SOLVING 2D QUANTUM MATTER WITH NEURAL QUANTUM STATES

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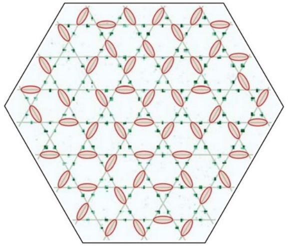
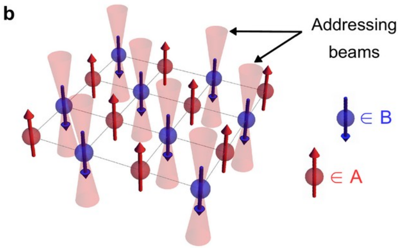
INTERACTING 2D QUANTUM MATTER

CURRENT FRONTIER IN EXPERIMENT

RYDBERG ATOM ARRAYS

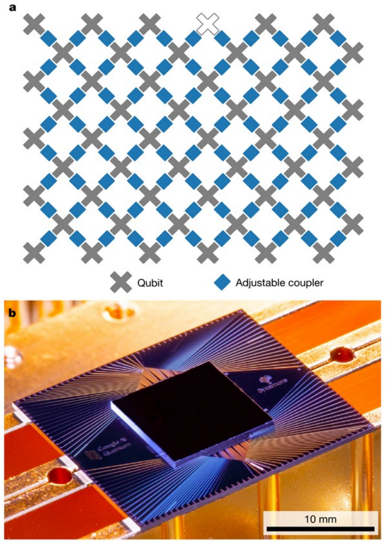


Semeghini *et al.*, Science '21



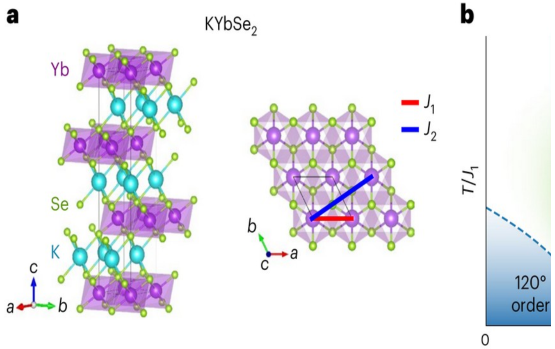
Chen *et al.*, Nature '23

SUPERCONDUCTING QUANTUM PROCESSORS



Arute *et al.*, Nature '19

SOLID-STATE SYSTEMS



Scheie *et al.*, Nature Physics '23

INTERACTING 2D QUANTUM MATTER

SOLVING THE 2D QUANTUM PROBLEM THEORETICALLY IS DIFFICULT

COMPLEXITY IS A MATTER OF THE METHOD

EXACT DIAGONALIZATION	TENSOR NETWORKS	QUANTUM MONTE CARLO
Curse of dimensionality	Entanglement Contraction complexity	Sign problem

NEURAL QUANTUM STATE (NQS)

NOVEL CLASS OF VARIATIONAL WAVE FUNCTIONS

QUANTUM STATES IN COMPUTATIONAL BASIS

$$|\psi\rangle = \sum_s \psi_s |s\rangle$$

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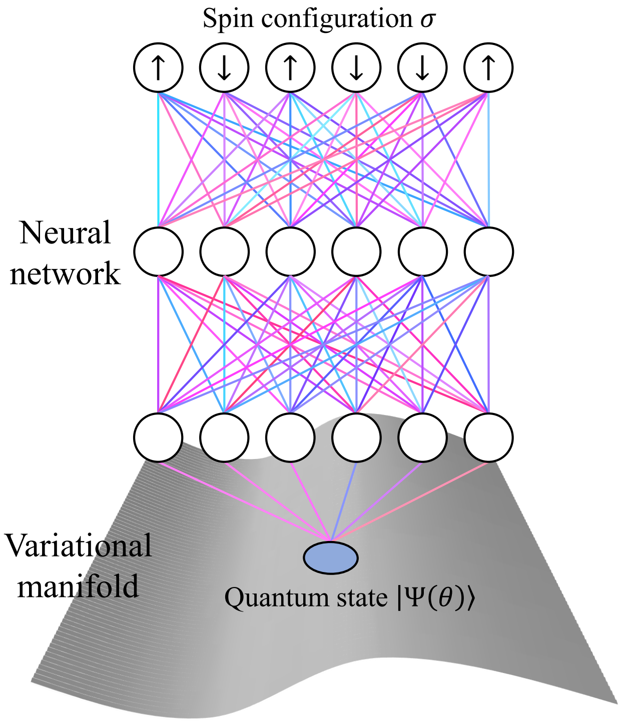
encode into an artificial neural network (ANN)

Carleo & Troyer, Science '17



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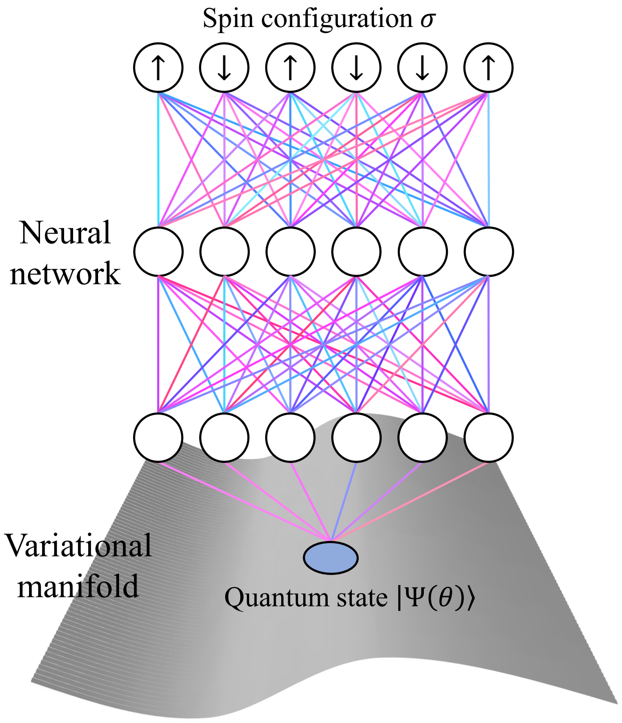

UNIVERSAL APPROXIMATION THEOREM

Numerically exact approach

Convergence parameter: size of ANN

GROUND STATES OF COMPLEX 2D QUANTUM MATTER

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GROUND STATES

STOCHASTIC RECONFIGURATION (SR)

NQS IS A VARIATIONAL WAVE FUNCTION

$$|\psi(\theta)\rangle = \sum_s \psi_s(\theta)|s\rangle$$

GROUND STATE: Minimize variational energy

$$\mathcal{E}(\theta) = \frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle}$$

SR: Imaginary time evolution (from random initial condition)

$$S\dot{\theta} = F \qquad \Rightarrow \dot{\theta} = S^{-1}F$$

KEY CHALLENGE IN SR

MATRIX INVERSION

$$S\dot{\theta} = F \qquad \Rightarrow \dot{\theta} = S^{-1}F$$

CHALLENGE: $S \in \mathbb{C}^{N_p \times N_p}$ N_p: number of variational parameters

Computational complexity for inversion: $\mathcal{O}(N_p^3)$

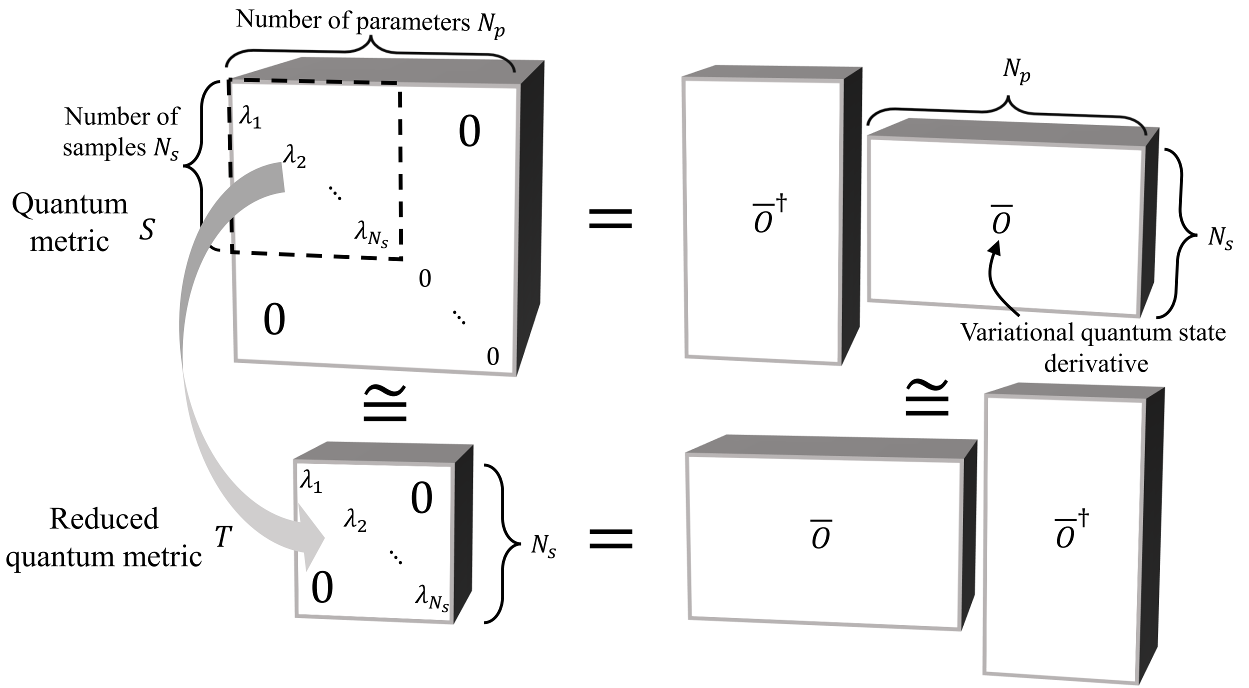
LIMITS CRITICALLY THE REACHABLE ANN SIZES

SOLUTION: Minimum-step stochastic Reconfiguration Chen & **MH** Nature Phys. '24

Reducing the computational complexity: $\mathcal{O}(N_p)$

A NEW OPTIMIZER: MINSR

NEURAL TANGENT KERNEL

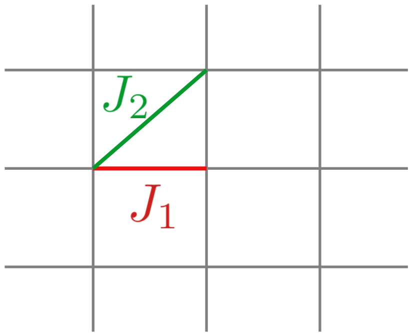


$$\delta\theta = S^{-1}\overline{O}^\dagger\overline{\epsilon} \quad \text{with}\, S = \overline{O}^\dagger\overline{O} \quad \rightarrow \quad \delta\theta = \overline{O}^\dagger T^{-1}\overline{\epsilon} \quad \text{with}\, T = \overline{O}\,\overline{O}^\dagger$$

ANTIFERROMAGNETIC HEISENBERG MODEL

SQUARE LATTICE

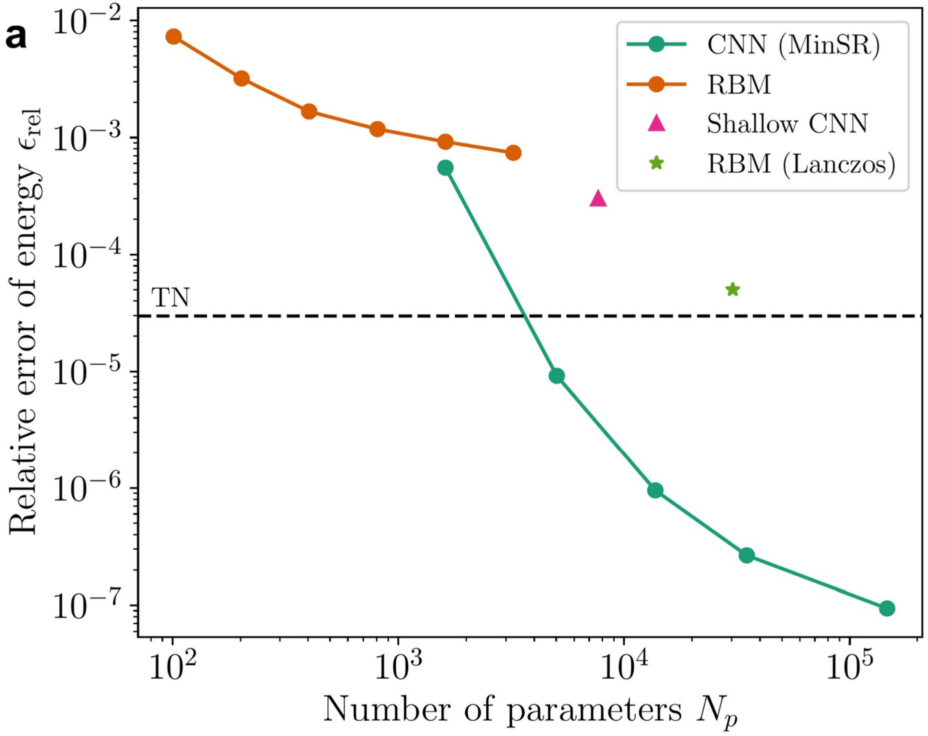
$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



HEISENBERG MODEL

APPROACHING MACHINE PRECISION

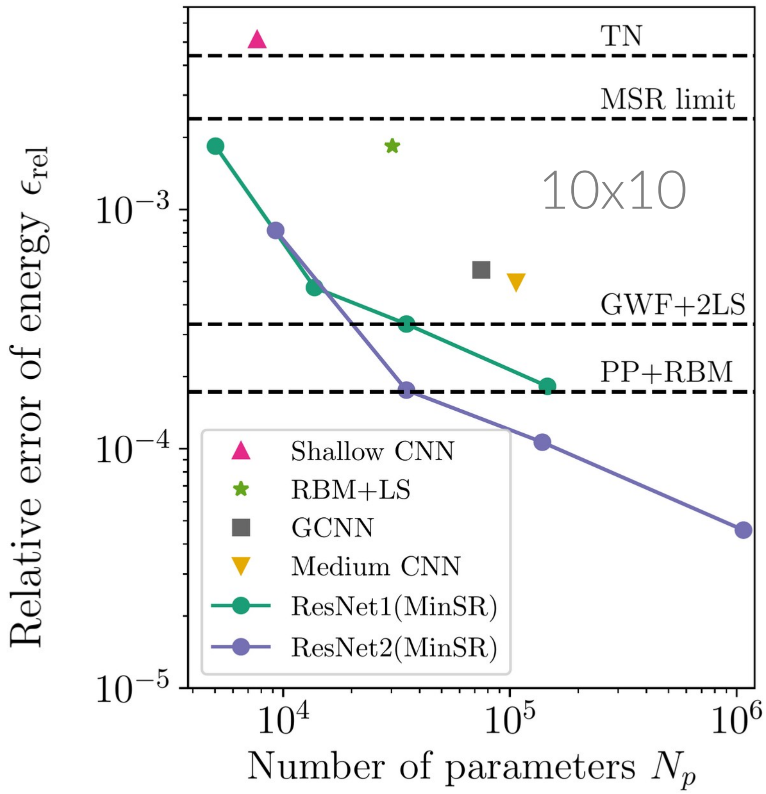
10x10

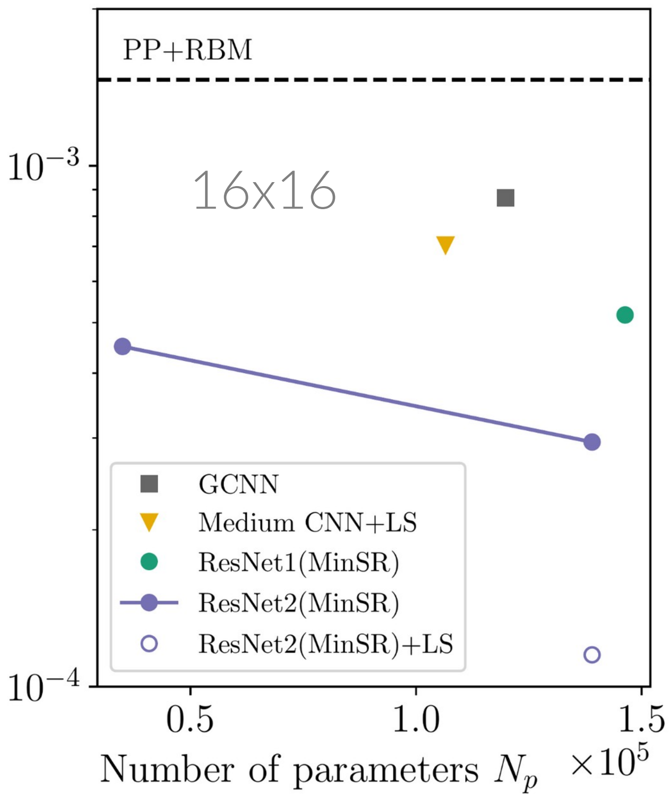


Chen & MH Nature Phys. '24

J1-J2 MODEL

FRUSTRATED POINT J2/J1=1/2





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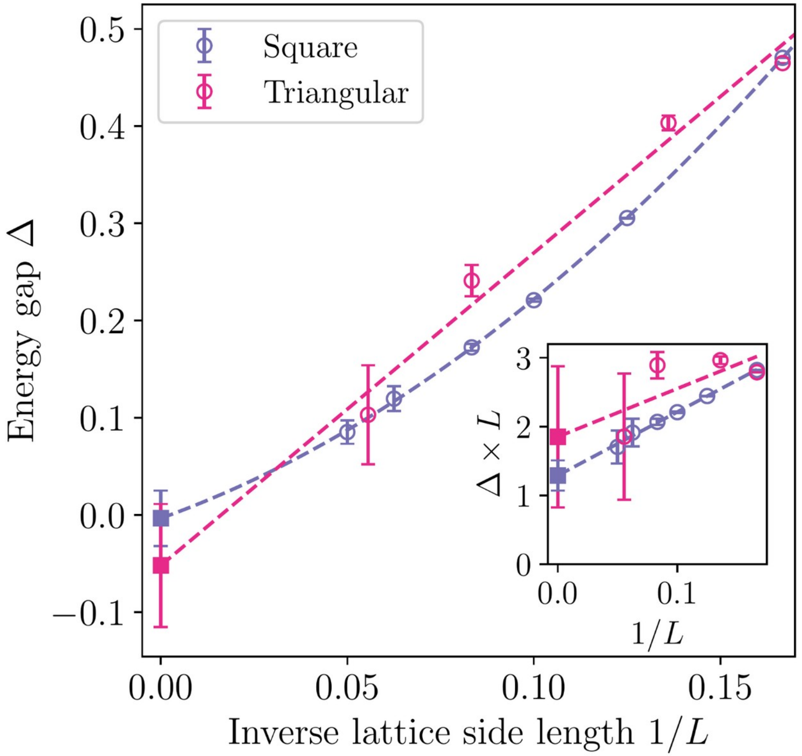
MEASURING GAPS IN THE J1-J2 MODEL

SQUARE AND TRIANGULAR LATTICES

GAPS
Measured between S=1 and S=0

SQUARE LATTICE
J2/J1=1/2
M-point at k=(π,π)

TRIANGULAR LATTICE
J2/J1=1/8
k=(4π/3,0)

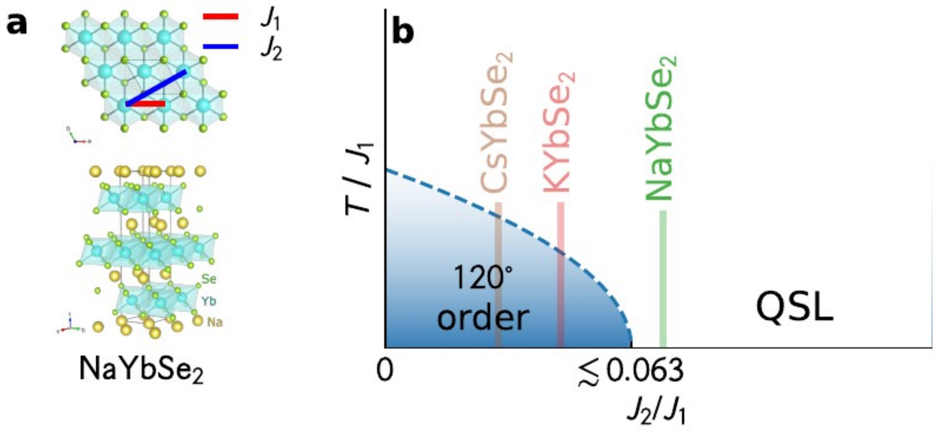


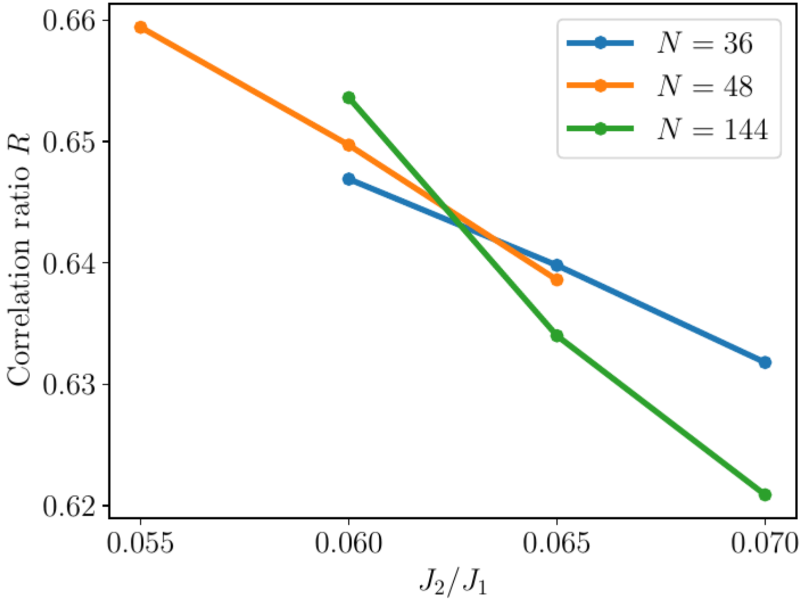
Chen & MH Nature Phys. '24

ACCURATE ESTIMATION OF PHASE DIAGRAMS

J1-J2 MODEL ON THE TRIANGULAR LATTICE

$$R = 1 - S(\mathbf{Q}_{\text{peak}} + \delta\mathbf{q})/S(\mathbf{Q}_{\text{peak}})$$





Scheie, **MH** et al. arXiv '24

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