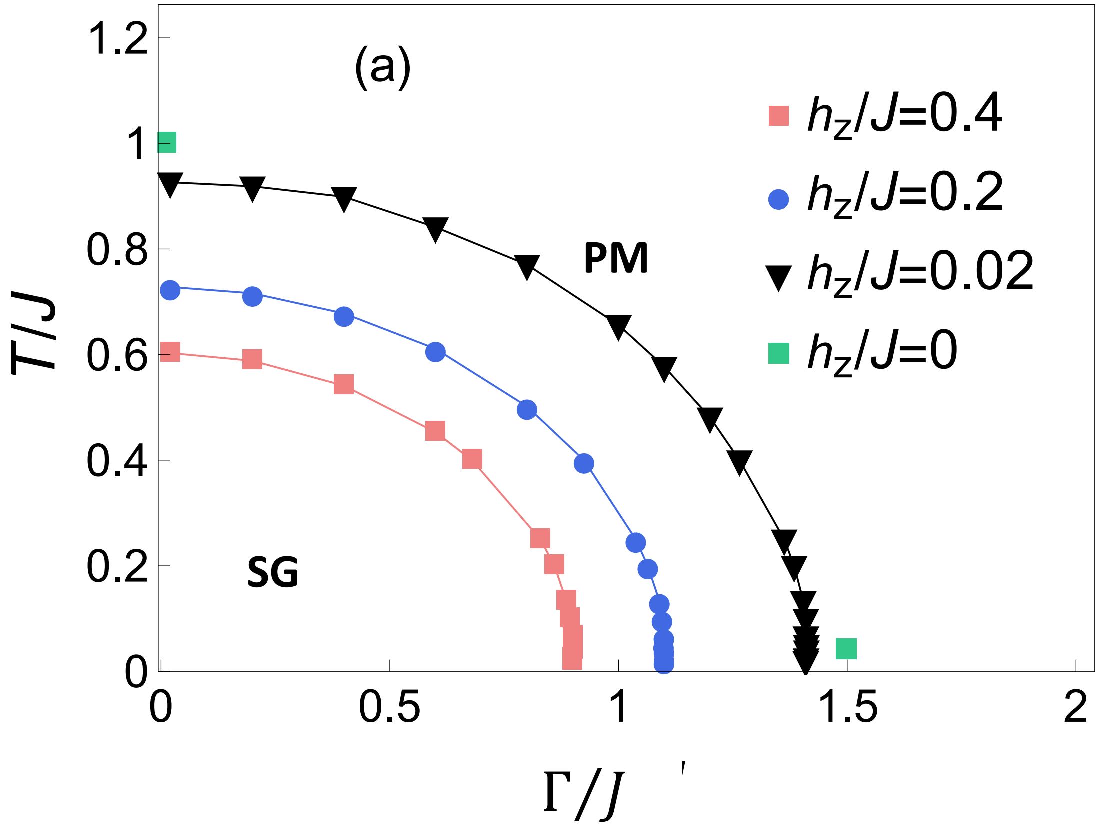
SP, Pieri, PRE (2020)

Quantum spin glasses

$$H = -\sum_{i<j} J_{i,j}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x - h_z\sum_i \sigma_i^z$$

- 1D, n.n. interactions: no frustration, no spin glass
- Finite D (e.g., 2D or 3D): spin glass, RSB vs droplet?
- Sherrington-Kirkpatrick: $J_{i,j} \sim \mathrm{Norm}[\mu = 0, \sigma = J/\sqrt{N}]$

Exact MF solution (classical), replica-symmetry breaking!



Quantum SK: **dynamical MFT**

A. Kiss et al. arXiv:2306.07337 (2023)

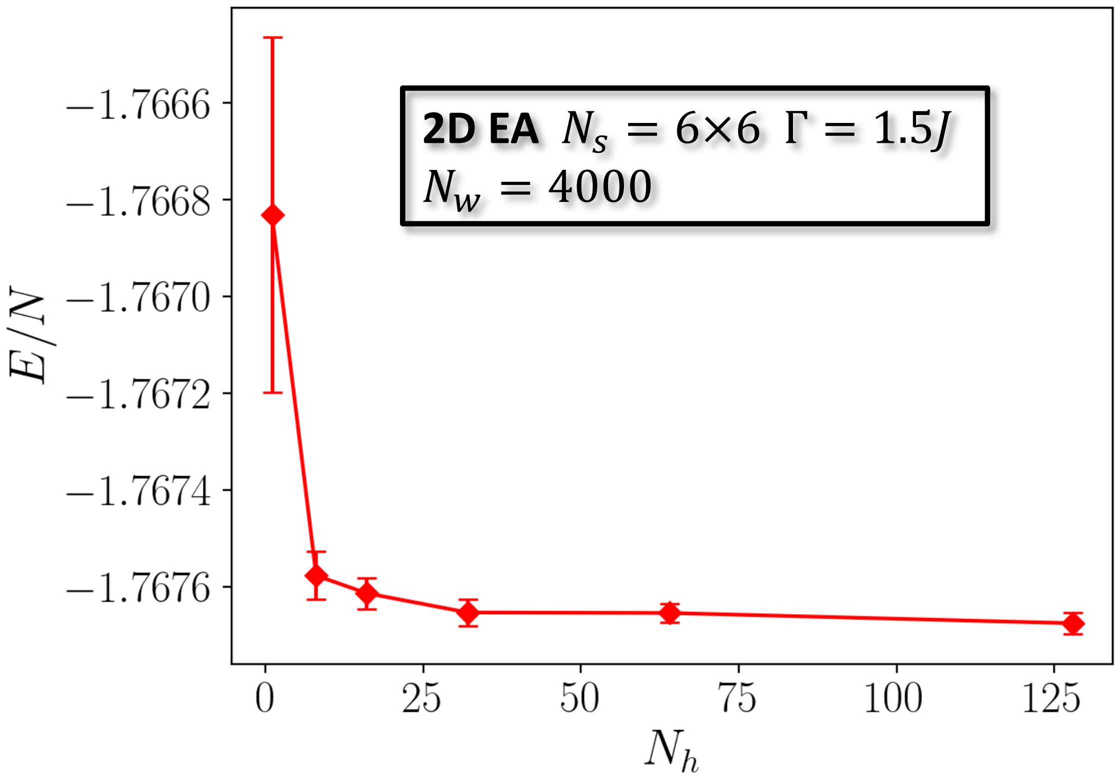
See also:

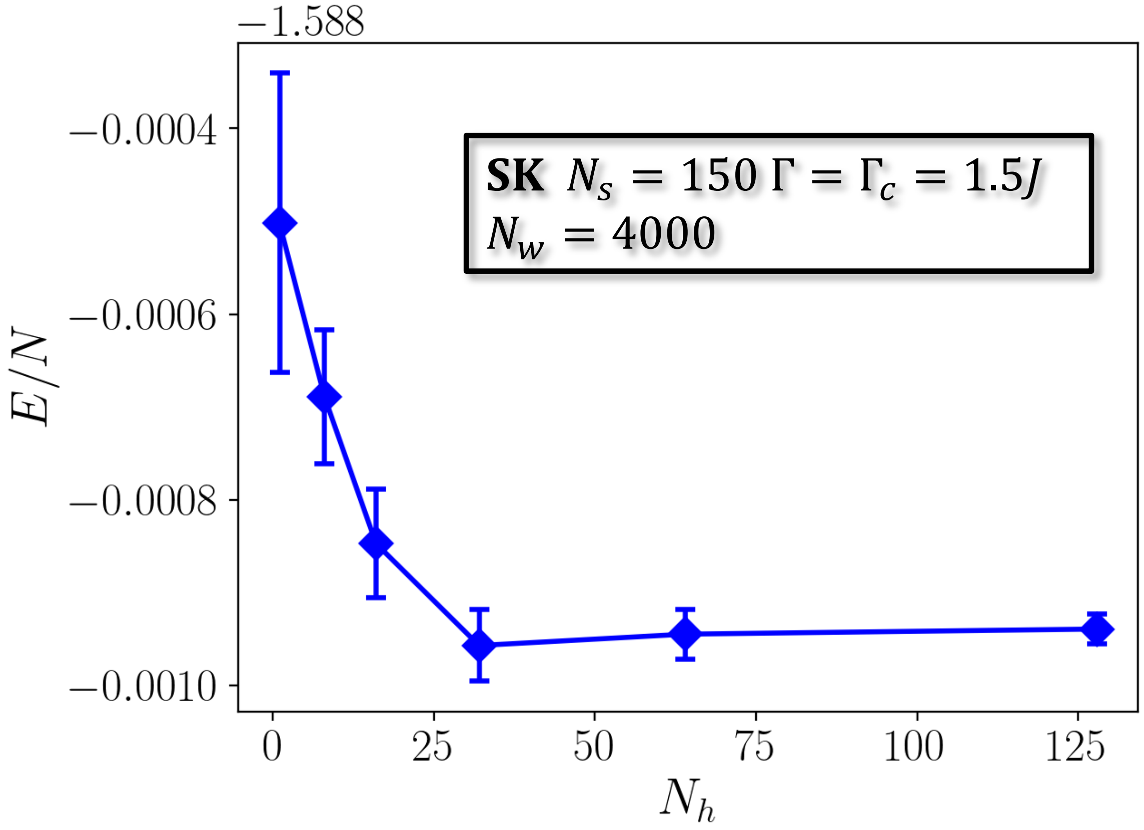
Leschke et al., PRL 127, 207204 (2021)

Schindler et al., PRL 129, 220401 (2022)

Population control bias

Self-learning DMC with N_w =4000 walkers guided by RBM with N_h hidden neurons





DMC for Quantum SK model: PRELIMINARY RESULTS!!!

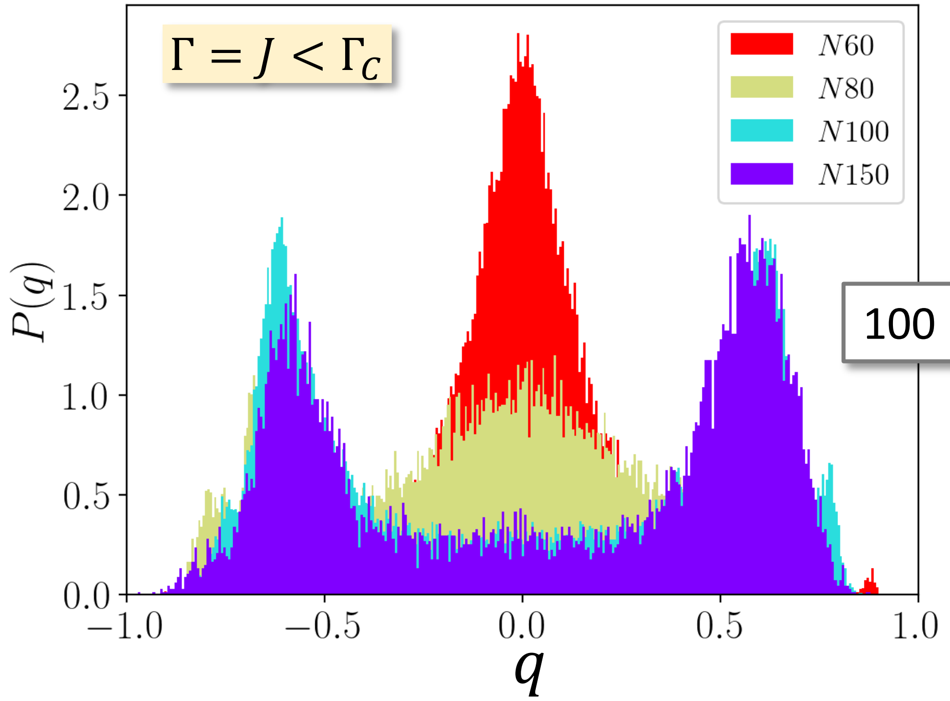
Edward-Anderson order parameter: $q_{EA} = \frac{1}{N}\sum_i \langle \sigma_i^Z \rangle^2$

Spin overlap: $q = \frac{1}{N}\sum_i \sigma_{iA}^Z \sigma_{iB}^Z$ Two copies: $H_{\text{TOT}} = H_A + H_B$ (separable RBM)

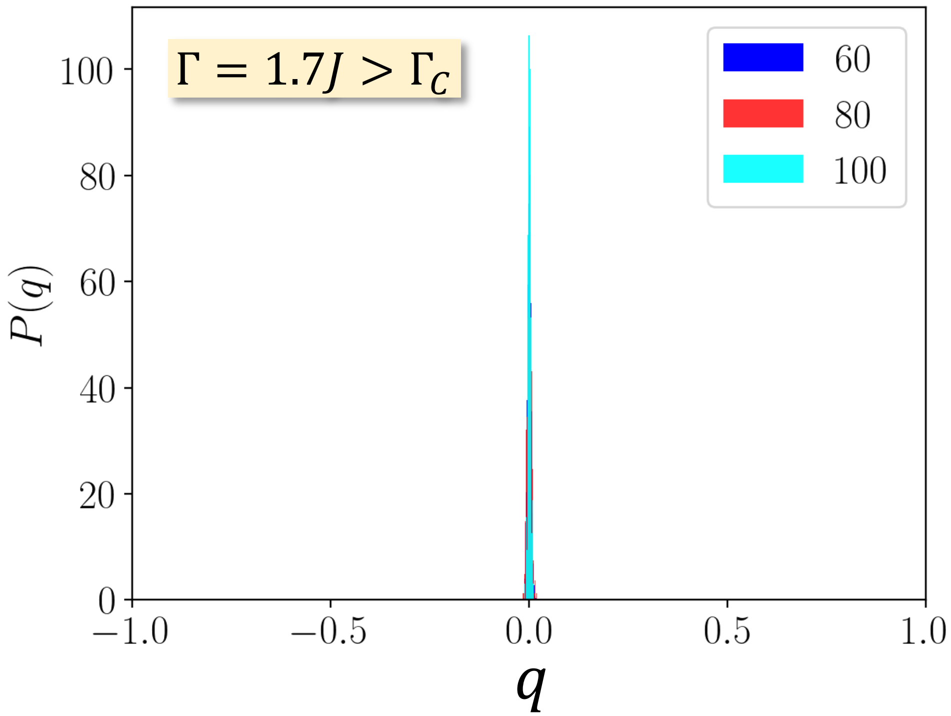
$\rightarrow \quad q_{EA} = \langle q \rangle$

Overlap distribution: Droplet picture $P(q) = \frac{1}{2}\delta(q - q_{EA}) + \frac{1}{2}\delta(q + q_{EA})$

Replica simmetry breaking $P(q = 0) > 0$



100 realizations



Summary:

- QMB physics via deep learning with NQS, DFT, supervised learning.
- Scalability matters.
- Sign problem is not the only problem.
- Promising results with neural DMC for quantum spin glasses.

- Scriva, Costa, McNaughton, SP, SciPost Phys. 15, 018 (2023)
- Costa, Fazio, SP, Phys. Rev. B (2023)
- Costa, Scriva, Fazio, SP, Phys. Rev. E 106 (4), 045309 (2022)
- Mujal, Martínez Miguel, Polls, Juliá-Díaz, S Pilati, SciPost Phys. 10 (3), 073 (2021)
- Saraceni, Cantori, SP, Phys. Rev. E 102, 033301 (2020)
- McNaughton, Milošević, Perali, SP, Phys. Rev. E 101 (5), 053312 (2020)
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- Inack, Giudici, Parolini, Santoro, SP, Phys. Rev. A 97 (3), 032307 (2018)