Time-Dependent Neural Quantum States

Giuseppe Carleo

CQSL: Computational Quantum Science Lab

QSE: Center for Quantum Science and Engineering

Institute of Physics, EPFL

Computational Quantum Science Lab.

01.

Out-of-Equilibrium.

Out of Equilibrium Protocols and Questions

Quantum Quenches

$$e^{-i\mathcal{H}t}|\Psi\rangle$$

Unitary dynamics of
a pure state

Driving Hamiltonian

$$\mathcal{T}e^{-i\int_0^t dt'\mathcal{H}(t')}\,|\Psi\rangle$$

Unitary dynamics with
a time-varying Hamiltonian

Fundamental Questions

How to reconcile Schrödinger with Boltzmann?

$$\mathrm{Tr}\, e^{-\frac{\mathcal{H}}{k_b T}}$$ *Which Temperature?*

How fast equilibrium is reached?

Defect production across a phase Transition

Consequences for Adiabatic State Preparation?

A Challenge in Computational Physics

Exact Approaches

Exact Diagonalization/ Lanczos

Limited to small systems

Path-Integral Monte Carlo

Severe Phase Problem

Ill-conditioned inversion

Quantum Computing

Strongly Affected by Noise

Error-Corrected Hardware Likely Needed to Access Regimes Truly Hard/Interesting for Physics

Tensor Network Methods

DMRG / Matrix Product States / PEPS

Mostly limited to 1D/ short time scales

Mostly lattice systems

Mean-Field Dynamics

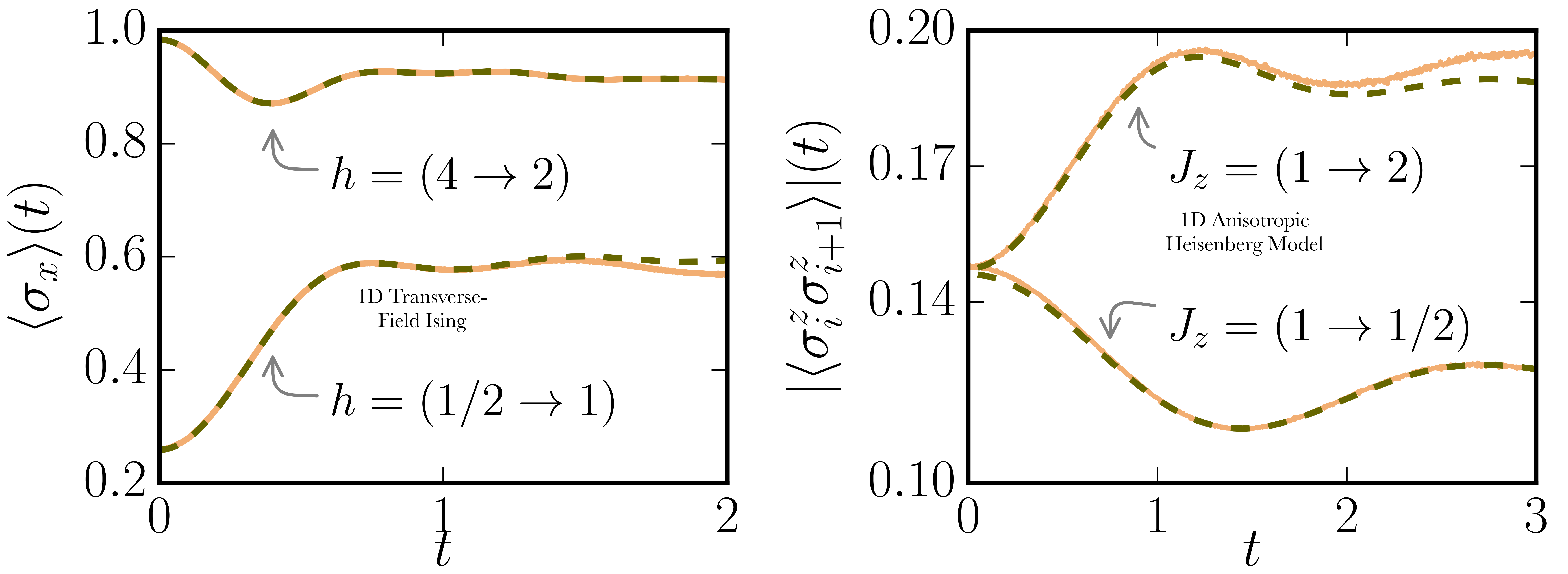
No limitations on geometry/timescales

Poor qualitative and quantitative accuracy

02.

Spin Dynamics.

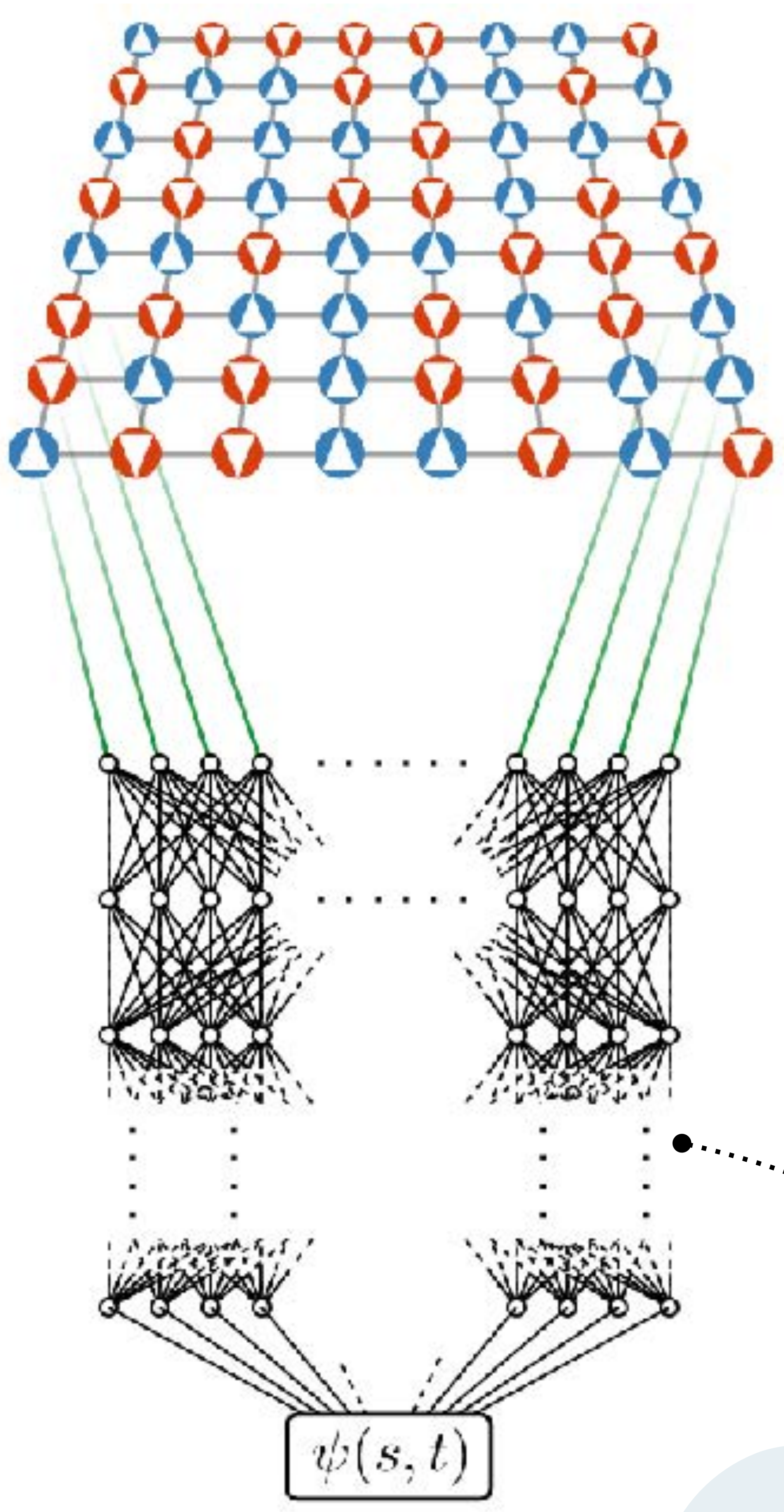
First Results with Time-Dependent RBM

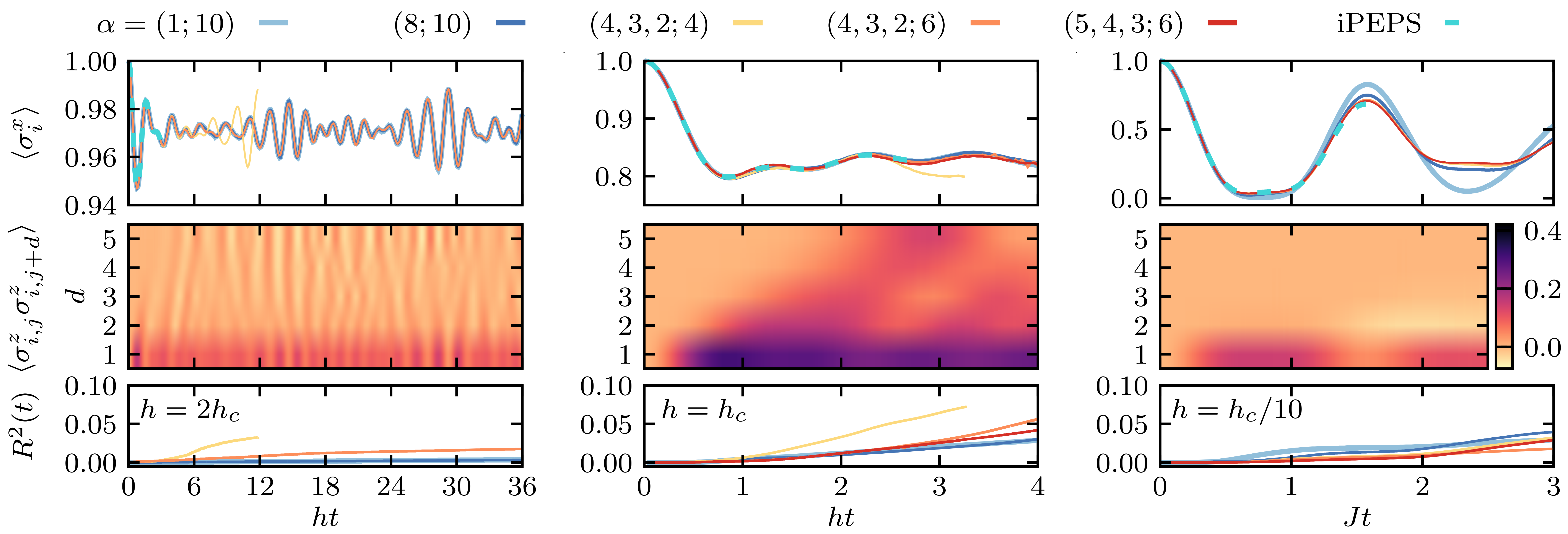


$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_j \sigma_j^x$$

Carleo and Troyer
Science 355, 602 (2017)

Explorations of 2D Quench Dynamics



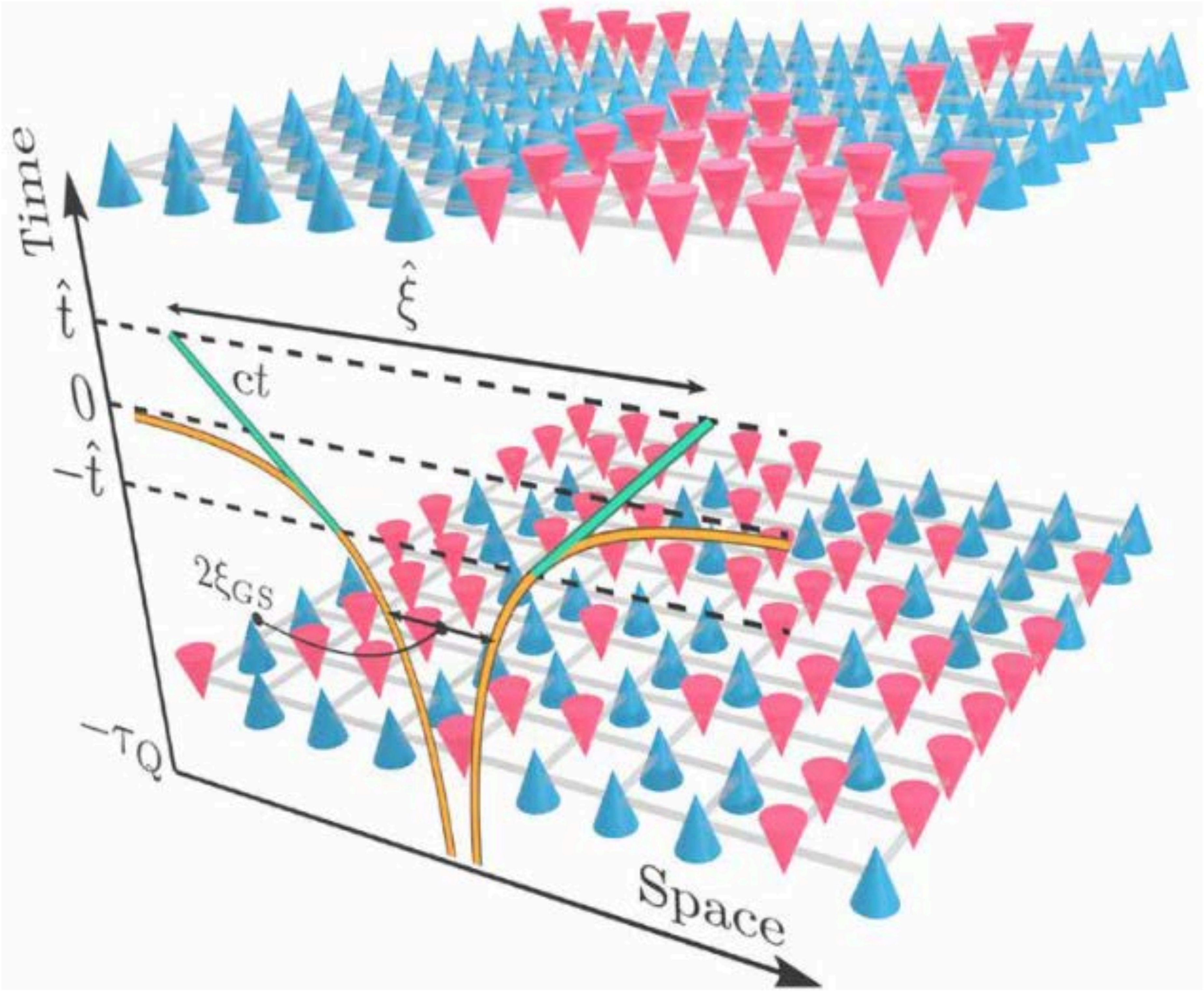


Two-Dimensional Convolutional Neural Networks

$$H = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - h\sum_j \sigma_j^x$$

Schmitt and Heyl, Phys. Rev. Lett. 125, 100503 (2020)

Time-Dependent Hamiltonians



$$H(t) = -J(t) \sum_{\langle m,n \rangle} \sigma_m^z \sigma_n^z - g(t) \sum_{m=1}^{L^2} \sigma_m^x$$

Kibble-Zurek mechanism

Defect formation near quantum phase transitions

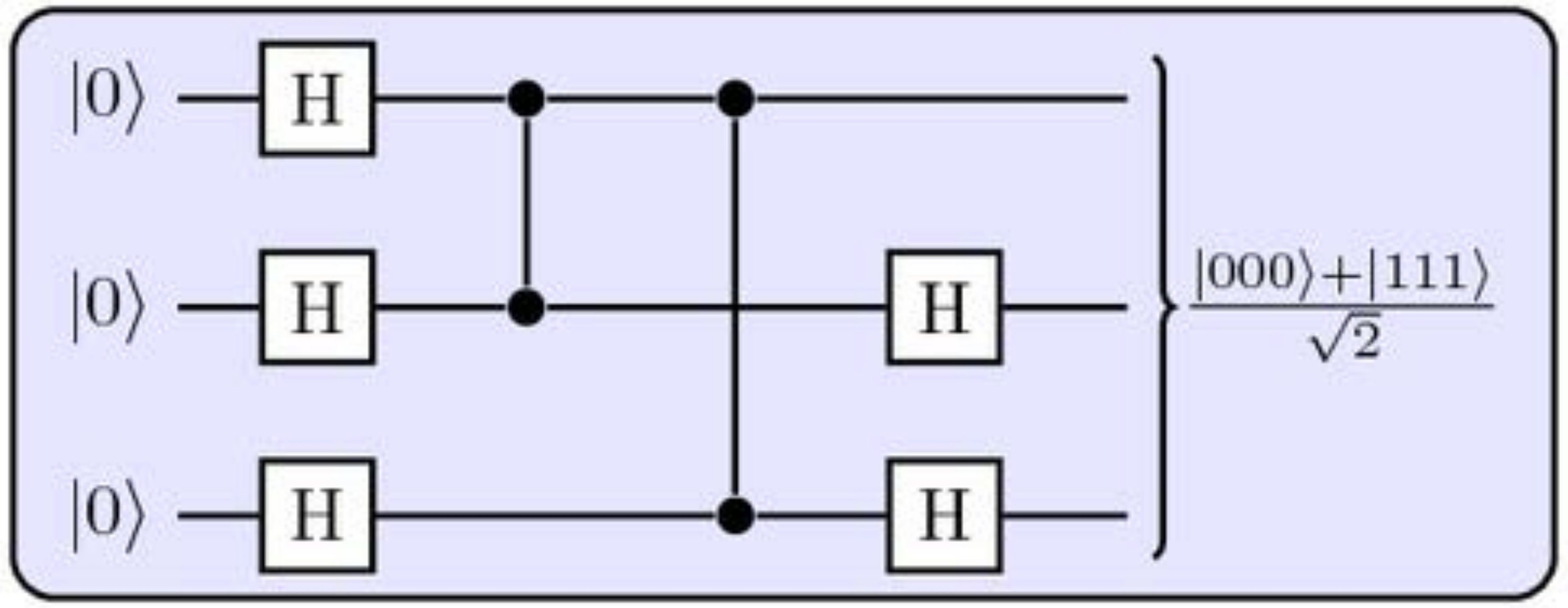
Violation to the mechanism found in 2D

Schmitt, Rams, Dziarmaga, Heyl, and Zurek
Science Advances 8, abl6850 (2022)

03.

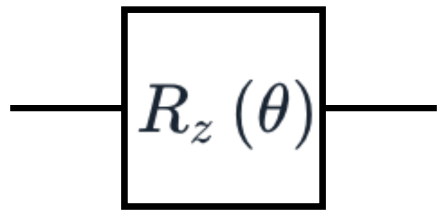
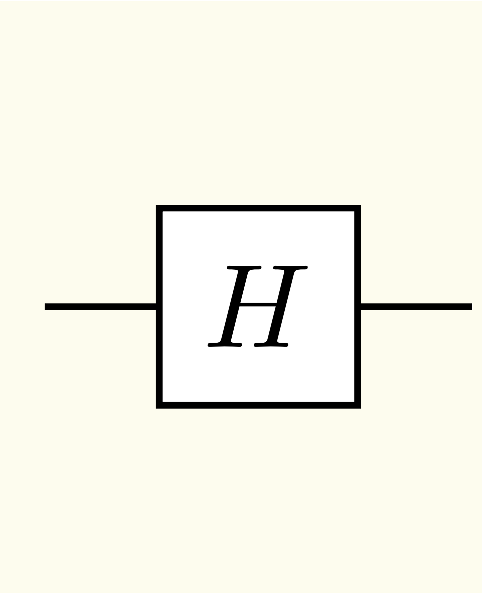
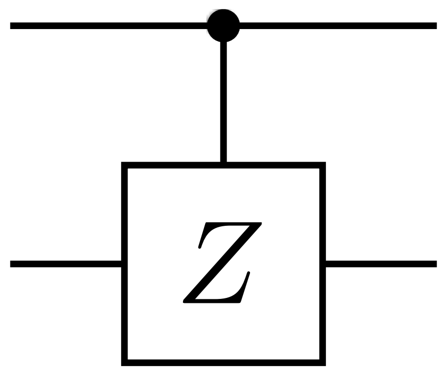
Simulating Quantum Circuits.

Quantum Circuits and Universal Gates

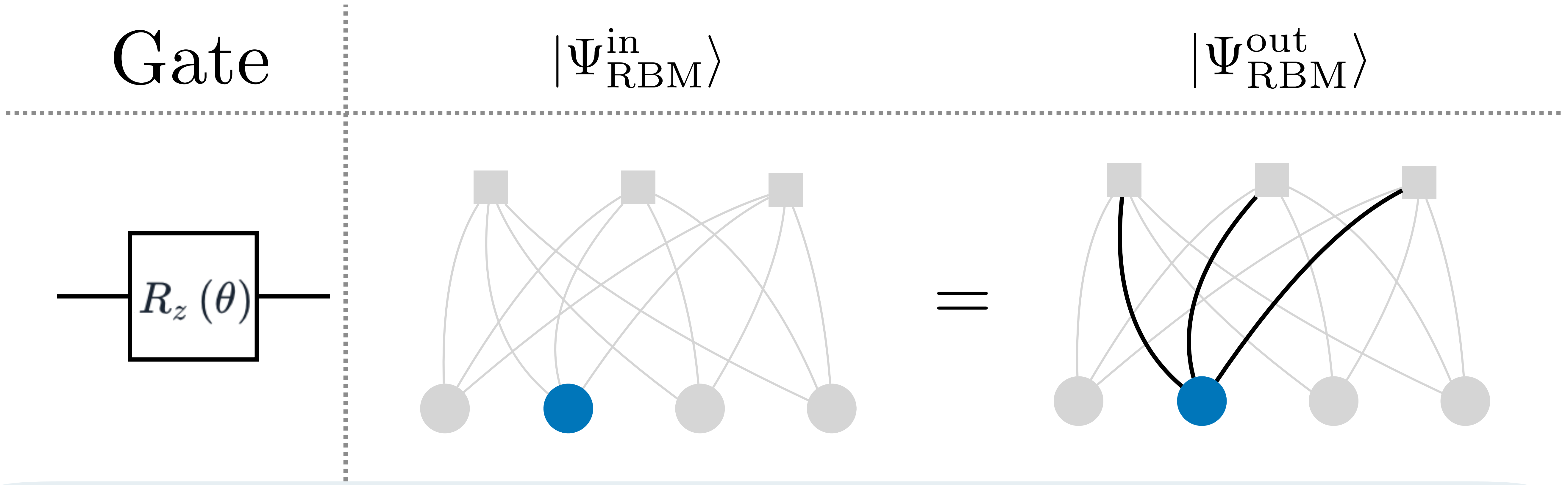


Elementary Gates

Any Quantum Circuit Can be Decomposed Into the Action of Few Elementary Gates

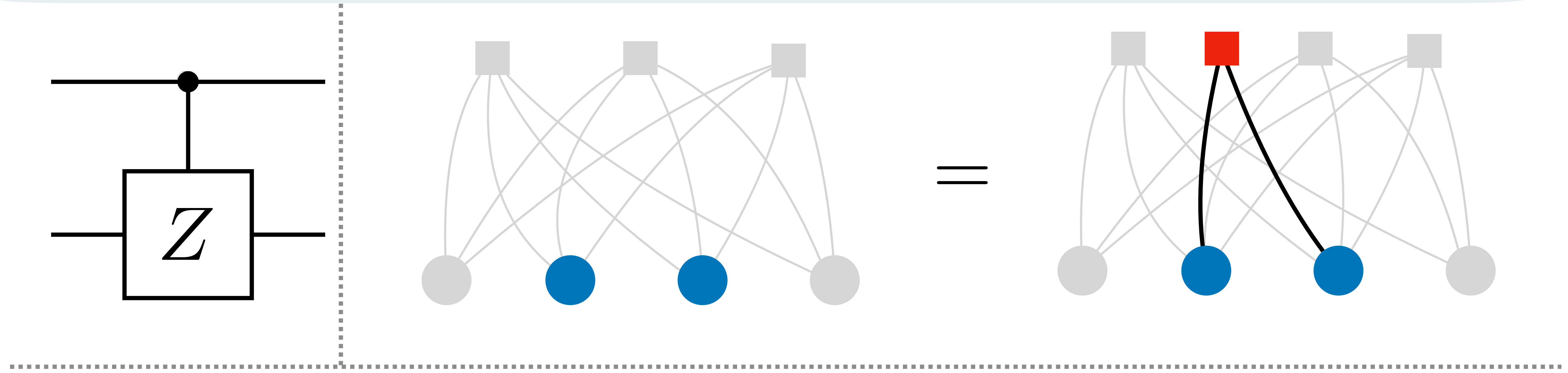
	Gate	
Rz Rotations		$\begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}$
Hadamard		$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
Controlled Z		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$

Applying Gates to a RBM



Can Be Performed Exactly

Give Rise To Local Modifications of Weights

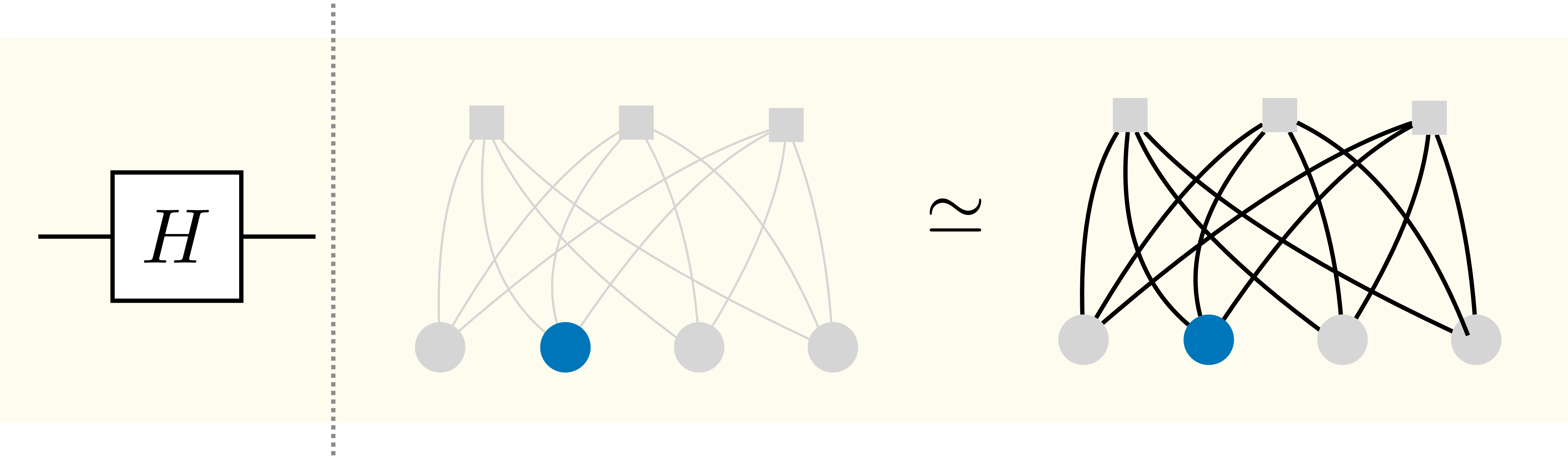


Many Other Gates Can Be Done Exactly

All Diagonal Gates, All Pauli Gates,...

Jonsson, Bauer, and Carleo
arXiv:1808.05232 (2018)

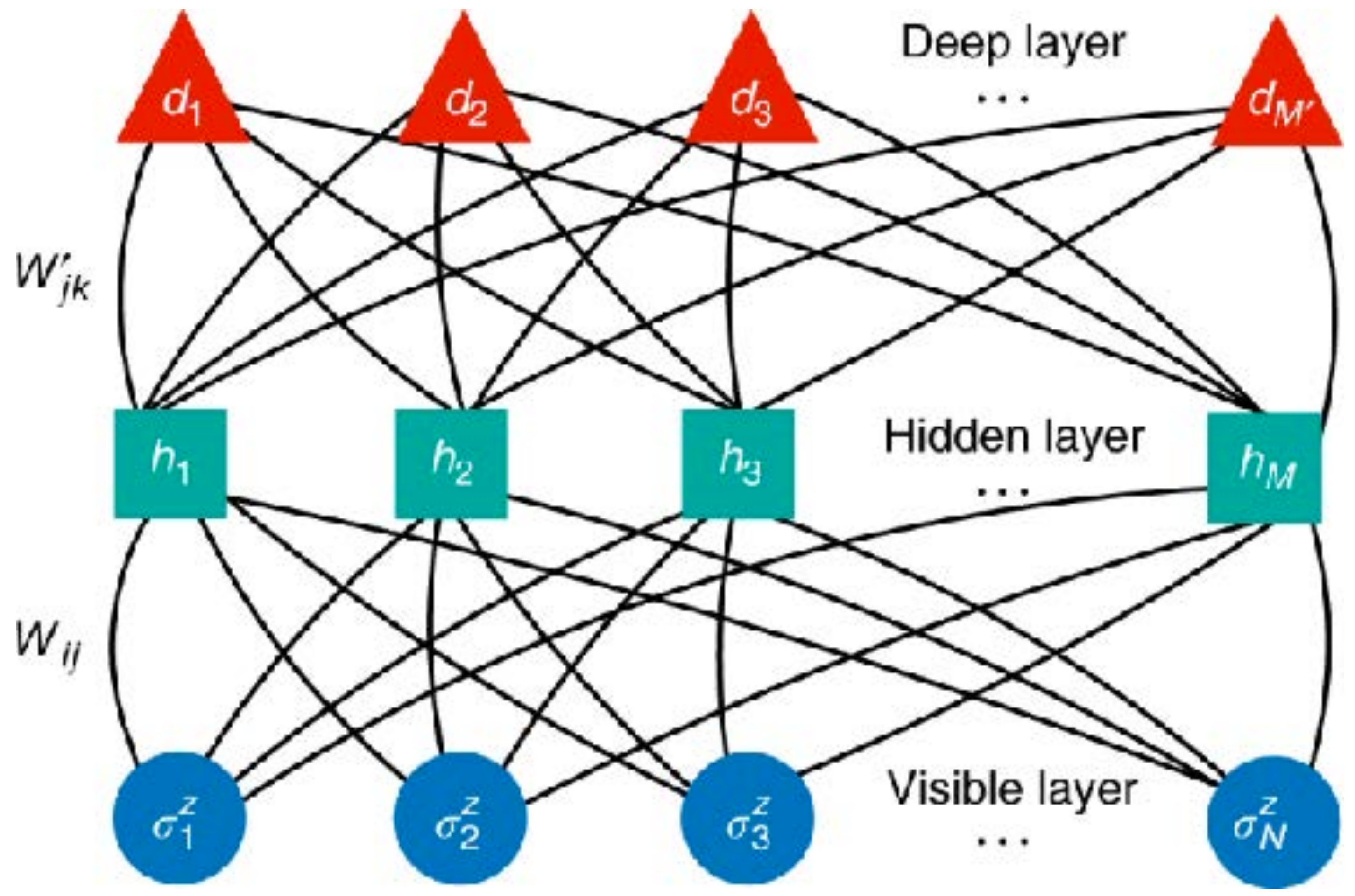
The Hadamard Gate is Hard



Mathematical Problem

The Sum of Two RBMs is not an RBM, in general, it is a DBM

Jonsson, Bauer, and Carleo
arXiv:1808.05232 (2018)



Approximating the Hadamard Gate

$$|\phi\rangle = H|\psi_\theta\rangle$$

$$|\psi_{\theta'}\rangle \simeq |\phi\rangle$$

$$\mathcal{D}(\phi, \psi_{\theta'}) = 1 - F(\phi, \psi_{\theta'})$$

Minimize infidelity

Jonsson, Bauer, and Carleo
arXiv:1808.05232 (2018)

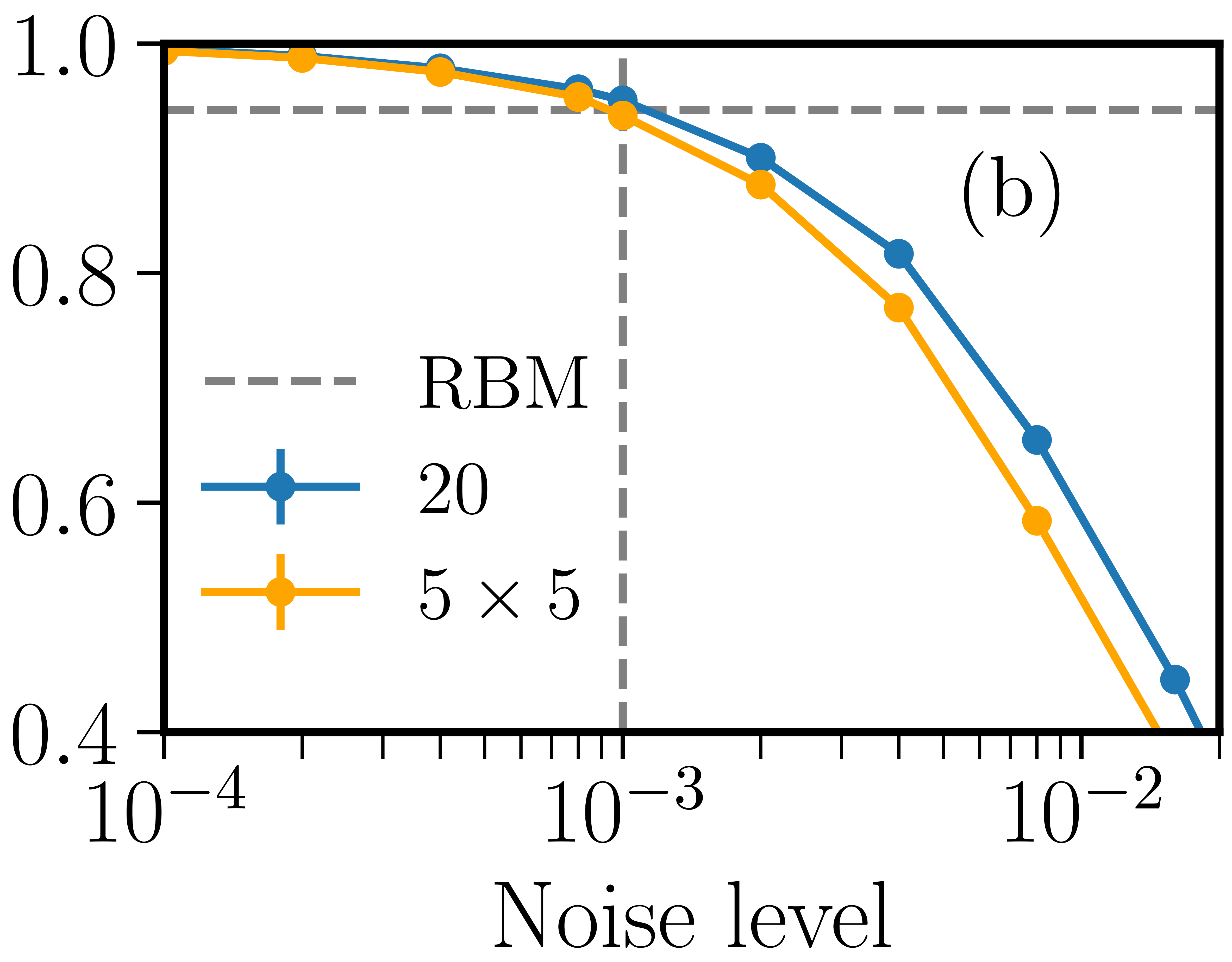
Infidelity as a Stochastic Average

$$F(\psi,\phi) = \frac{|\langle\phi|\psi\rangle|^2}{\langle\phi|\phi\rangle\langle\psi|\psi\rangle} = \left\langle \frac{\phi}{\psi} \right\rangle_{\psi} \left\langle \frac{\psi}{\phi} \right\rangle_{\phi}$$

Statistical Expectation Values

$$\frac{\partial \mathcal{D}}{\partial \theta_l^*} = \left\langle \frac{\phi}{\psi_\theta} \right\rangle_{\psi_\theta} \left\langle \frac{\psi_\theta}{\phi} \right\rangle_{\phi} \left[\langle \mathcal{O}_k^* \rangle_{\psi_\theta} - \frac{\left\langle \frac{\phi}{\psi_\theta} \mathcal{O}_k^* \right\rangle_{\psi_\theta}}{\left\langle \frac{\phi}{\psi_\theta} \right\rangle_{\psi_\theta}} \right]$$

Variational Error Versus Hardware Error

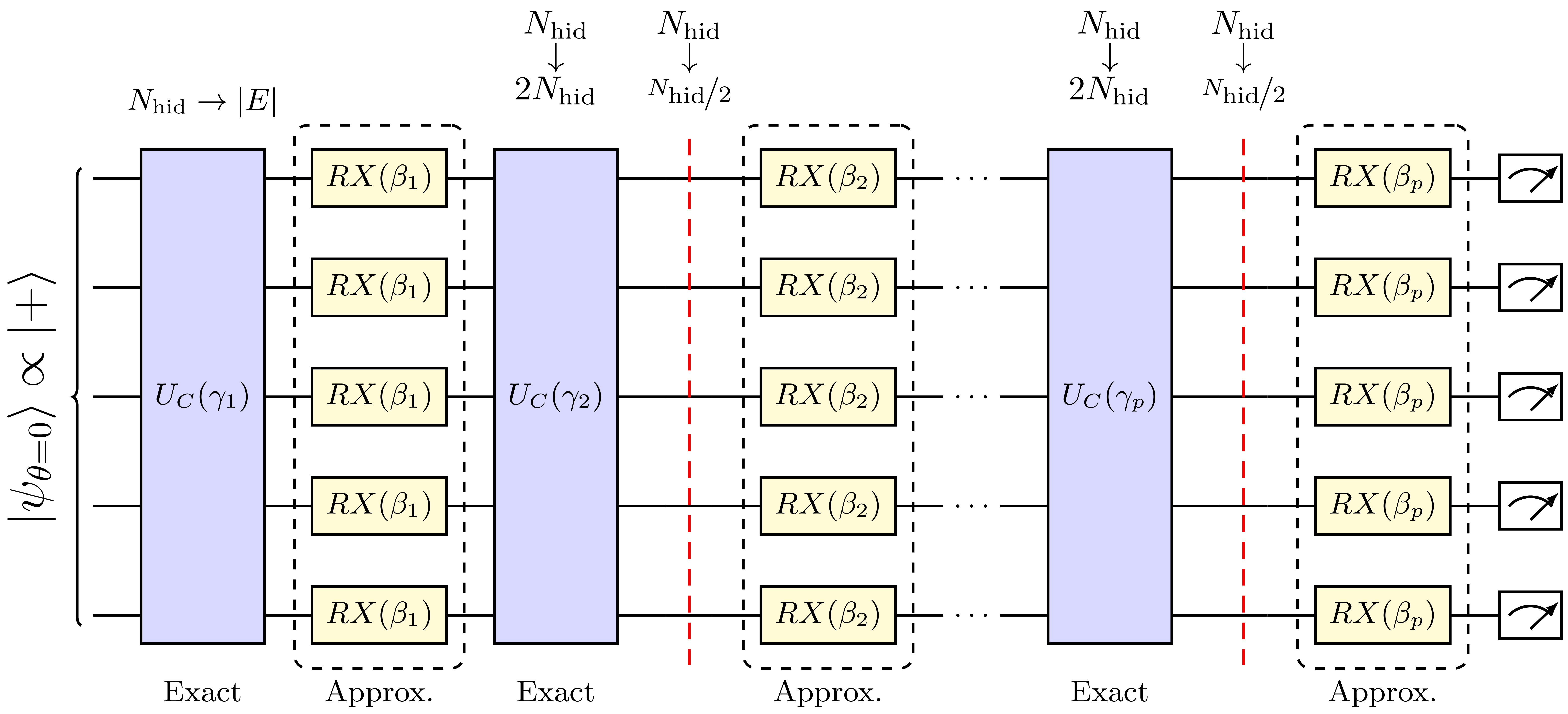


Comparing Variational Error with Depolarization Noise

Jonsson, Bauer, and Carleo
arXiv:1808.05232 (2018)

see also
Zhou et al PRX 10, 041038 (2020)

Simulating QAOA



$$U_C(\gamma) = e^{-i\gamma\mathcal{C}} = \prod_{i,j \in E(G)} e^{-i\gamma w_{ij} Z_i Z_j}$$

$$U_B(\beta) = \prod_{i \in G} e^{-i\beta X_i}$$

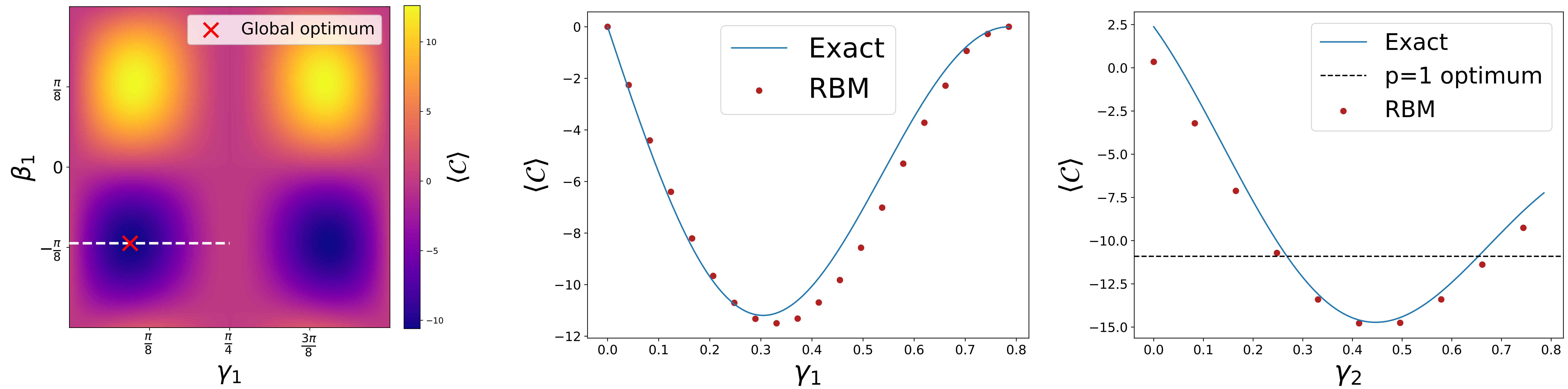
Medvidovic, and Carleo

Npj Quantum Info 7, 101 (2021)

Computational Quantum Science Lab.

Columbia University in the City of New York

Benchmarks

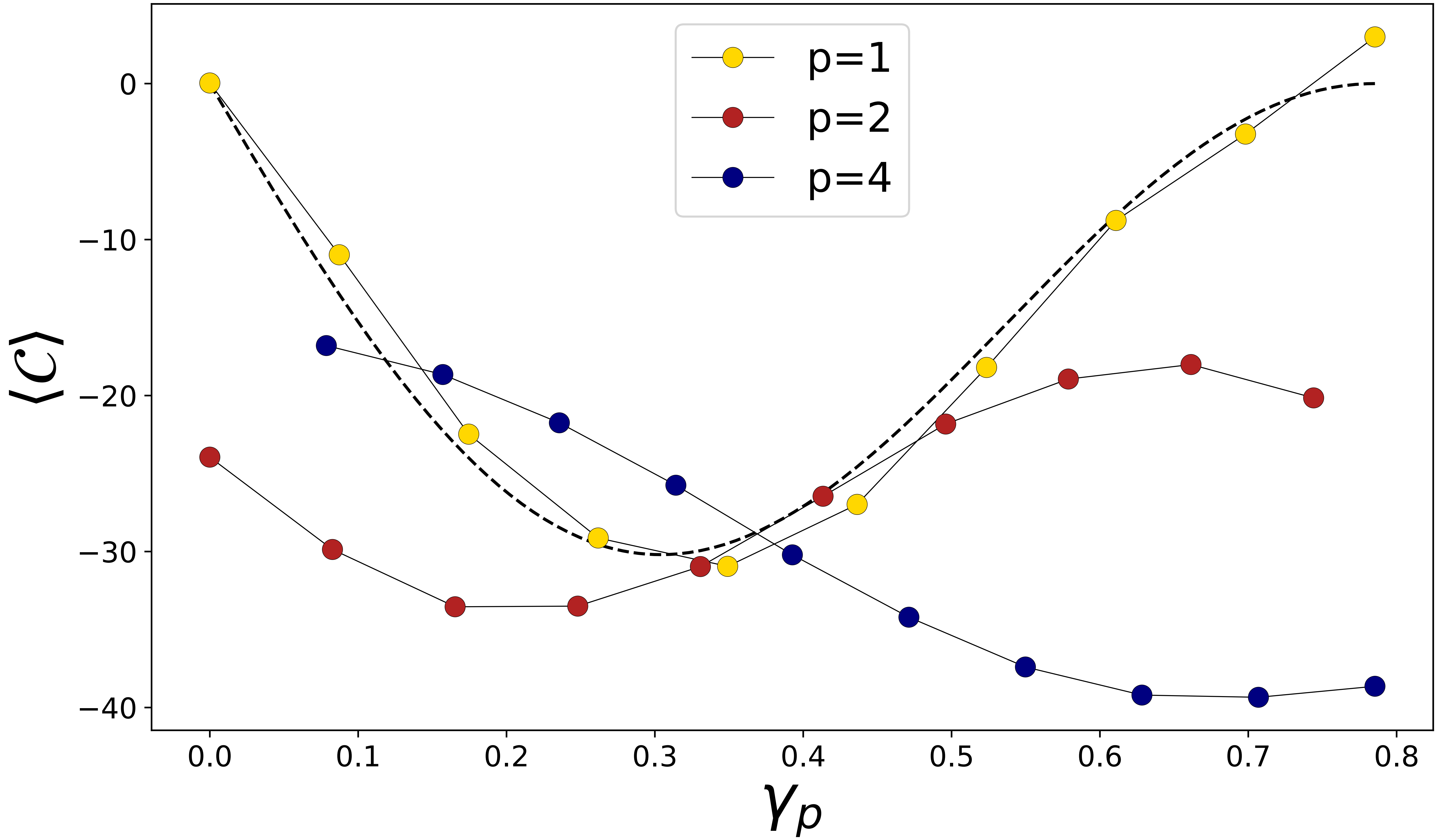


20 Qubits

3-Random Regular Graph

Medvidovic, and Carleo
Npj Quantum Info 7, 101 (2021)

Scaling to 54 Qubits



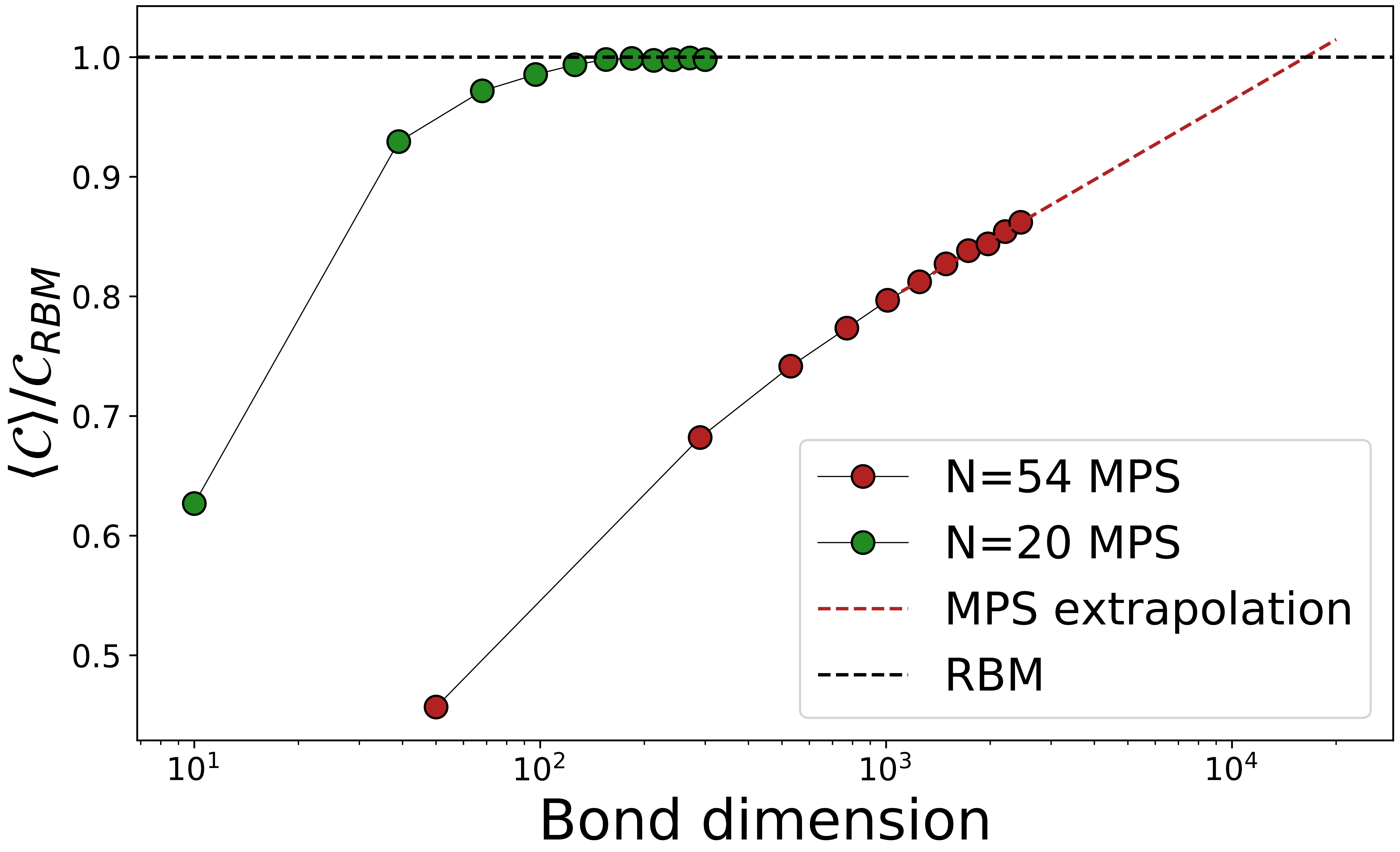
4 Layers

324 RZZ Gates

216 RX Gates

Medvidovic, and Carleo
Npj Quantum Info 7, 101 (2021)

Comparison With Matrix Product States



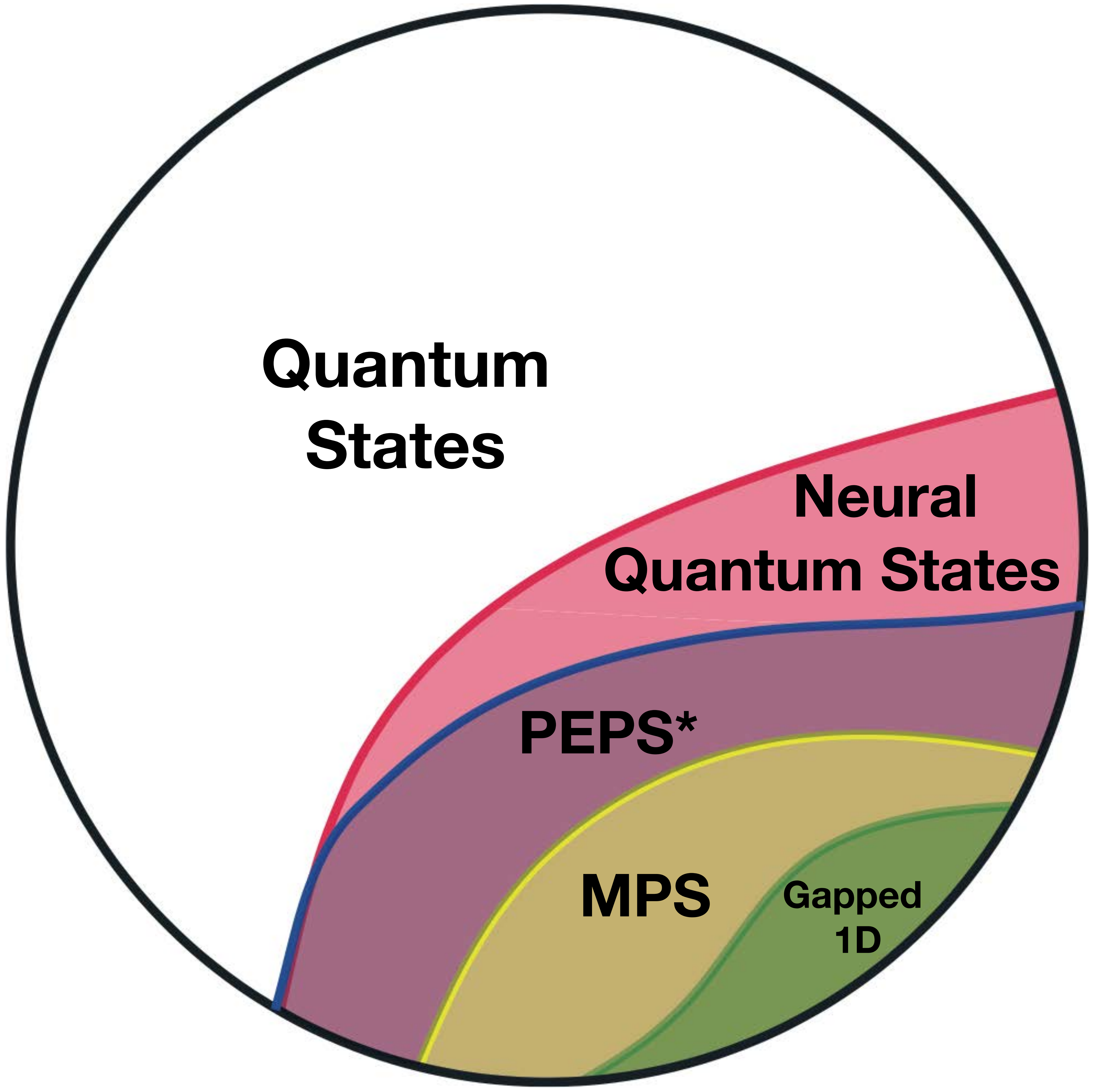
Estimated Bond Dimension of ~10^4 for similar accuracy

Remark: competitive tensor contraction schemes on similar problems typically yield only cost function not samples/ wave functions like for MPS/NQS

Medvidovic, and Carleo
Npj Quantum Info 7, 101 (2021)

General Representation Diagram

Sharir, Shashua, and Carleo
Phys. Rev. B 106, 205136 (2022)



04.

Unitary Dynamics with Measurements.

A Problem with Stochastic Estimators?

$$F_k = \frac{\langle \partial_{\theta_k} \Psi_\theta | \mathcal{H} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} - \frac{\langle \partial_{\theta_k} \Psi_\theta | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \frac{\langle \Psi_\theta | \mathcal{H} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle}$$

$$S_{kk'} = \frac{\langle \partial_{\theta_k} \Psi_\theta | \partial_{\theta_{k'}} \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} - \frac{\langle \partial_{\theta_k} \Psi_\theta | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \frac{\langle \Psi_\theta | \partial_{\theta_{k'}} \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle}$$

$$F_k^{\mathrm{MC}} = \mathbb{E}_\Pi[O_k^*(\sigma) E_{\mathrm{loc}}(\sigma)] - \mathbb{E}_\Pi[O_k^*(\sigma)]\mathbb{E}_\Pi[E_{\mathrm{loc}}(\sigma)]$$

$$S_{kk'}^{\mathrm{MC}} = \mathbb{E}_\Pi[O_k^*(\sigma)(O_{k'}(\sigma)] - \mathbb{E}_\Pi[O_k^*(\sigma)]\mathbb{E}_\Pi[O_{k'}(\sigma)]$$

Assumption behind Estimators

Gradients of state vanish if state vanishes

Sinibaldi, Giuliani, Carleo, and Vicentini
In Preparation (2023)

Bias Term is Non-Negligible In Some Applications

$$F_k = \underbrace{\sum_{\sigma|\Psi_\theta(\sigma)=0} \frac{\langle \partial_{\theta_k} \Psi_\theta|\sigma\rangle \langle \sigma|\mathcal{H}|\Psi_\theta\rangle}{\langle \Psi_\theta|\Psi_\theta\rangle}}_{\text{bias}\, b_F} + F_k^{\text{MC}},$$

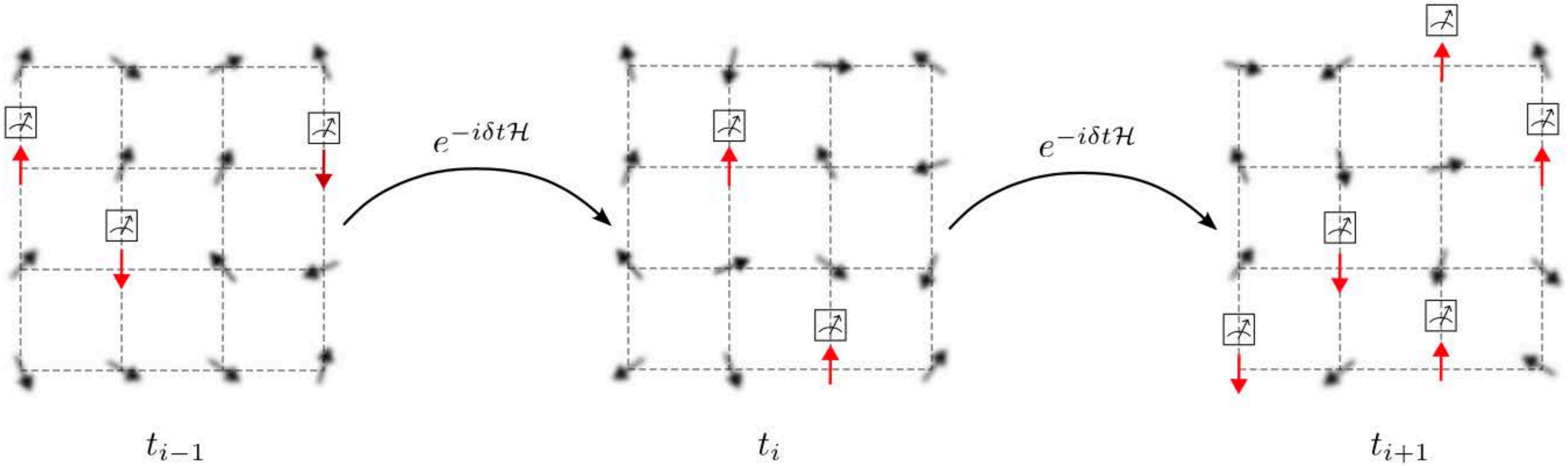
$$S_{kk'} = \underbrace{\sum_{\sigma|\Psi_\theta(\sigma)=0} \frac{\langle \partial_{\theta_k} \Psi_\theta|\sigma\rangle \langle \sigma|\partial_{\theta_{k'}} \Psi_\theta\rangle}{\langle \Psi_\theta|\Psi_\theta\rangle}}_{\text{bias}\, b_S} + S_{kk'}^{\text{MC}}$$

Directly Minimise Infidelity Instead

$$\min_{\tilde{\theta}} \mathcal{I}(\,|\Psi_{\tilde{\theta}}\rangle\,, \mathcal{U}\,|\Psi_\theta\rangle)$$

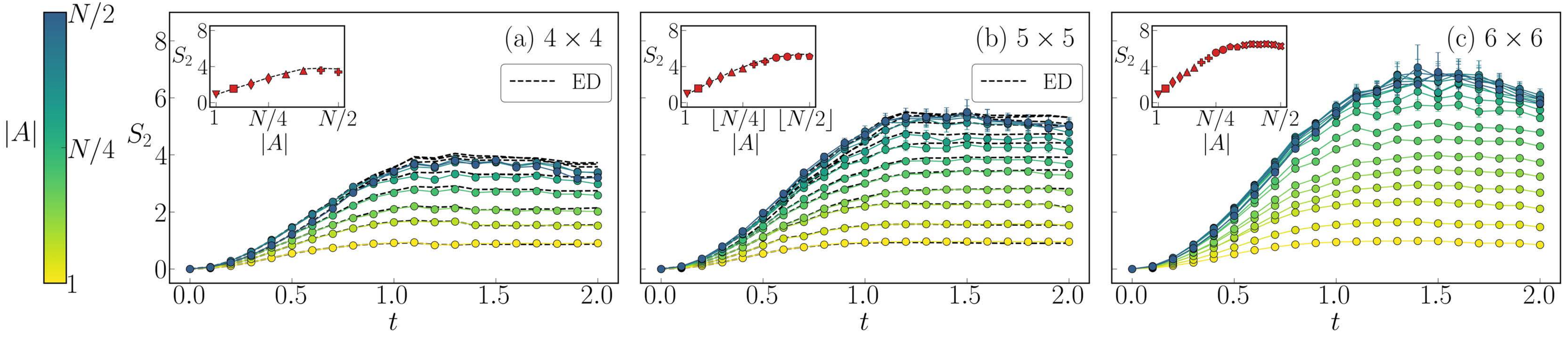
Sinibaldi, Giuliani, Carleo, and Vicentini
In Preparation (2023)

Application: Interleaving Dynamics with Measurements



$$\mathcal{H}_{\mathrm{TFI}} = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^x$$

Preliminary Exploration of Entanglement Entropy



The initial state is $\prod_i^N |+\rangle_i$ and the parameters of $\mathcal{H}_{\mathsf{TFI}}$ are $J = 1/2$ and $h = h_c/4$.

Low Measurement Regime

Measurement rate of p=0.01, dt=0.1

Violation of Area Law

Preliminary date indicates Area Law is Violated

05.

Final Thoughts.

Ground States with Neural Quantum States

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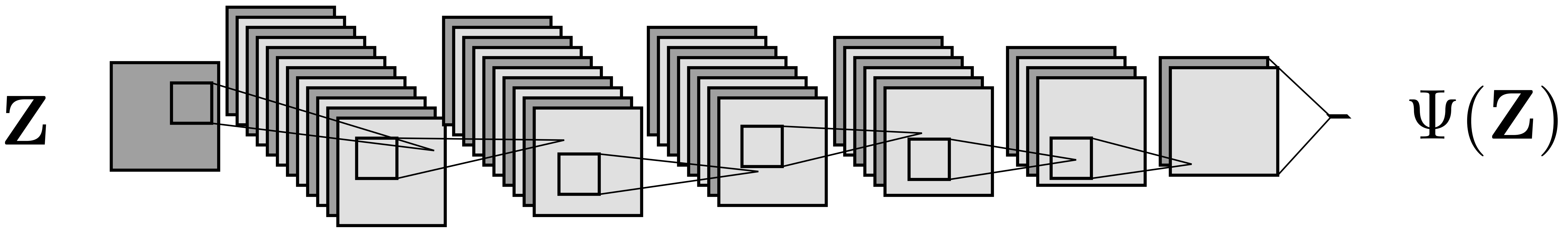
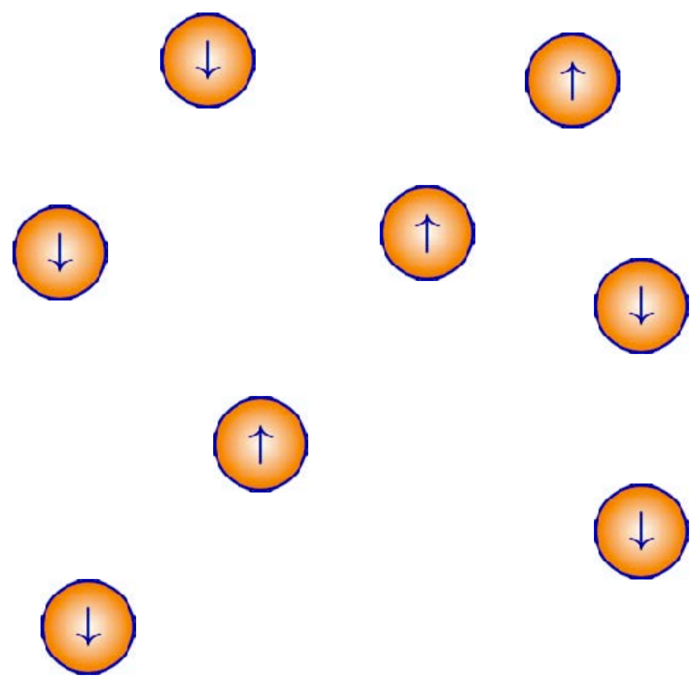


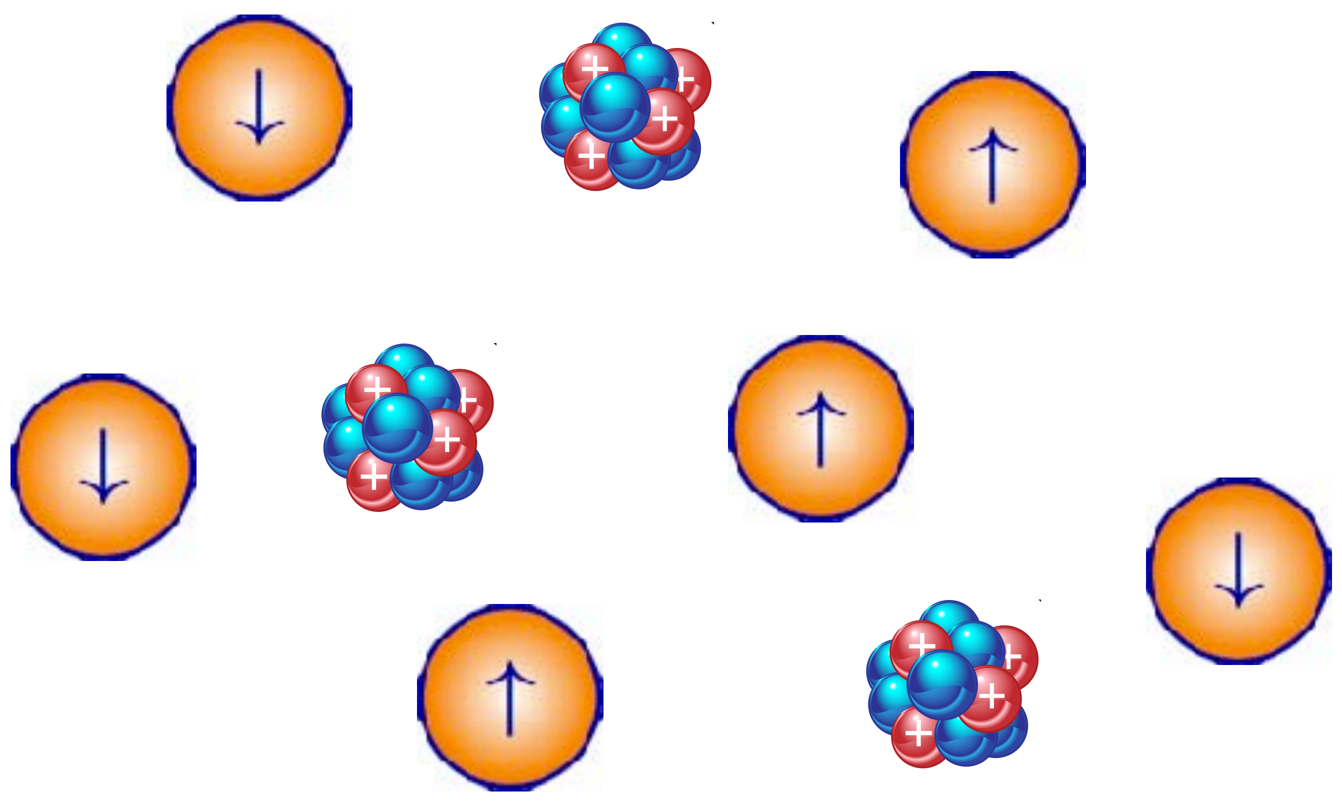
Neural Quantum States

Carleo, and Troyer
Science 355, 602 (2017)

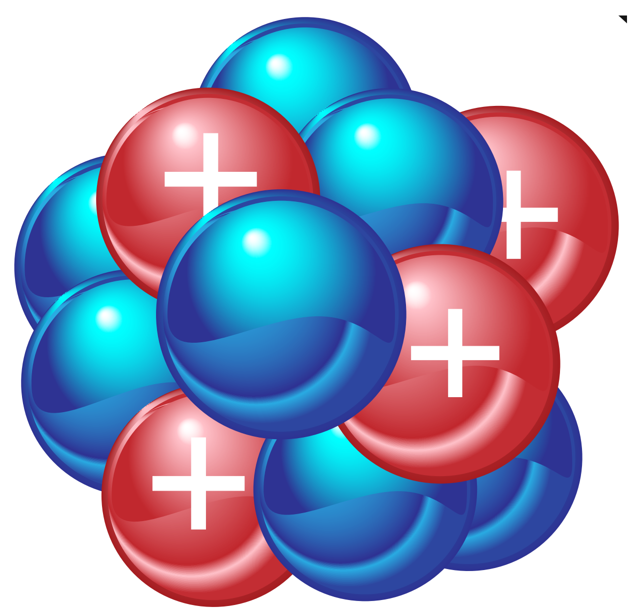
State of the art many-body wave functions in spin models, quantum chemistry, nuclear matter



Robledo Moreno, Carleo, Georges, and Stokes
PNAS 119, e2122059119 (2022)



Choo, Mezzacapo, and Carleo
Nature Comm. 11, 2368 (2020)



Adams, Carleo, Lovato, and Rocco
Phys. Rev. Lett. 127, 022502 (2021)

Pescia, Nys, Kim, Lovato, and Carleo
arXiv:2305.07240 (2023)

Dynamics : Challenges and Opportunities

In its present formulation, variational dynamics is a much heavier counterpart to ground state search

Great progress has been made, with suitable improvements NQS are on track to become state of the art **general-purpose quantum simulators**

By **combining** the full power of classical simulation and QPU accelerators, progress can happen faster

What you Cannot Expect in The Near Future

GC

Can you please compute, as a function of time, the average value of the interaction energy after a quench in the two-dimensional transverse-field Ising model on the square lattice? The initial state is the ground-state for h=0 and the final transverse field for the time evolution is h=2, assume the coupling is J=1.

To compute the average value of the interaction energy as a function of time after a quench in the two-dimensional transverse-field Ising model on a square lattice, we need to perform time evolution of the initial ground state under the final transverse field. The time evolution of the quantum state is given by the Schrödinger equation:

$$i\, \partial\psi/\partial t = H\, \psi$$

where ψ is the state vector and H is the Hamiltonian. In this case, the Hamiltonian is time-independent as it only depends on the final transverse field.

The Hamiltonian for the two-dimensional transverse-field Ising model on a square lattice is given by:

$$H = -J \sum_{<i,j>} \sigma_{zi}\sigma_{zj} - h \sum_i \sigma_{xi}$$

where σ_{xi} and σ_{zi} are the Pauli matrices acting on site i, J is the coupling constant, and h is the transverse field strength. The sum $\sum_{<i,j>}$ is taken over neighboring lattice sites.

We can numerically simulate the time evolution by discretizing time and using a time-evolution algorithm such as the Trotter-Suzuki decomposition or the time-dependent variational principle (TDVP). Here, let's use the Trotter-Suzuki decomposition, which approximates the time evolution operator by a product of exponential operators.

The time evolution operator for a time step Δt is given by:

$$U(\Delta t) = e^{-iH\Delta t}$$

To compute the average value of the interaction energy as a function of time, we can follow these steps:

1. Initialize the system in the ground state for h = 0, which corresponds to all spins aligned along the z-direction, $\sigma_{zi} = +1$ for all sites i.
2. Set the final transverse field strength h = 2.
3. Choose a time step Δt.
4. Apply the time evolution operator U(Δt) to the initial state iteratively, for a desired number of time steps.
5. At each time step, calculate the interaction energy by evaluating the expectation value of the interaction term for each pair of neighboring spins.
6. Take the average of the interaction energy over the desired number of time steps.

By repeating steps 4-6 for different time steps and plotting the results, you can obtain the average value of the interaction energy as a function of time after the quench in the transverse-field Ising model on the square lattice.

Thank you!

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