Neural-Network Quantum States

New Computational Possibilities for the Quantum Many-Body Problem

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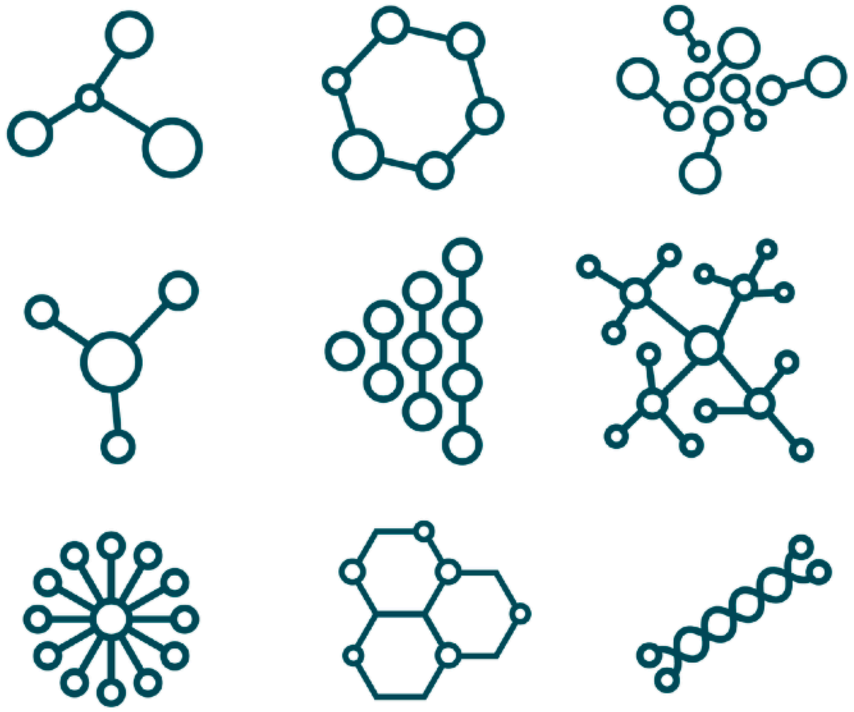
Computational Quantum Science Lab.

EPFL

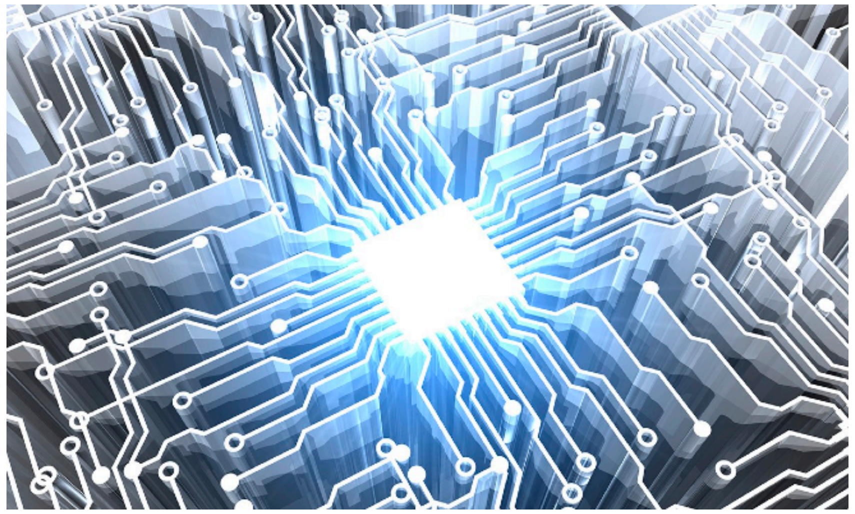
01.

The Quantum Many-Body Problem.

01.1 - Interacting Quantum Matter



E.g.
Interacting Particles in Chemistry, Material Science, Atomic Physics, Nuclear Physics...

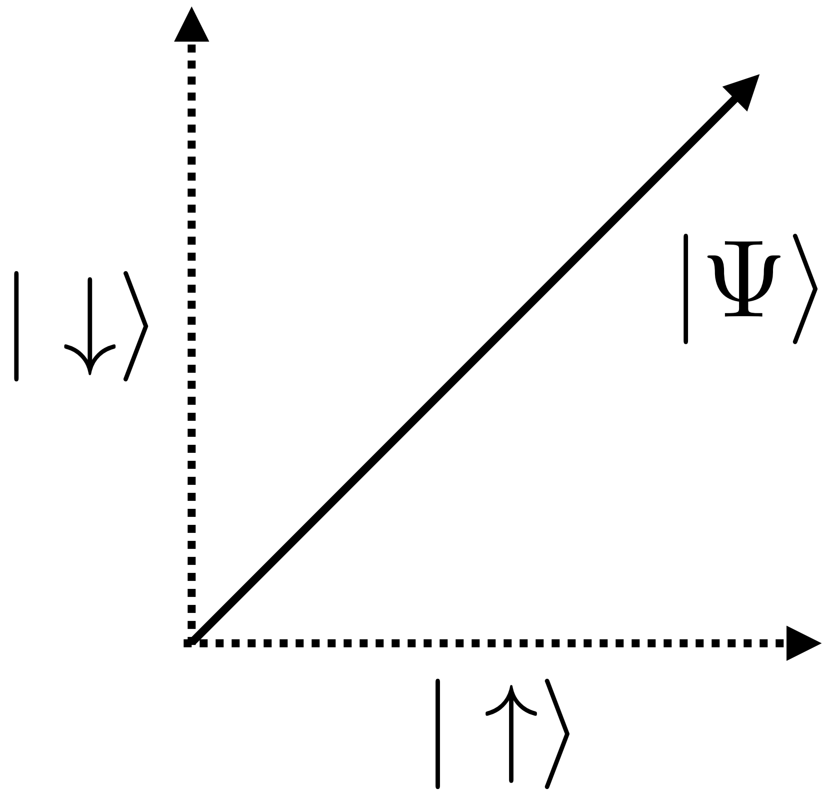


E.g.
Harnessing Entanglement in Quantum Computers, Quantum Simulators...

01.2 - Refresher: Quantum States

The state of a
quantum spin is
a complex-valued
vector

$$|\Psi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$$



Probability of Observing a Given State

$$P(\uparrow) = |c_{\uparrow}|^2$$

$$P(\downarrow) = |c_{\downarrow}|^2$$

A quantum spin can be found
in either up or down state
with a given probability

01.3 - The Many-Body Wave Function

$$|\Psi\rangle = c_{\uparrow\uparrow\dots\uparrow}|\uparrow\uparrow\dots\uparrow\rangle + c_{\downarrow\uparrow\dots\uparrow}|\downarrow\uparrow\dots\uparrow\rangle + \dots c_{\downarrow\downarrow\dots\downarrow}|\downarrow\downarrow\dots\downarrow\rangle$$

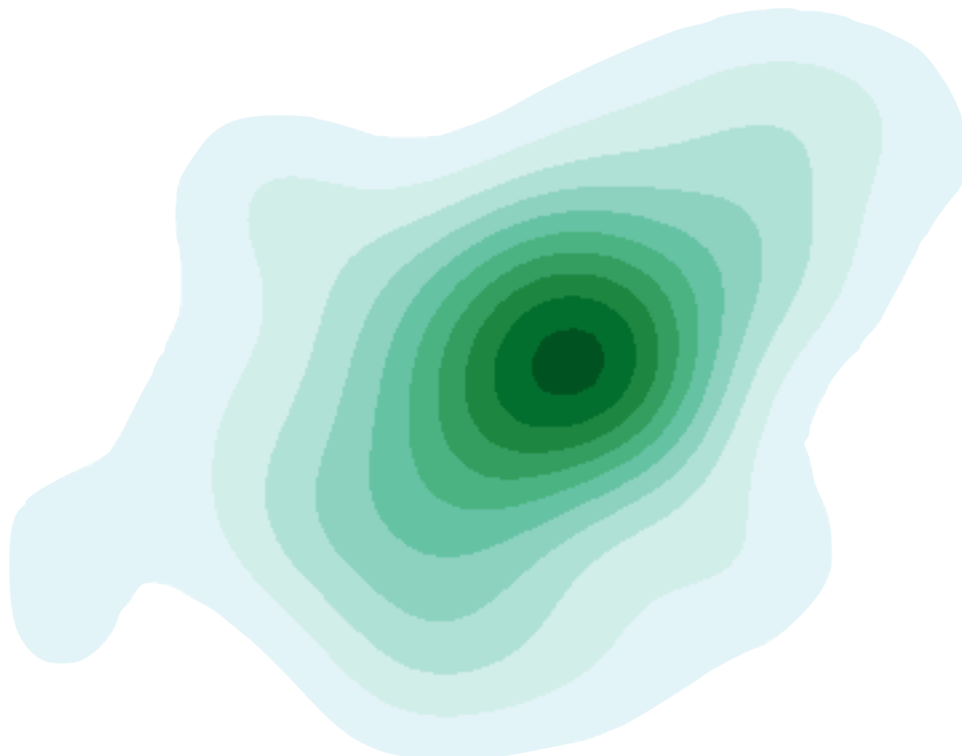
Complex-Valued Coefficients

The Wave Function is a Vector in a Huge (2^N) Space

The state of N quantum particles is a high-dimensional "monster"

"In general the many-electron wave-function for a system of many electrons is not a legitimate scientific concept"

W. Kohn, Nobel Lecture



01.4 - Time-Independent Schrödinger Equation

$$\mathcal{H}\big|\Psi_n\big\rangle = E_n\big|\Psi_n\big\rangle$$

Eigenvalue Problem
for given Hamiltonian

$\mathcal{H}$: Hamiltonian

$\big|\Psi_n\big\rangle$: Eigenstates

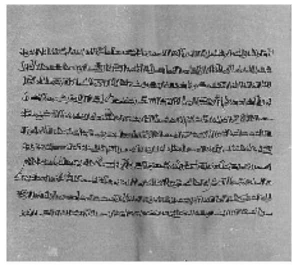
$$\mathcal{H} \doteq \begin{pmatrix} \bullet & & & & \bullet & & & \\ & & \bullet & & & & & \\ & & & \bullet & & & & \\ & & & & \bullet & & & \\ & & \bullet & & \bullet & & \bullet & \\ & & & & \bullet & & \bullet & \\ & & \bullet & & & & & \bullet \\ & \bullet & & & \bullet & & & \end{pmatrix}$$

"Row-Sparse"
Matrix for
Physical
Interactions

01.5 - Exact Solutions Limited to Small Systems

[3000 BCE]

Papyrus



10 Qubits

[1455]

Book

15 Qubits

[1973]

IBM 3340

23 Qubits

[1993]

IBM 3390

35 Qubits

[2002]

Earth Simulator

46 Qubits

[2019]

Summit

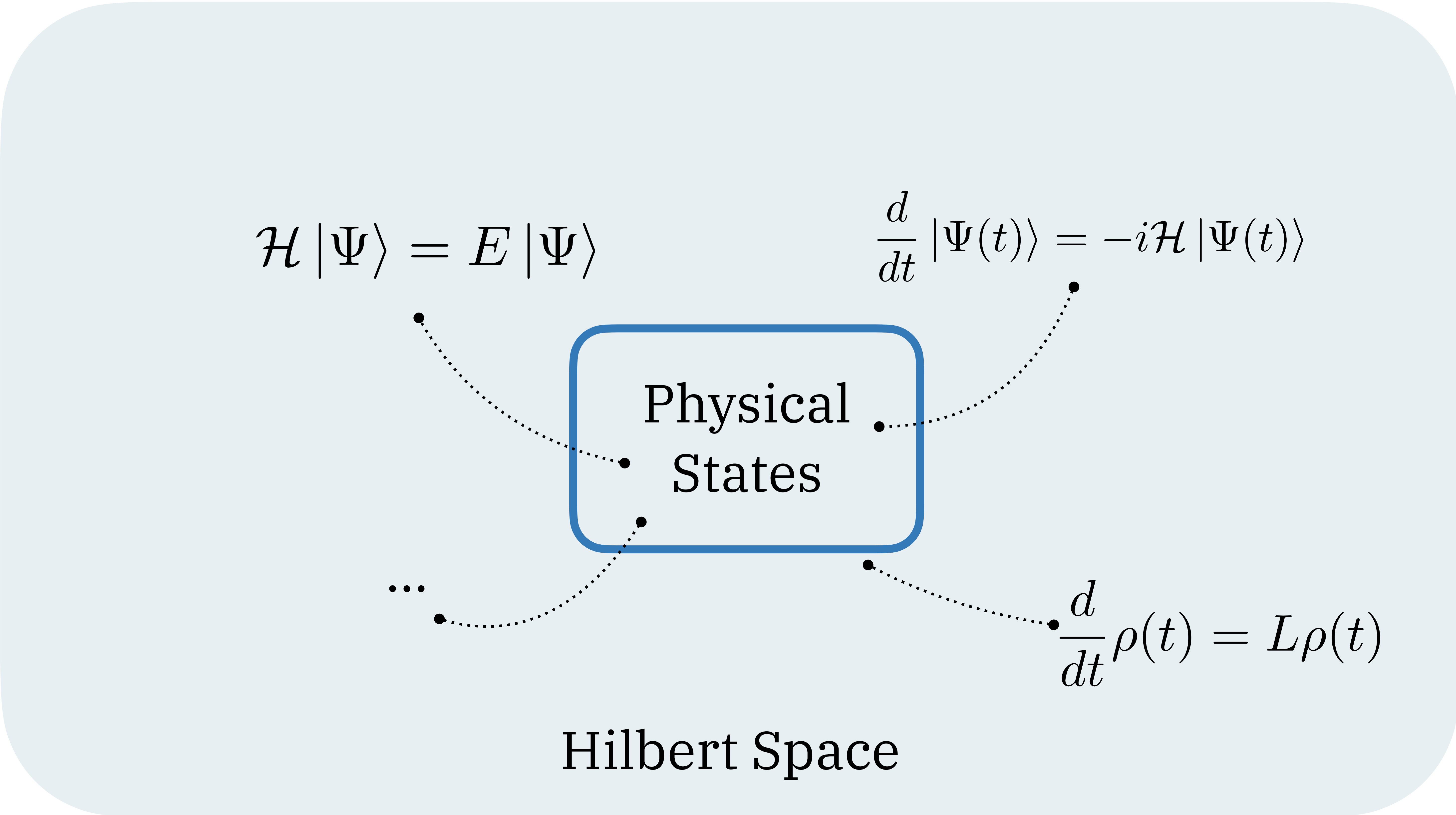
54 Qubits

Time →

02.

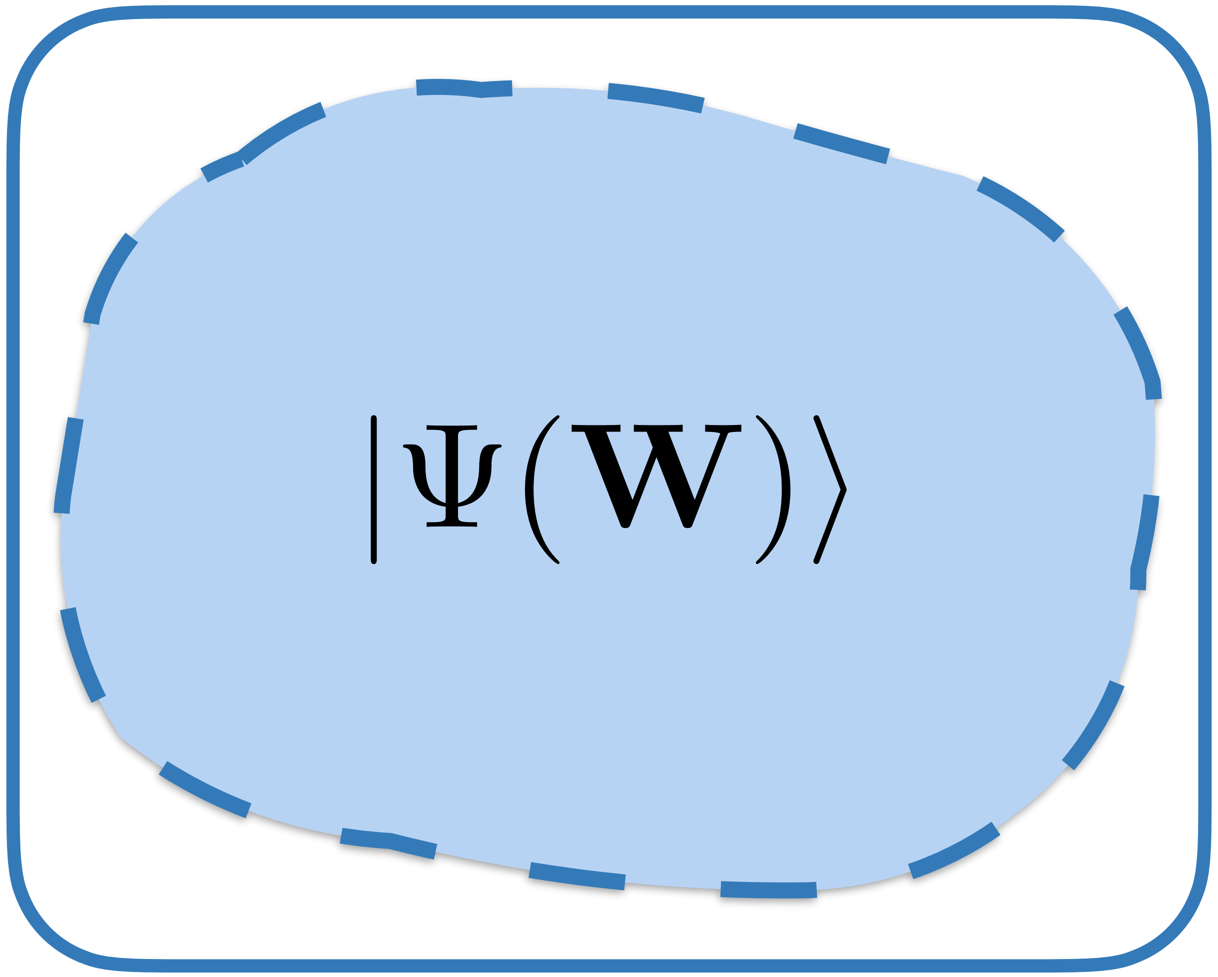
Variational Representations.

02.1 - Corners of the Hilbert space



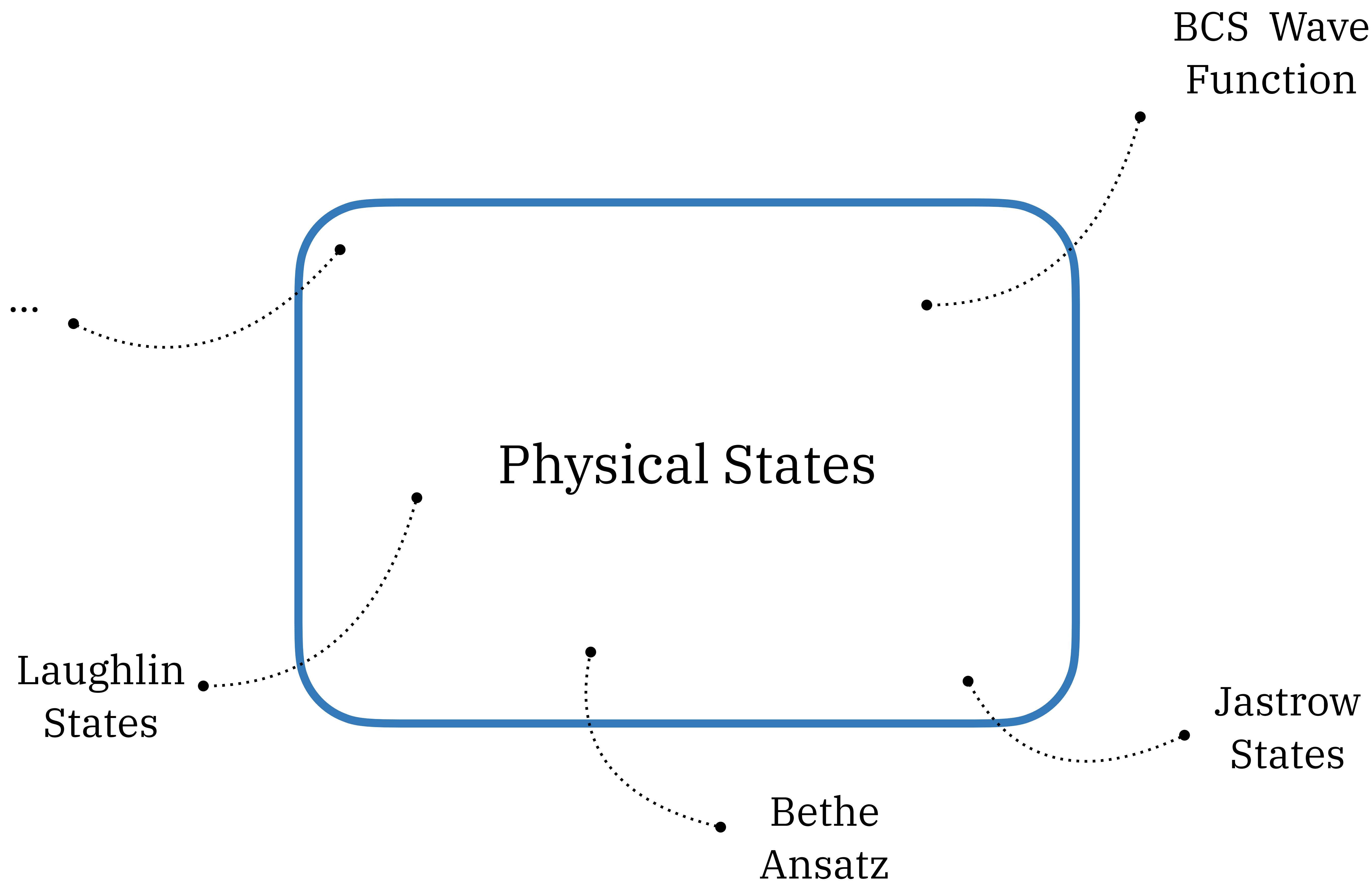
O2.2 - Variational Representations

$$|\Psi(W)\rangle = c_{\uparrow\uparrow\ldots\uparrow}(W)|\uparrow\uparrow\ldots\uparrow\rangle + c_{\downarrow\uparrow\ldots\uparrow}(W)|\downarrow\uparrow\ldots\uparrow\rangle + \ldots c_{\downarrow\downarrow\ldots\downarrow}(W)|\downarrow\downarrow\ldots\downarrow\rangle$$



$$\langle Z_1 Z_2 \ldots Z_n|\Psi(W)\rangle = \Psi(Z_1, Z_2 \ldots Z_N; W) = c_{Z_1, Z_2, \ldots Z_N}(W)$$

02.3 - Physics-Inspired Representations

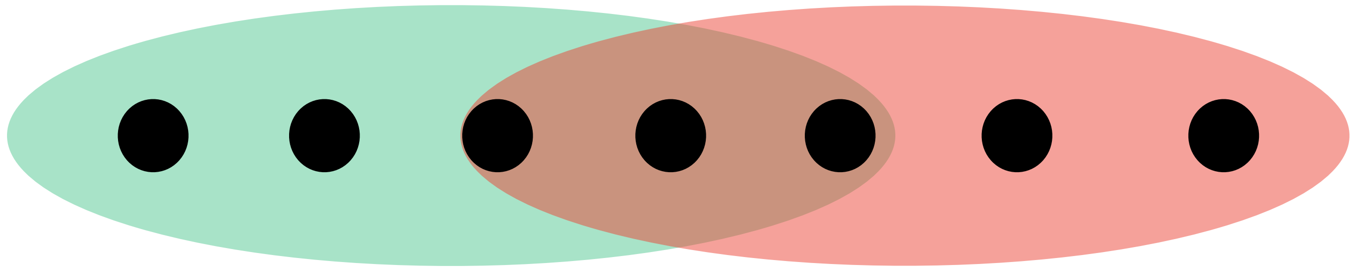


02.4 - General Purpose: Matrix Product States

$$\langle Z_1 Z_2 \ldots Z_n | \Psi(W) \rangle = \mathrm{Tr}\left[M(Z_1; W) M(Z_2; W) \ldots M(Z_n; W) \right]$$

Matrices
DxD

S. White
Phys. Rev. Lett. 69, 2863 (1992)



Simple Algebra

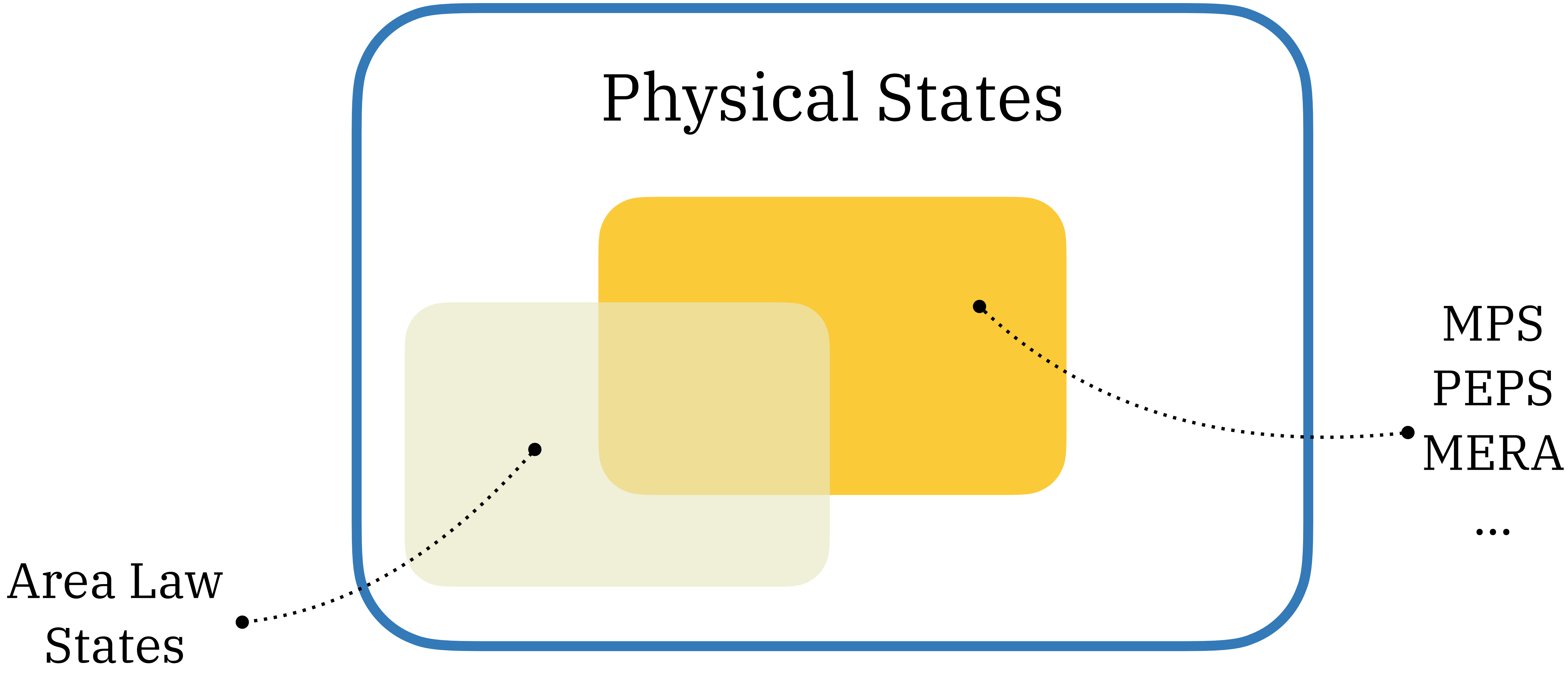
Efficient Compression
of Wave-Function

"Polynomial"
complexity

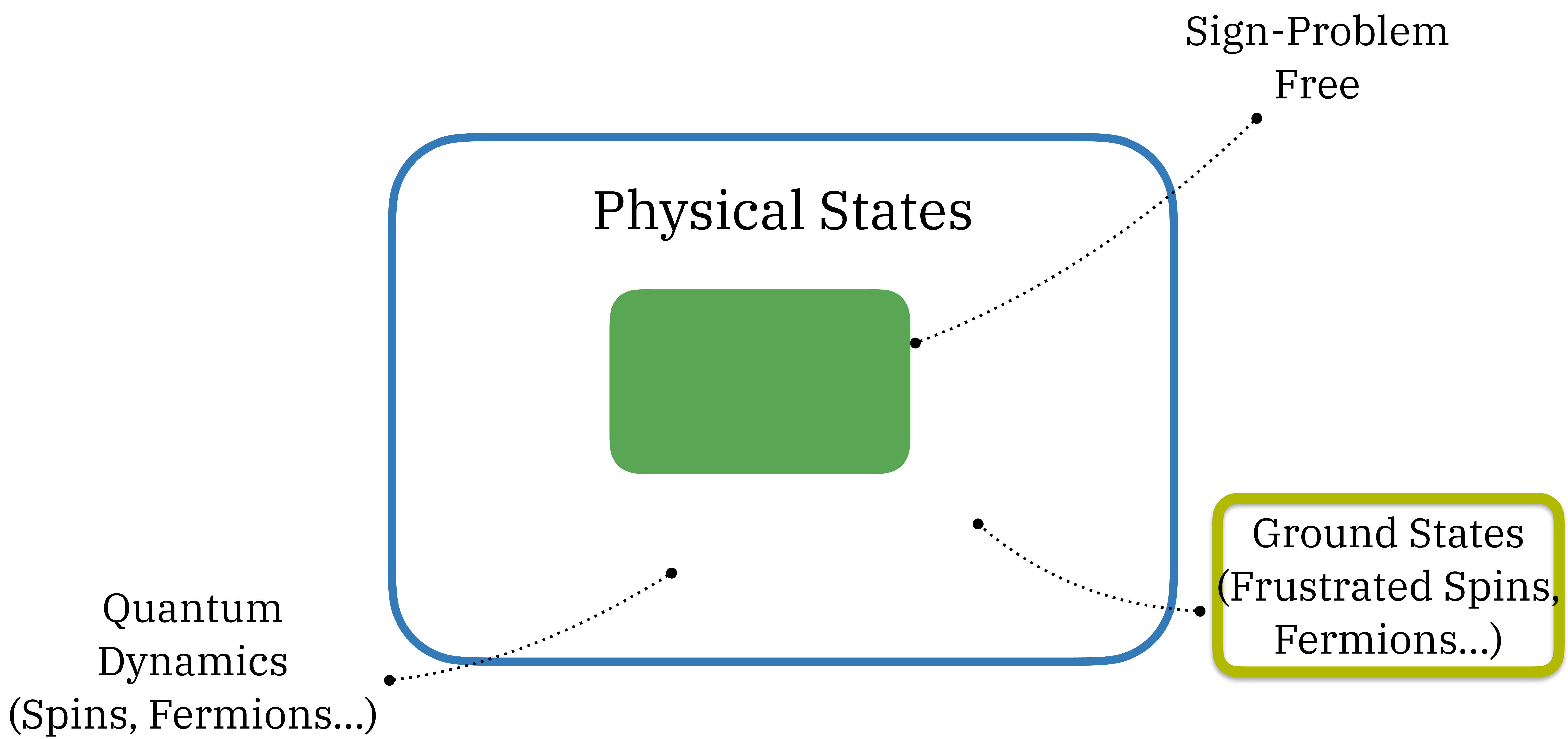
Low Entanglement

Many-Body State
Specified by Small Set
of Local Quantities

02.5 - Tensor Networks Representations



O2.6 - Traditionally Hard Problems In 2D and 3D

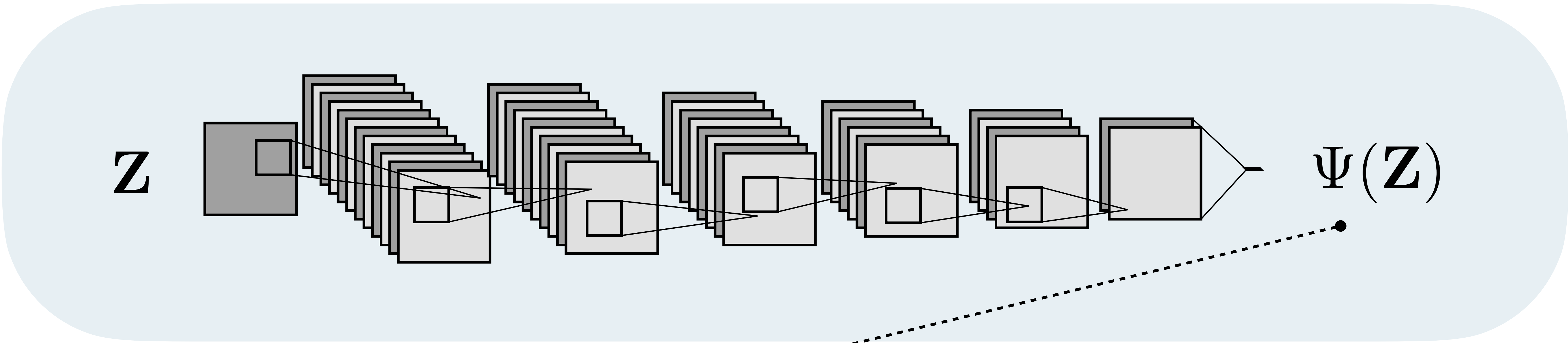


03.

Neural-Network Representations.

03.1 - Neural Quantum States

Carleo, and Troyer
Science 355, 602 (2017)



$$\langle Z_1 Z_2 \ldots Z_N | \Psi \rangle = g^{(L)} \circ W^{(L)} \ldots g^{(2)} \circ W^{(2)} g^{(1)} \circ W^{(1)} \mathbf{Z}$$

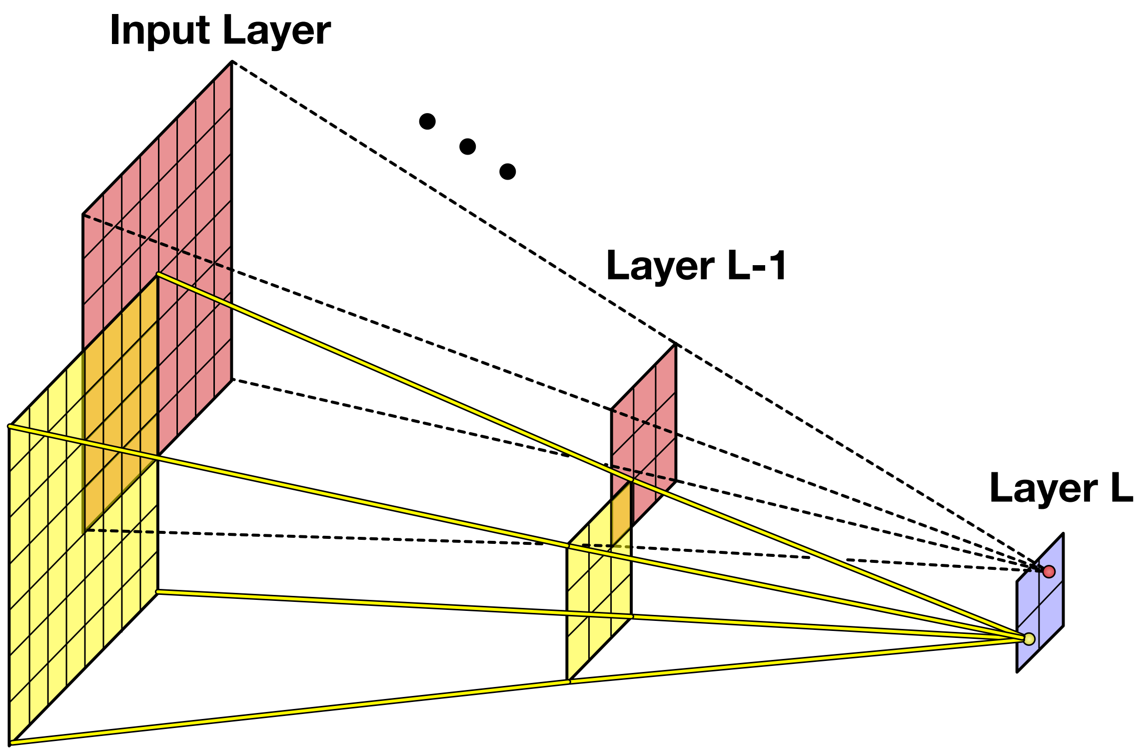
03.2 - Representation and Entanglement Properties

$$\langle \mathbf{Z} | \Psi \rangle = \sum_{q=0}^{2n} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(Z_p) \right)$$

Universal Approximation Theorems

Kolmogorov and Arnold (1956)

Cybenko (1989)



Volume-Law States

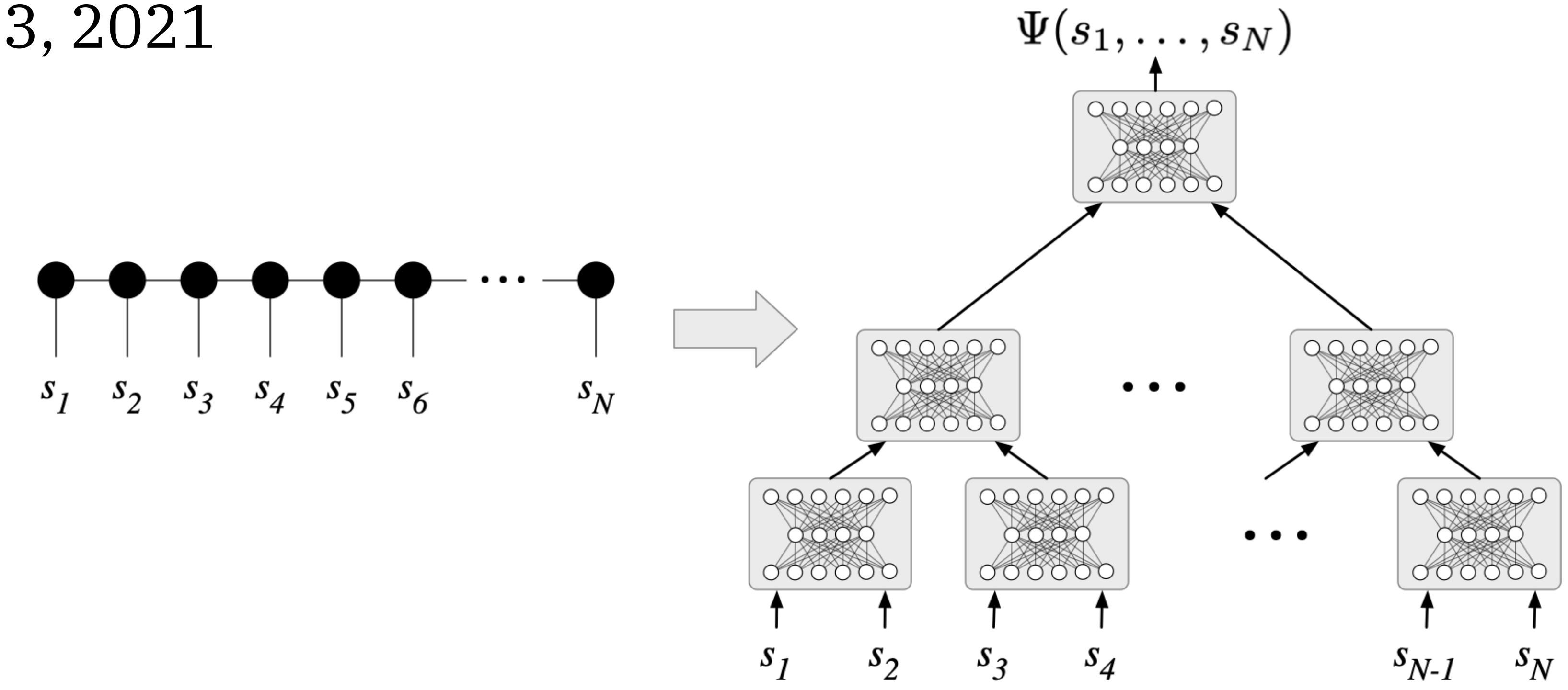
Deng, Li, and Das Sarma PRX *7, 021021 (2017)*

....

Levine, Sharir, Cohen, and Shashua PRL *122, 065301 (2019)*

03.3 - Neural-Tensor Contractions

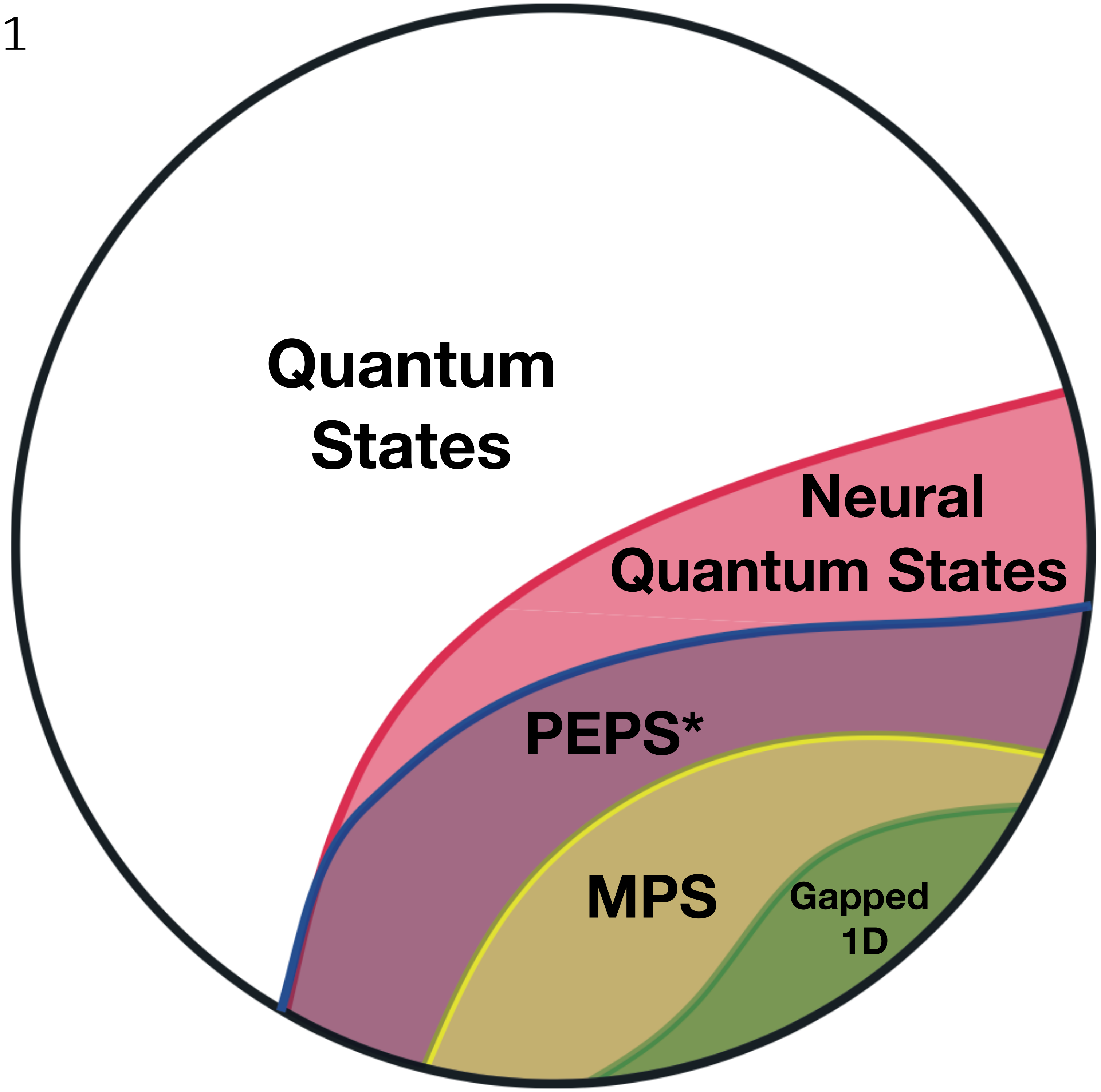
Sharir, Shashua, and Carleo
arXiv:2103.10293, 2021



Corollary 1 *For any tensor network quantum state with a contraction scheme of run-time k, and at most b bits of precision in computations and parameters, there exists a neural network that approximate it with a maximal error of ϵ and of run-time (number of edges)* $O\left(k + \ln^2\left(\frac{kb}{\epsilon}\right) + \ln\left(\frac{1}{\epsilon}\right)\sqrt{\frac{1}{\epsilon}}\right)$.

03.4 - Representability Diagram

Sharir, Shashua, and Carleo
arXiv:2103.10293, 2021



04.

Learning the Ground State.

04.1 - Variational Formulation

$$E(\mathbf{W}) = \frac{\langle \Psi(\mathbf{W}) | \mathcal{H} | \Psi(\mathbf{W}) \rangle}{\langle \Psi(\mathbf{W}) | \Psi(\mathbf{W}) \rangle} \geq E_0$$

Rayleigh Quotient

Exact Ground-State Energy

Expectation Minimization

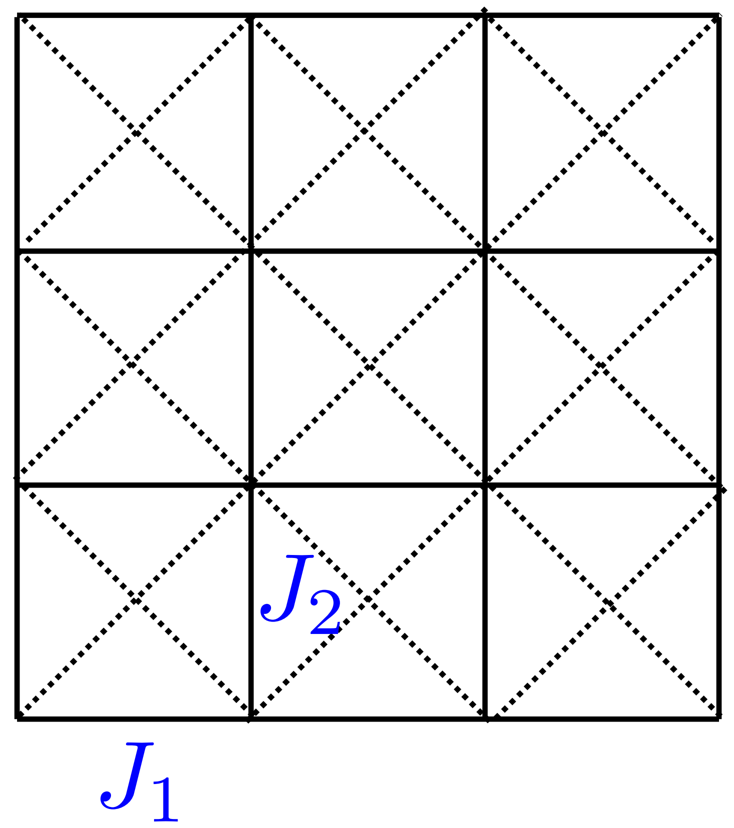
$$E(\mathbf{W}) = \frac{\sum_Z |\Psi(Z; W)|^2 E_{\text{loc}}(Z; W)}{\sum_Z |\Psi(Z; W)|^2}$$

McMillan, Phys. Rev. 138, *A442 (1965)*

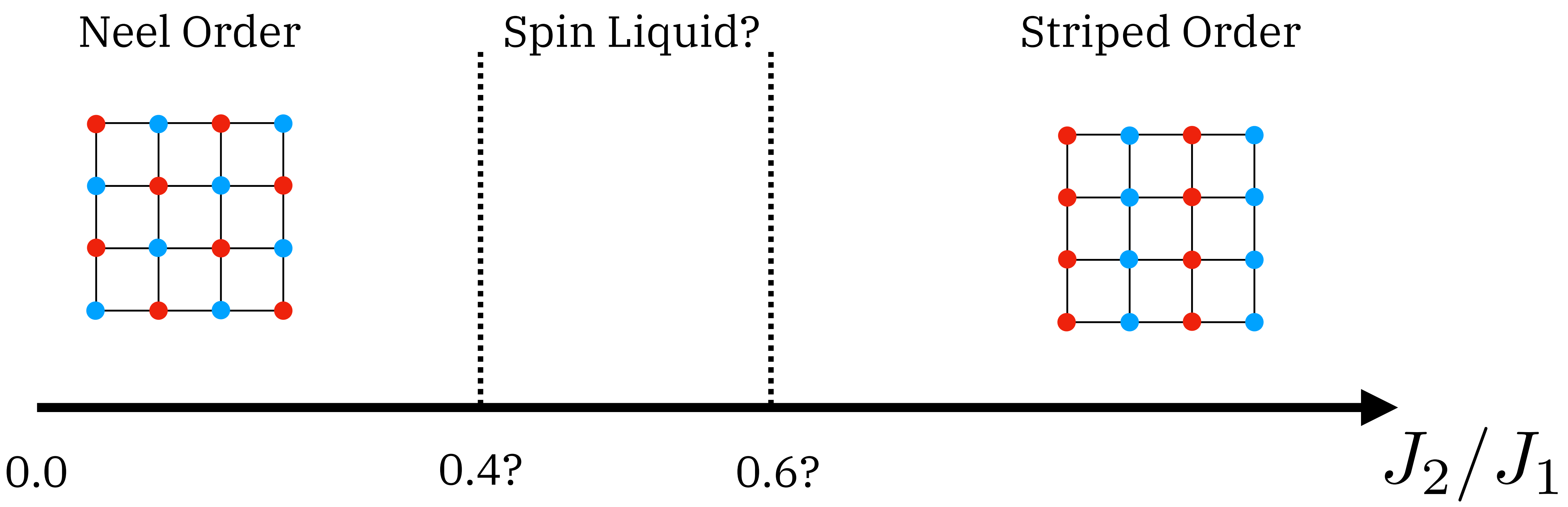
04.2 - Example Application: Frustrated Spins

J1-J2 Model

$$\hat{H} = J_1 \sum_{\langle ij \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j$$

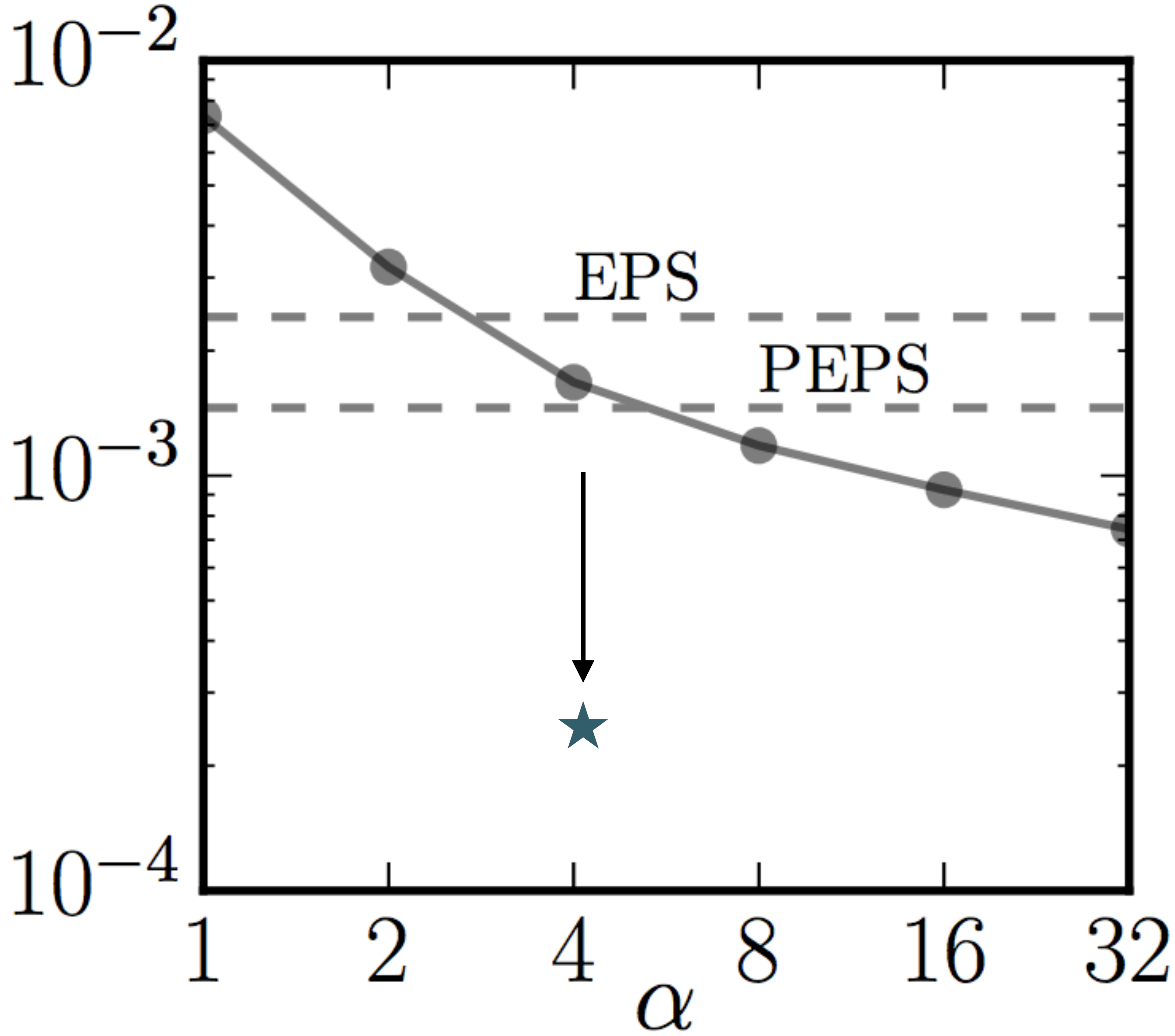


Phase Diagram



04.3 - Heisenberg Limit - From RBM to ARN

Carleo, and Troyer
Science 355, 602 (2017)



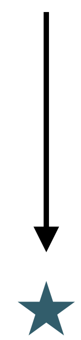
10 by 10 cluster

Choo, Neupert, and Carleo
Phys. Rev. B 100,
125124 (2019)

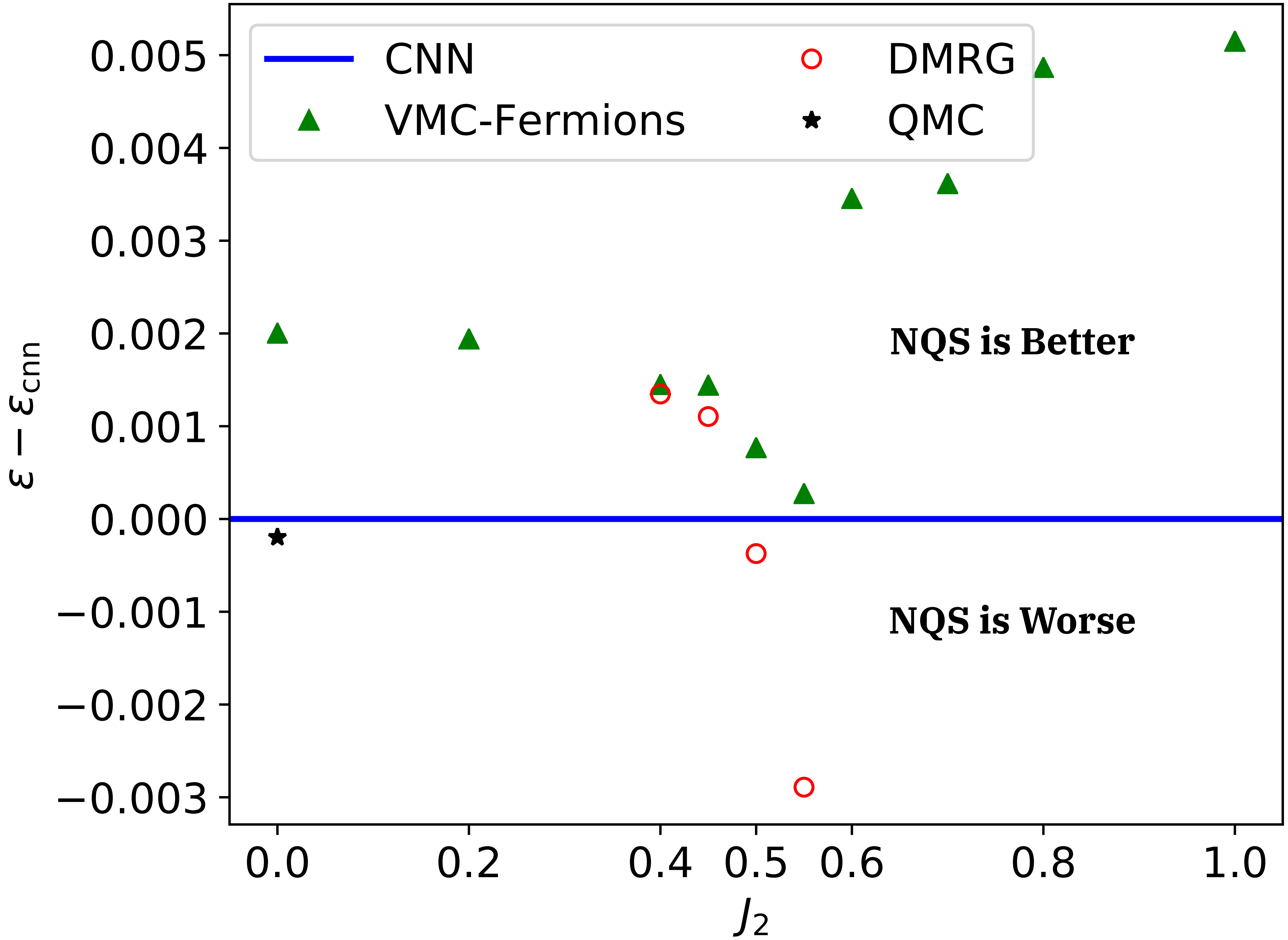
Sharir, Levine, Wies,
Carleo, and Shashua
Phys. Rev. Lett. 124,
020503 (2020)

Significantly Higher Accuracy Than
Shallow Networks

~4x10^-5



04.4 - Frustrated Case: Accuracy Diagram



10 by 10 cluster

Choo, Neupert, and Carleo
Phys. Rev. B 100, 125124 (2019)

04.5 - Continuous Improvements...

TABLE II. Comparison of ground-state energy for the 10×10 lattice at $J_2 = 0.5$ among different wave functions. The wave functions in bold font use neural networks. In Ref. [18], p-th order Lanczos steps are applied to the VMC wave function.

Energy per site	Wave function	Reference
$-0.494757(12)$	**Neural quantum state**	65
$-0.49516(1)$	**CNN**	60
$-0.49521(1)$	VMC(p=0)	18
-0.495530	DMRG	22
$-0.49575(3)$	**RBM-fermionic w.f.**	63
$-0.497549(2)$	VMC(p=2)	18
$-0.497629(1)$	**RBM+PP**	present study

Nomura, and Imada
Phys. Rev. X 11, 031034 (2021)

05.

Fermions

05.1 - Fermions: Back to the Spin Problem

Map Fermions to Spins

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

Jordan-Wigner Mapping

Pro: Simple Mapping

Con: N-Body, non-local Spin Operators

Bravyi-Kitaev Mapping

Pro: log(N)-Body, quasi-local Spin Operators

Con: More Involved Mapping

05.2 - Jordan-Wigner Mapping

$$c_j \rightarrow \left(\prod_{i=0}^{j-1} \sigma_i^z \right) \sigma_j^-$$

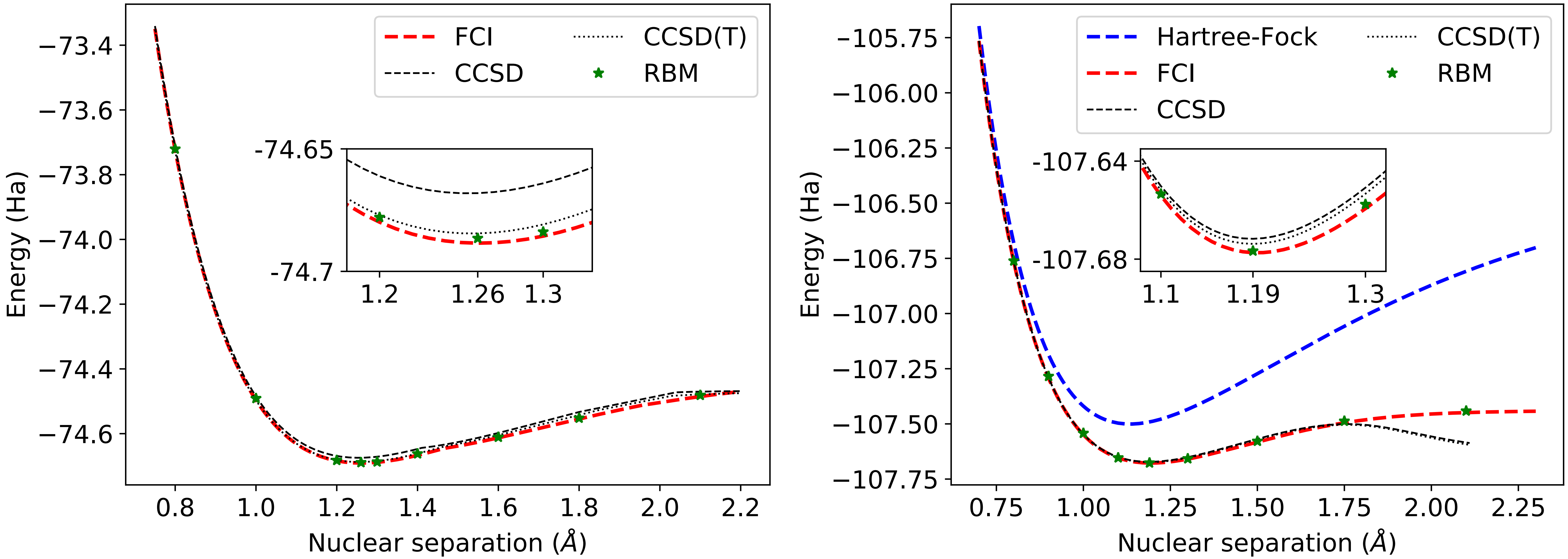
$$c_j^\dagger \rightarrow \left(\prod_{i=0}^{j-1} \sigma_i^z \right) \sigma_j^+$$

Jordan Wigner “strings” take into account exchange symmetry

$$H_q = \sum_{j=1}^{r} h_j \boldsymbol{\sigma}_j$$

Spin Hamiltonian is a sum of product of Pauli matrices

05.3 - Dissociation Curves for C_2 and N_2

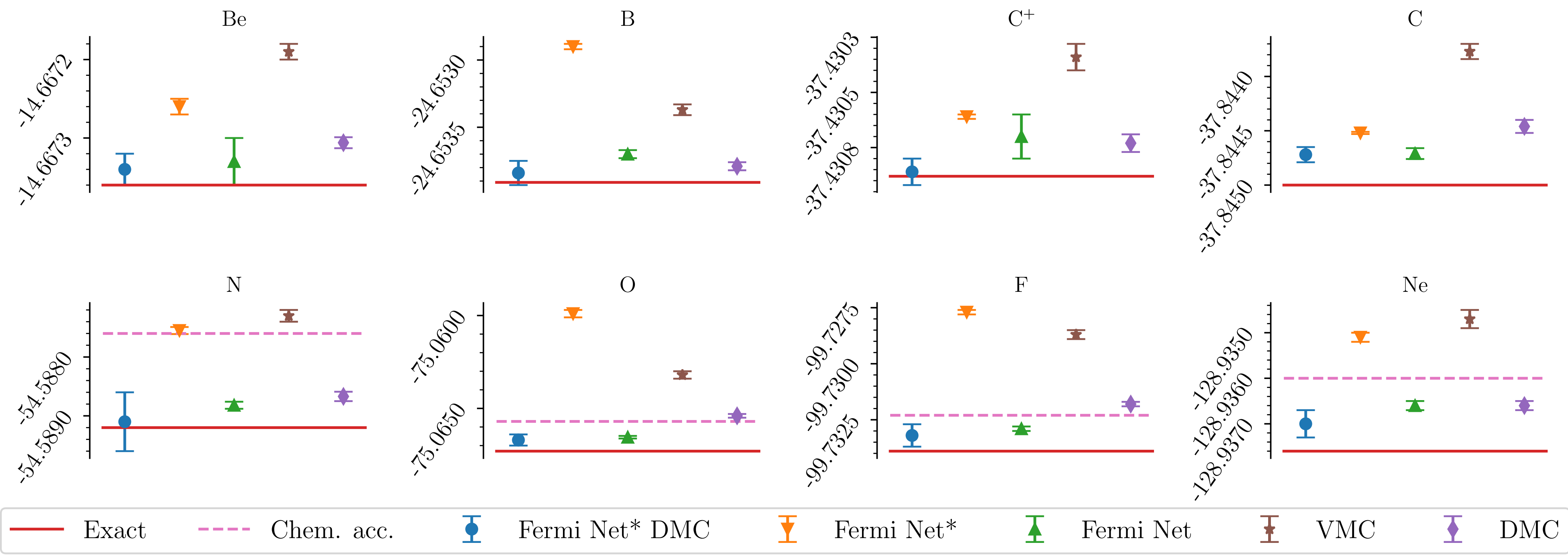


STO-3G Basis Set
Single-Layer Network

O5.4 - Alternative Approach to Chemistry Problems

Neural-Network Backflow: change nodal structure

$$\phi^b_{k\sigma}(r_{i,\sigma};\boldsymbol{r}) = \phi_{k\sigma} + \sum_j \eta_{ij,\sigma}\phi_{k\sigma}(r_{j,\sigma})$$



M. Wilson, N. Gao,
F. Wudarski, E. Rieffel, N. Tubman
arXiv:2103.12570 (2021)

M. Ruggeri, S. Moroni,
M. Holzmann
PRL, 120, 205302 (2018)

D. Luo, and B. Clark
PRL, 122, 226401 (2019)

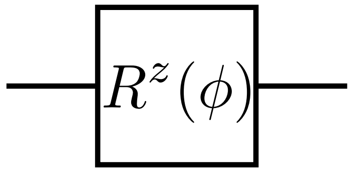
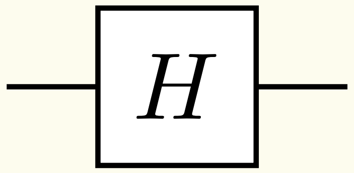
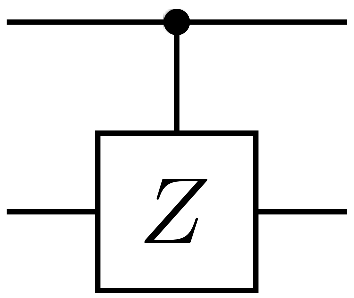
D. Pfau, J. Spencer,
A. Matthews, W. Foulkes
Phys. Rev. Research, 2, 033429 (2020)

J. Hermann, Z. Schätzle, F. Noé
Nature Chemistry, 12, 891 (2020)

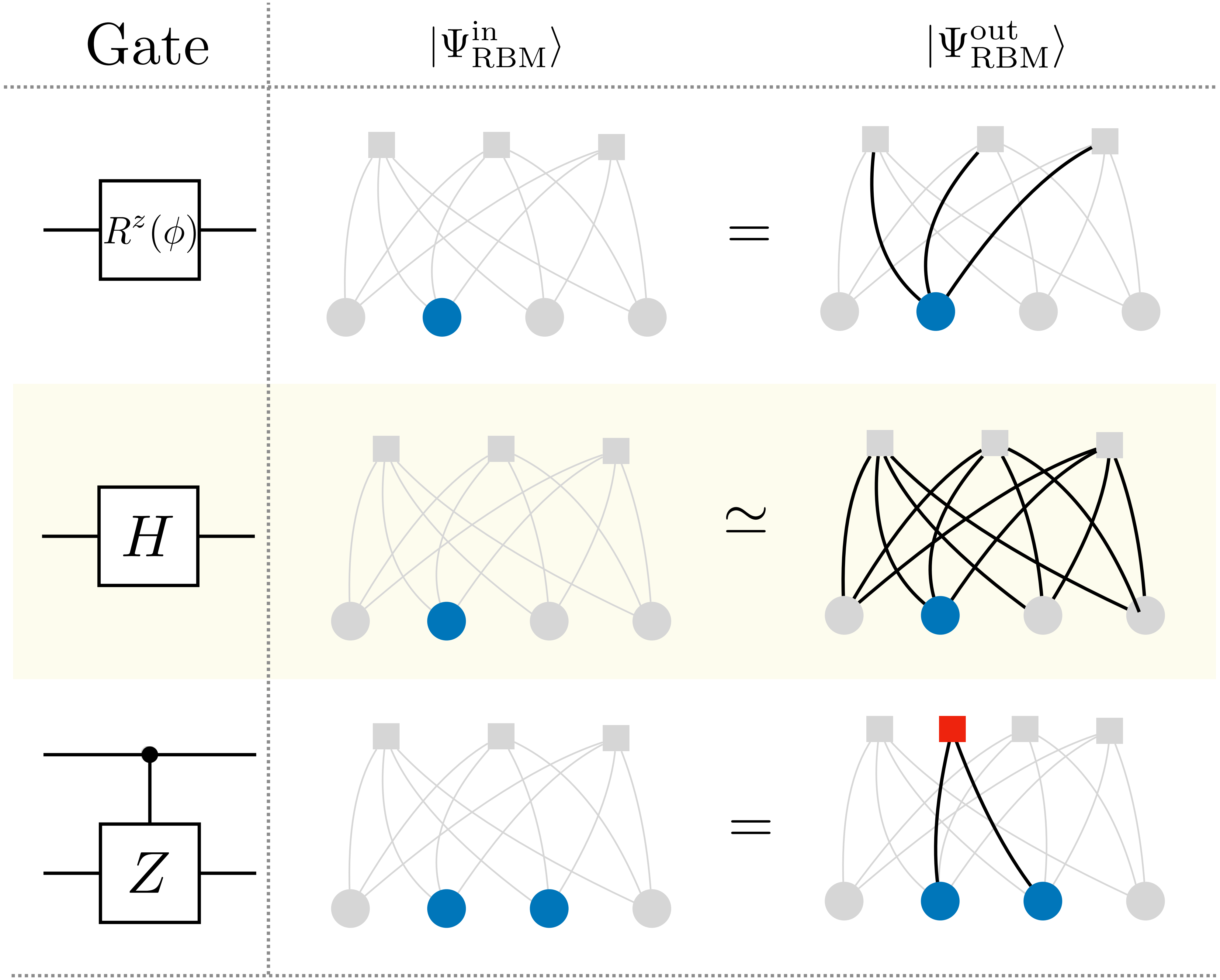
06.

Classical Simulation of Quantum Circuits.

06.1 - Universal Gate Set

Gate	
	Single-Qubit Z Rotations
	Hadamard Gate
	Two-Qubit Controlled Z Rotations

06.2 - Action on a NQS



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

06.3 - Learning the Hadamard

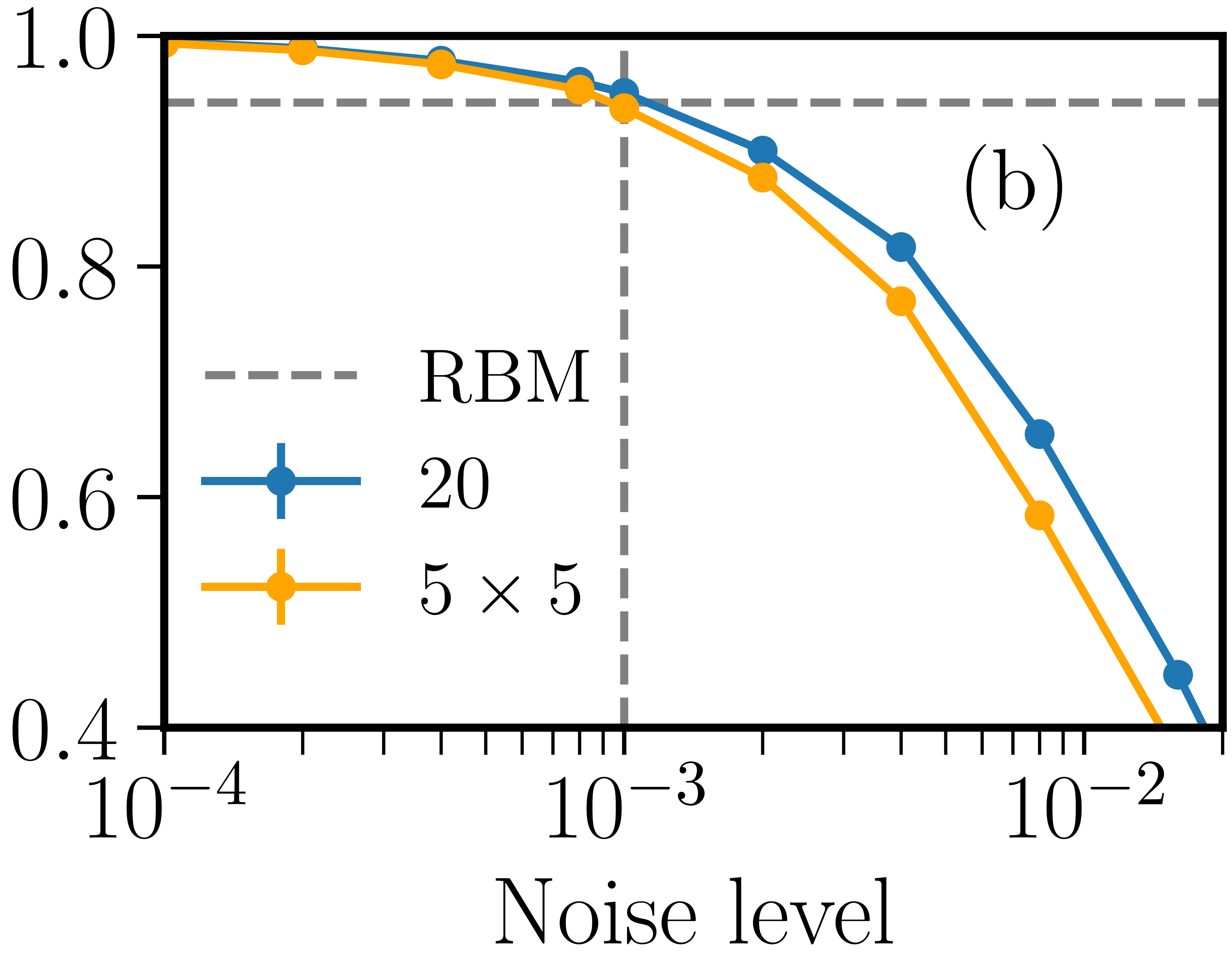
$$|\Phi\rangle = H|\Psi_{\mathcal{W}}\rangle \qquad |\Psi_{\mathcal{W}'}\rangle \simeq |\Phi\rangle$$

$$L(\Psi_{\mathcal{W}'}, \Phi) = -\log\left[\frac{|\langle\Psi_{\mathcal{W}'}|\Phi\rangle|}{||\Psi_{\mathcal{W}'}\rangle||\,|\Phi\rangle|}\right]$$

Minimize log infidelity

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

06.4 - Noise Versus Error

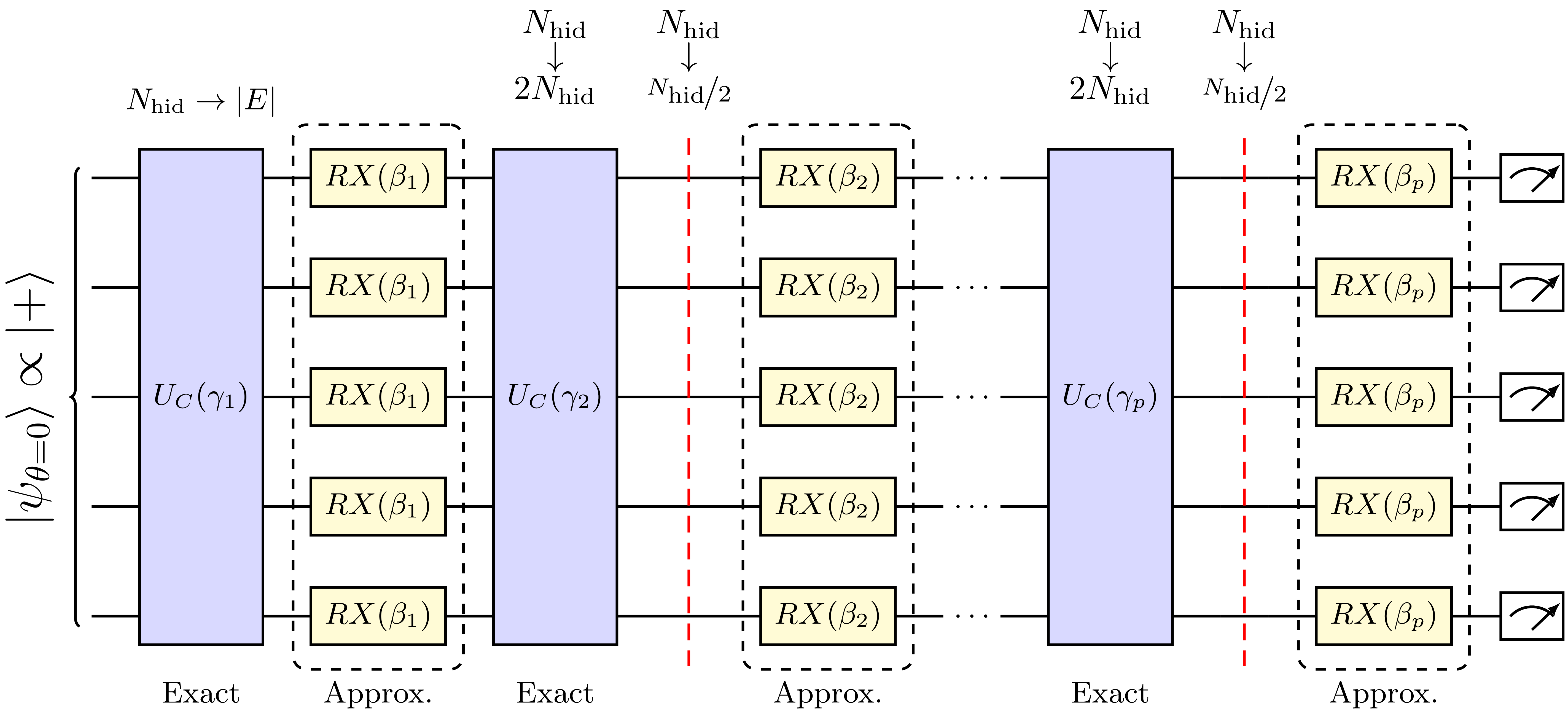


Comparing Variational Error with Depolarization Noise

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

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

O6.5 - Simulating QAOA

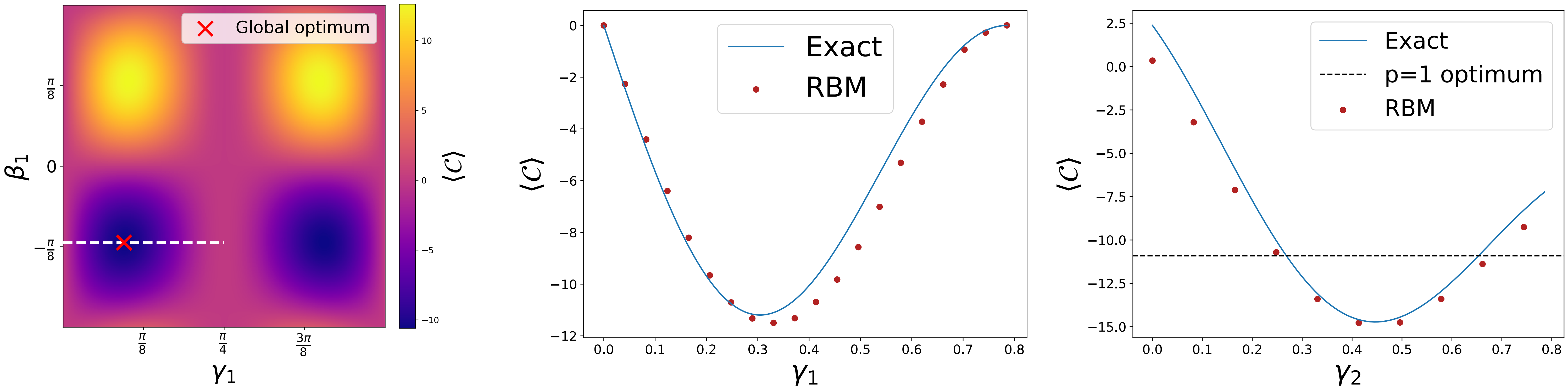


$$U_C(\gamma) = e^{-i\gamma\mathcal{C}} = \prod_{i,j\in E(G)} e^{-i\gamma w_{ij} Z_i Z_j}$$

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

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

06.6 - Benchmark of Small Circuits

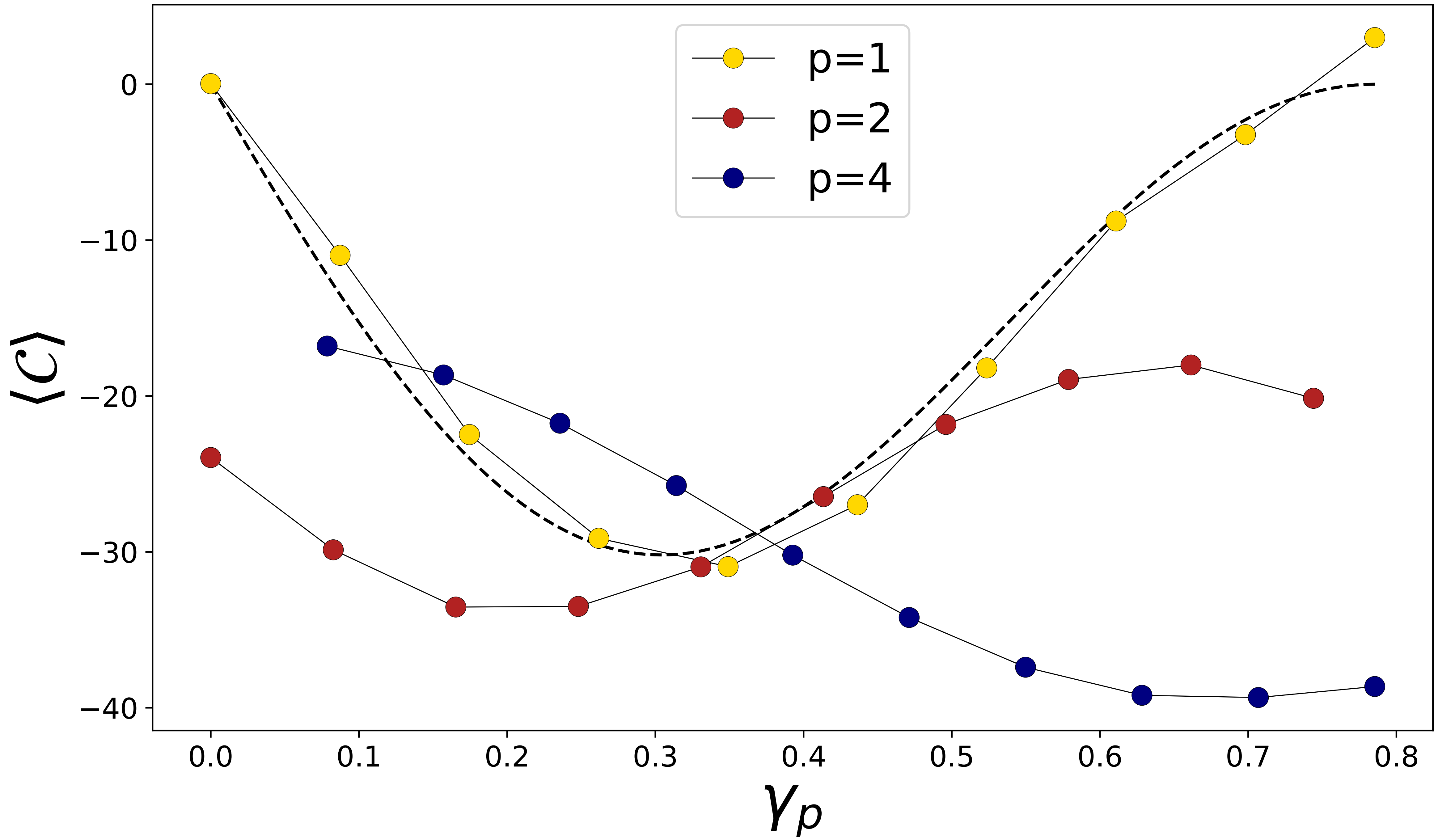


20 Qubits

3-Random Regular Graph

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

O6.7 - Simulating 54 Qubits



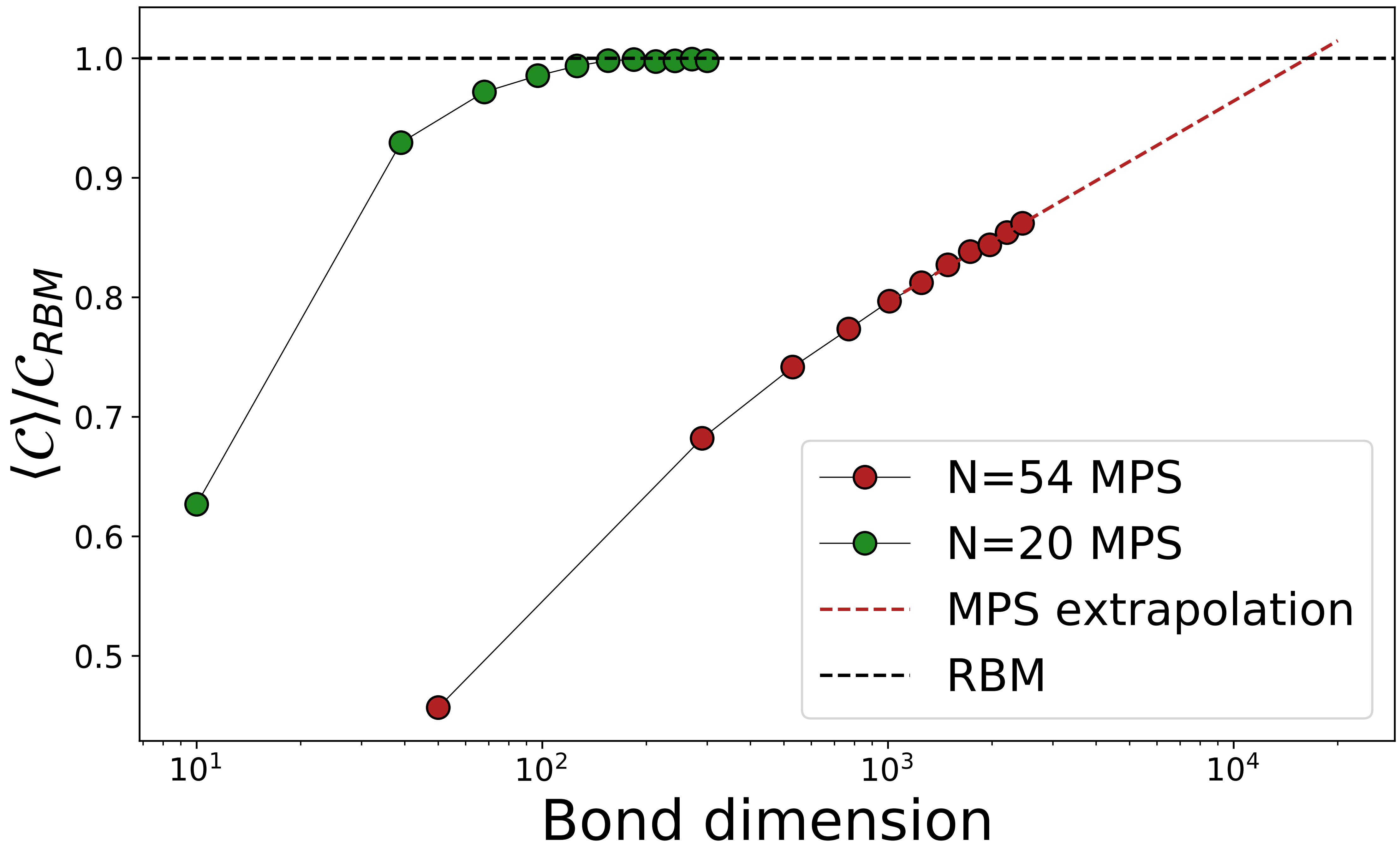
4 Layers

324 RZZ Gates

216 RX Gates

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

O6.8 - Comparing with tensor networks



Estimated Bond Dimension of ~10^4 for similar accuracy

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

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

07.

Outlook.

Neural Quantum States

Highly Entangled State

Exact Sampling [Autoregressive]

General Guiding Principle for Networks?

Efficiently Enforce Symmetries

Fermions

Several Approaches

Exciting new tool for correlated fermions

Imposing Locality

Still ~small systems

The NetKet Project

www.netket.org

NetKet: A Machine Learning Toolkit for Many-Body Quantum Systems

Giuseppe Carleo,[1] Kenny Choo,[2] Damian Hofmann,[3] James E. T. Smith,[4] Tom Westerhout,[5] Fabien Alet,[6] Emily J. Davis,[7] Stavros Efthymiou,[8] Ivan Glasser,[8] Sheng-Hsuan Lin,[9] Marta Mauri,[1,10] Guglielmo Mazzola,[11] Christian B. Mendl,[12] Evert van Nieuwenburg,[13] Ossian O'Reilly,[14] Hugo Théveniaut,[6] Giacomo Torlai,[1] and Alexander Wietek[1]

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[3] *Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany*
[4] *Department of Chemistry, University of Colorado Boulder, Boulder, Colorado 80302, USA*
[5] *Institute for Molecules and Materials, Radboud University, NL-6525 AJ Nijmegen, The Netherlands*
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[7] *Department of Physics, Stanford University, Stanford, California 94305, USA*
[8] *Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching bei München, Germany*
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[12] *Technische Universität Dresden, Institute of Scientific Computing, Zellescher Weg 12-14, 01069 Dresden, Germany*
[13] *Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, CA 91125, USA*
[14] *Southern California Earthquake Center, University of Southern California, 3651 Trousdale Pkwy, Los Angeles, CA 90089, USA*

```python
import netket as nk

# 1D Lattice
g = nk.graph.Hypercube(length=20, n_dim=1, pbc=True)

# Hilbert space of spins on the graph
hi = nk.hilbert.Spin(s=0.5, graph=g)

# Ising spin hamiltonian
ha = nk.operator.Ising(h=1.0, hilbert=hi)

# RBM Spin Machine
ma = nk.machine.RbmSpin(alpha=1, hilbert=hi)
ma.init_random_parameters(seed=1234, sigma=0.01)

# Metropolis Local Sampling
sa = nk.sampler.MetropolisLocal(machine=ma)
```

Numba

2.0: SoftwareX 10, 100311 (2019)

3.0: arXiv:2112.10526, (2021)

Computational Quantum Science Lab.

Sharir, Shashua, and Carleo
arXiv:2103.10293, 2021

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

Robledo Moreno, Carleo, Georges, and Stokes
arXiv:2111.10420 (2021)

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