Variational Simulation In The Age of Machine Learning.

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01.

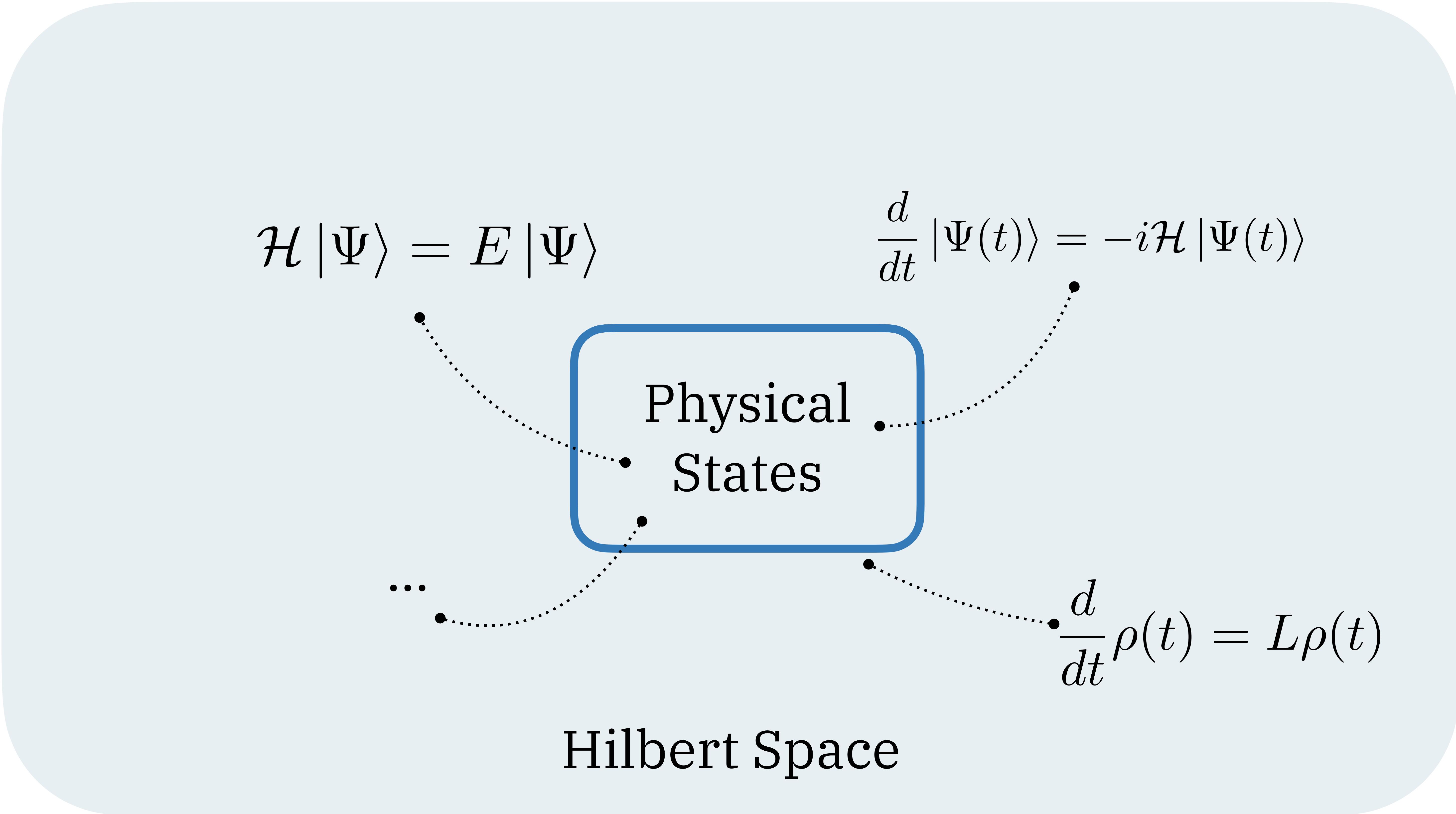
Corners of Hilbert Spaces.

01.1 - All The Many-Qubit Quantum States

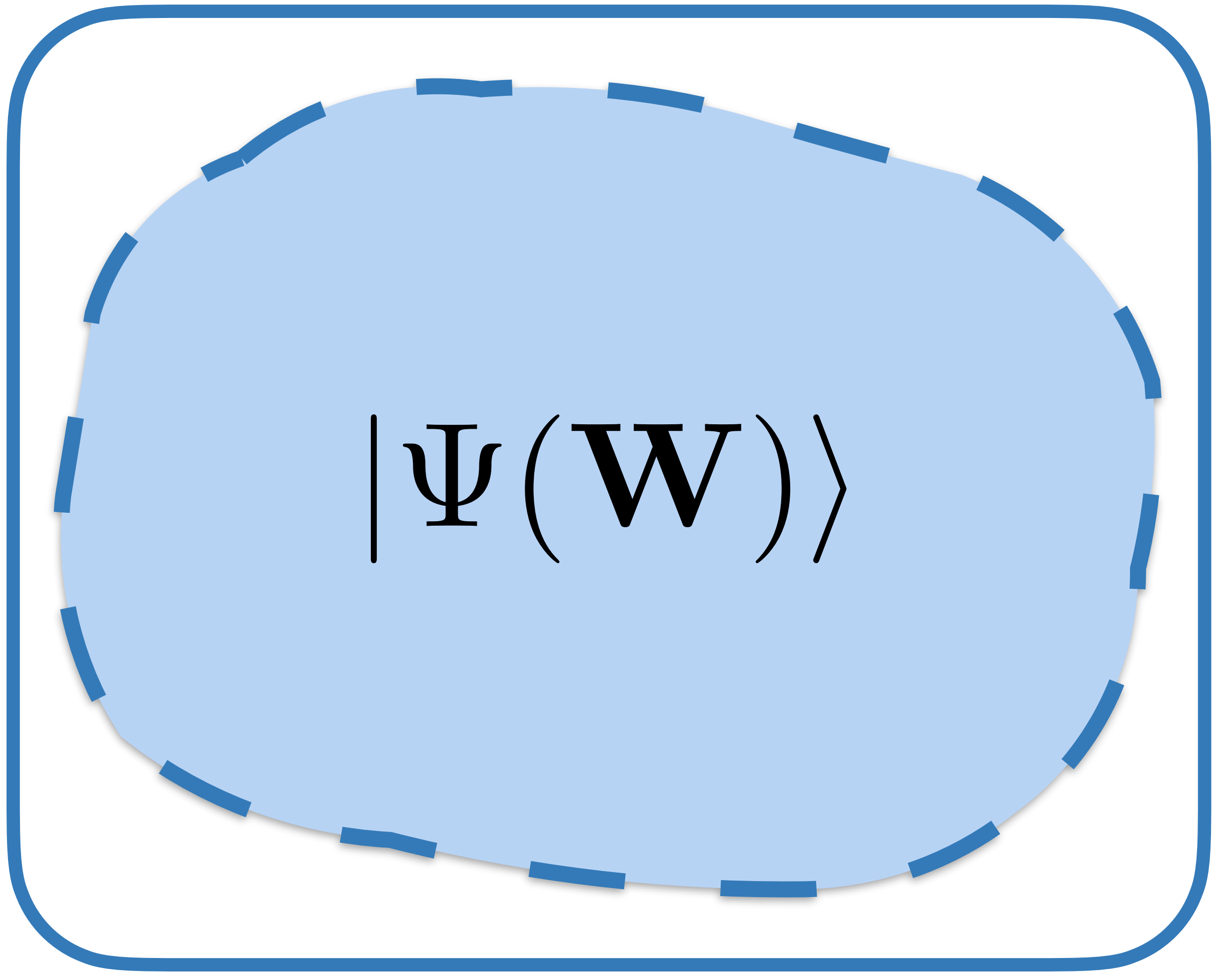
$$|\Psi\rangle$$

Hilbert Space

01.2 - All The States We Care About



01.3 - Variational Representations



Classical Variational States

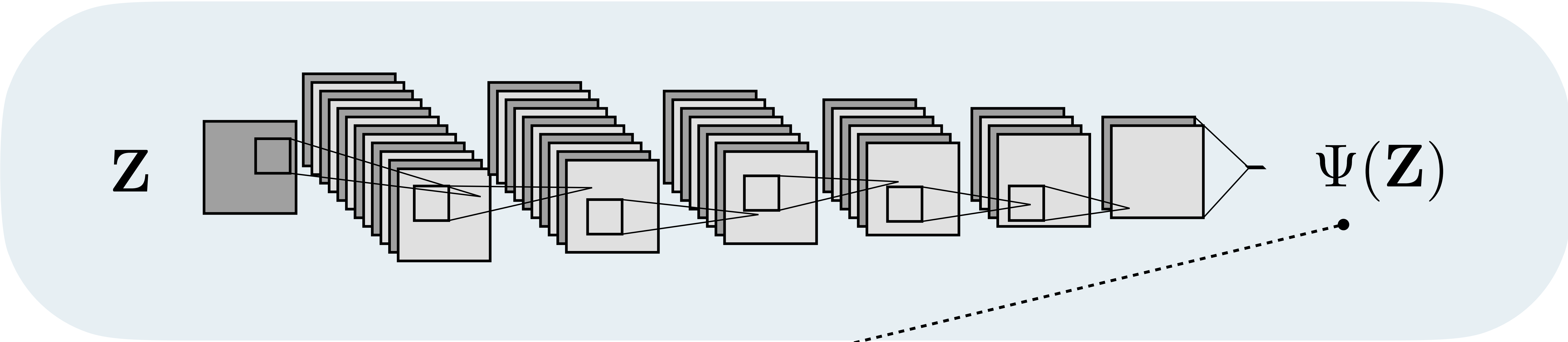
Parameterized Quantum Circuits

02.

Classical Variational Representations.

02.1 - Neural Quantum States

Carleo, and Troyer
Science 355, 602 (2017)



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

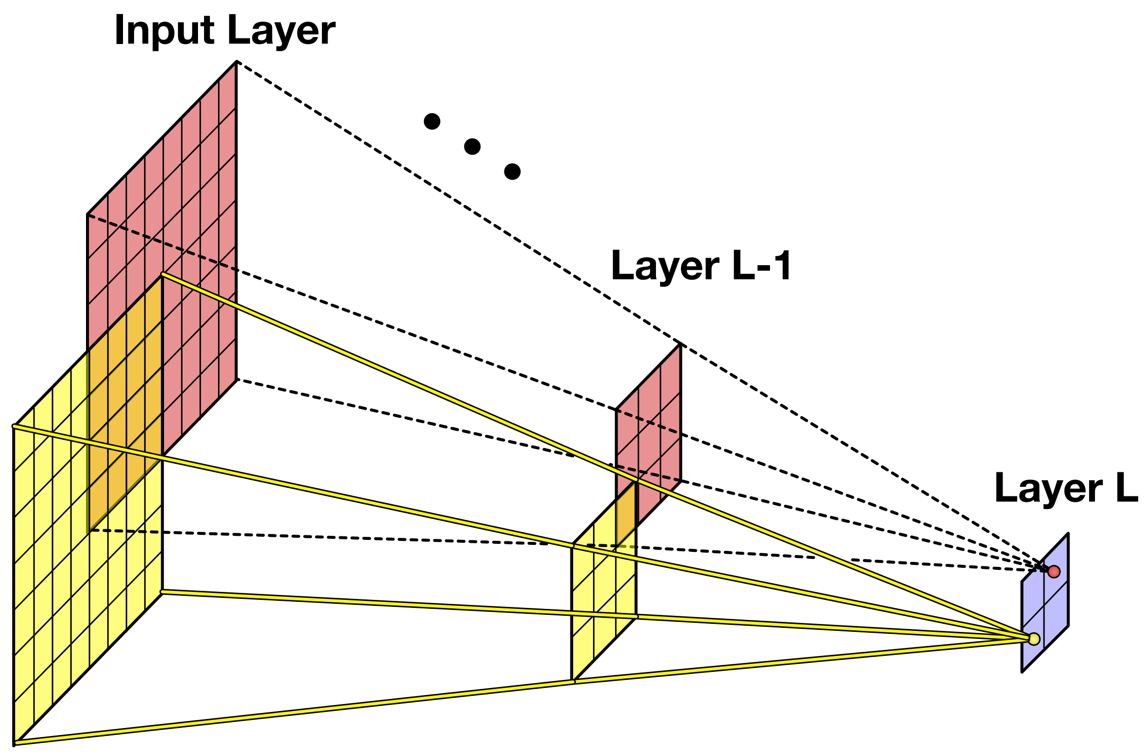
02.2 - Entanglement Properties

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

Universal Approximation Theorems

Kolmogorov and Arnold (1956)

Cybenko (1989)



Volume-Law States

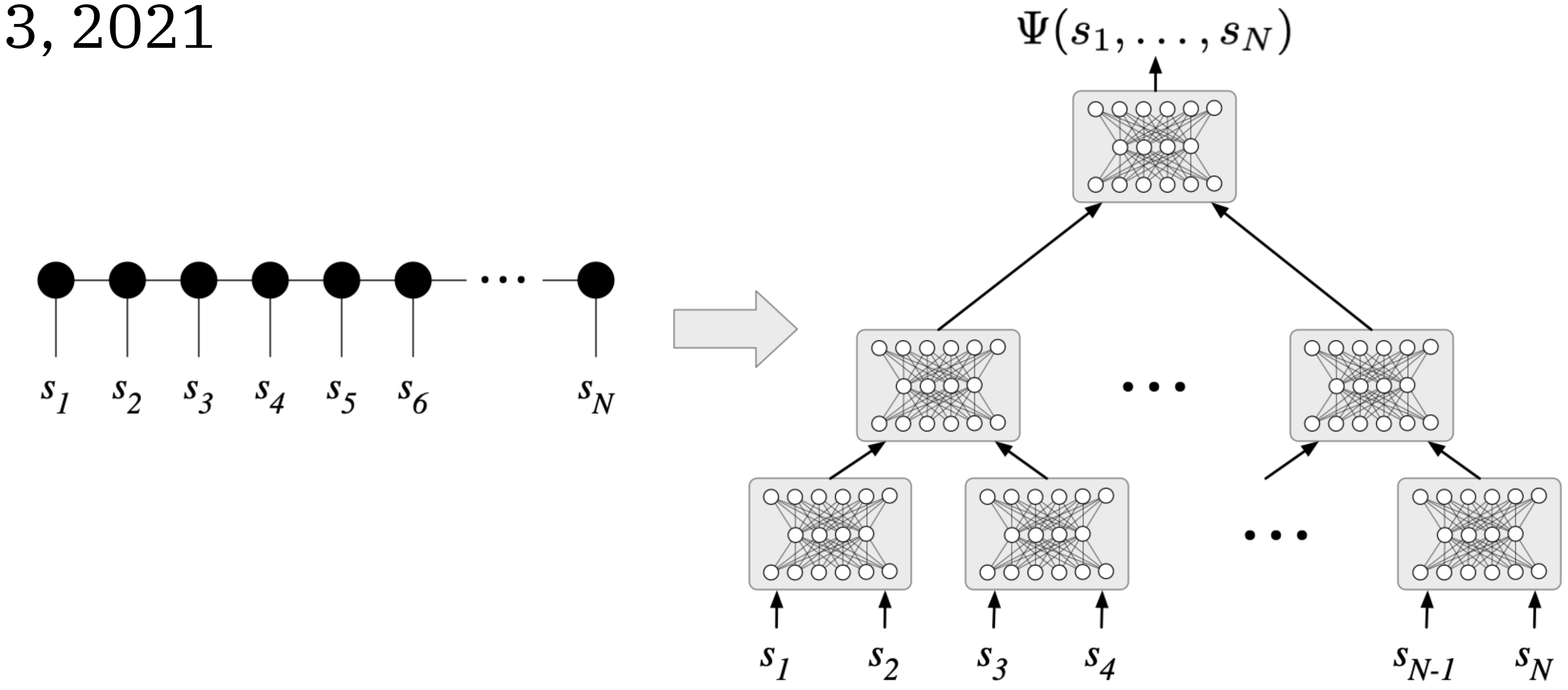
Deng, Li, and Das Sarma
PRX *7, 021021 (2017)*

....

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

02.3 - Neural-Tensor Contractions

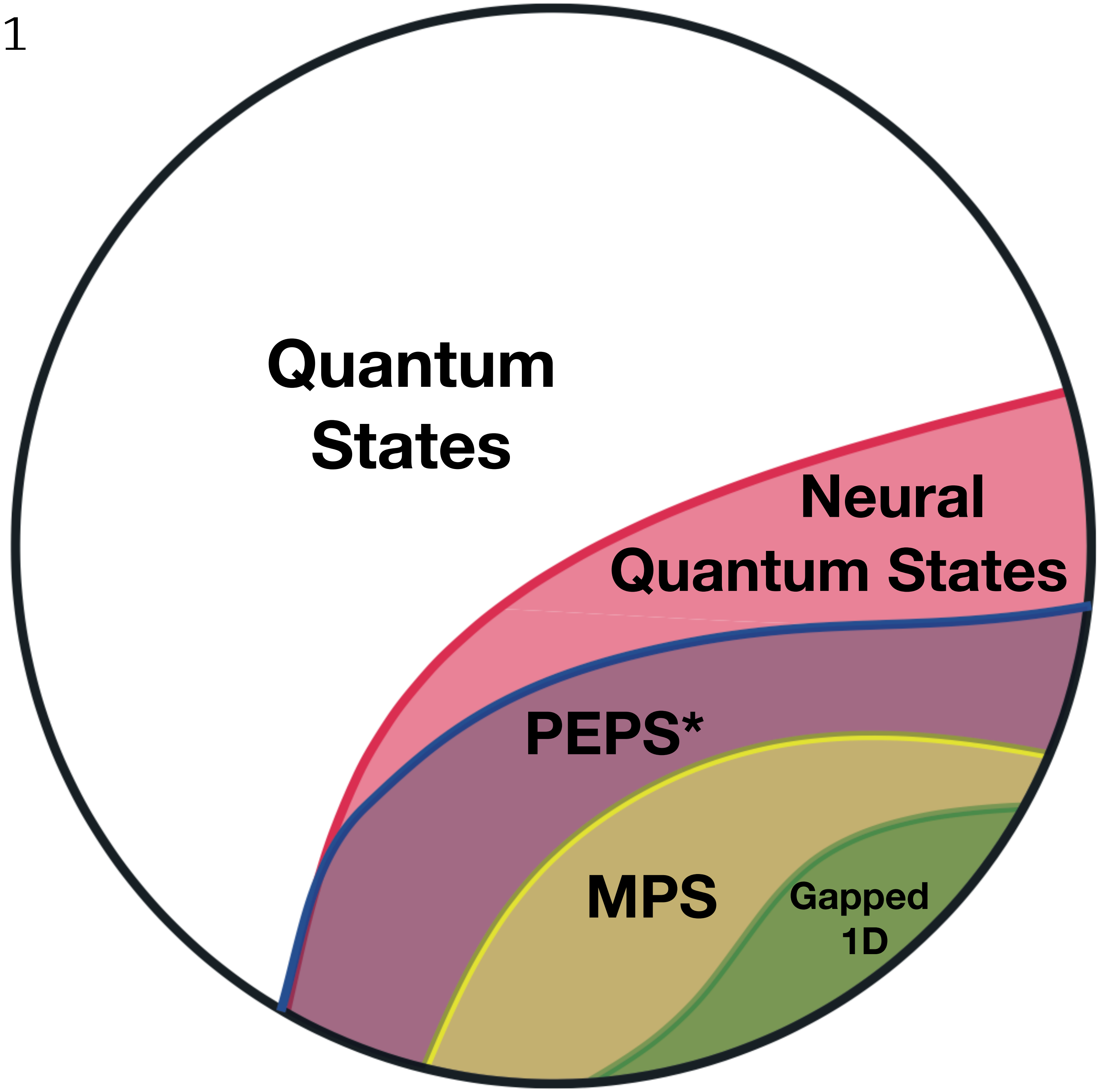
Sharir, Shashua, and Carleo
arXiv:2103.10293, 2021



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)* $O\left(k + \ln^2\left(\frac{kb}{\epsilon}\right) + \ln\left(\frac{1}{\epsilon}\right)\sqrt{\frac{1}{\epsilon}}\right)$.

O2.3 - Representability Diagram

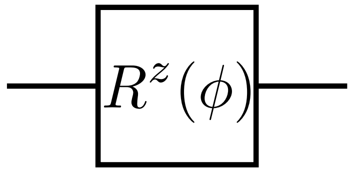
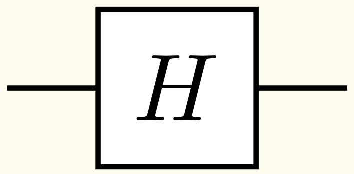
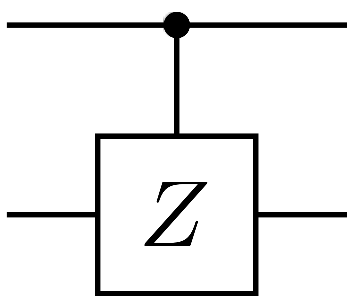
Sharir, Shashua, and Carleo
arXiv:2103.10293, 2021



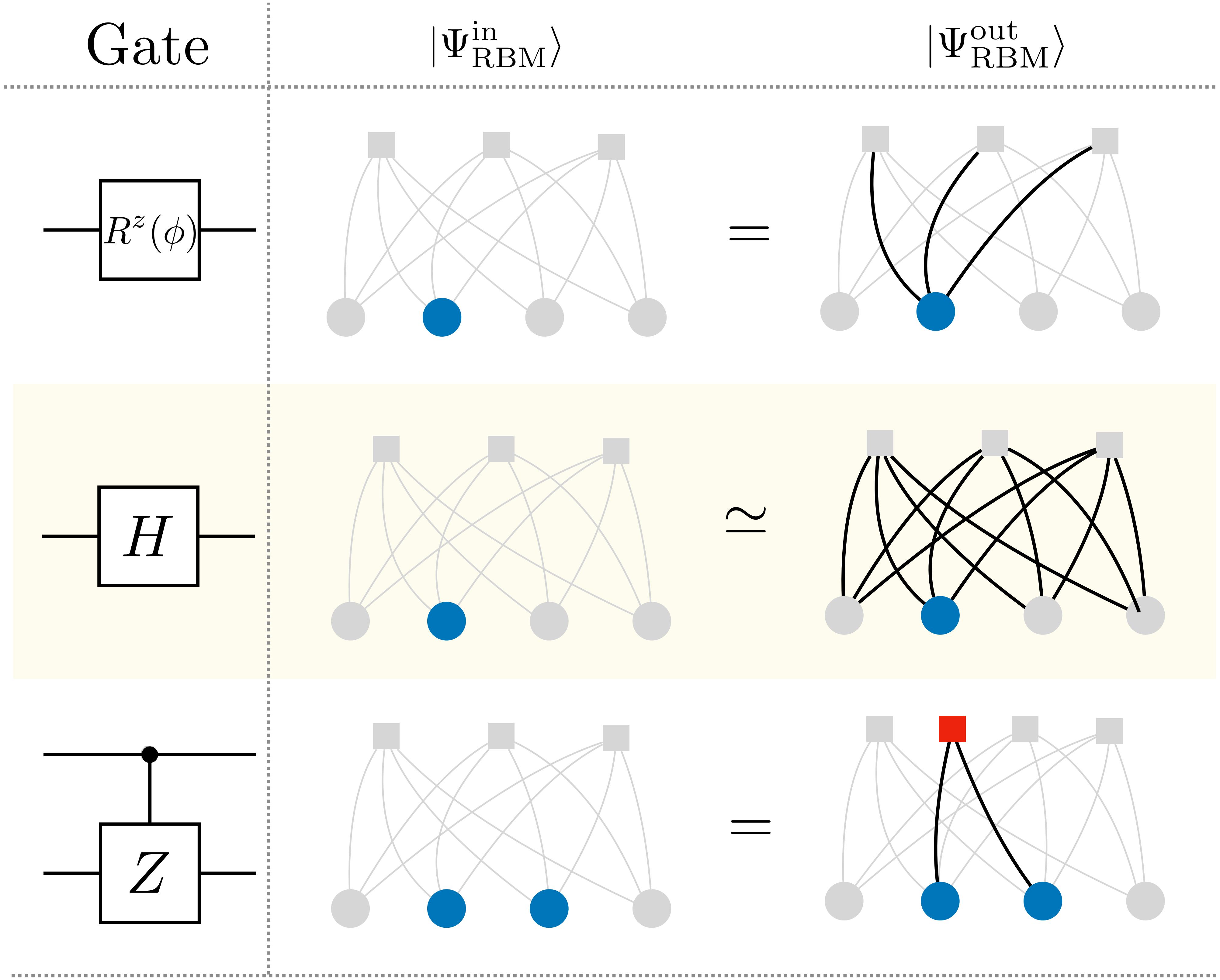
03.

Classical Simulation of Quantum Circuits.

03.1 - Universal Gate Set

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

03.2 - Action on a NQS



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

03.4 - Learning the Hadamard

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

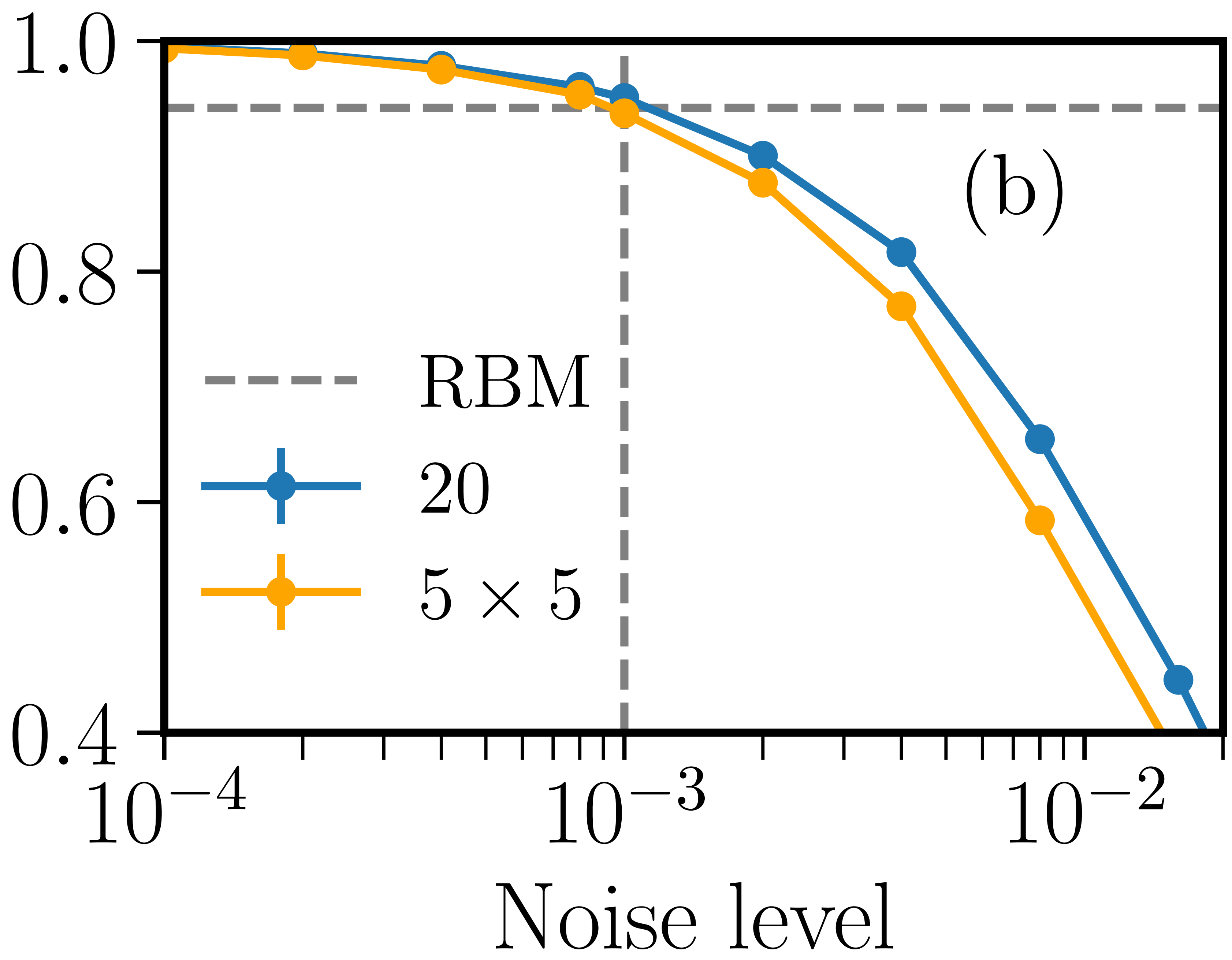
$$|\Psi_{\mathcal{W}'}\rangle \simeq |\Phi\rangle$$

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

Minimize log infidelity

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

03.5 - Noise Versus Error

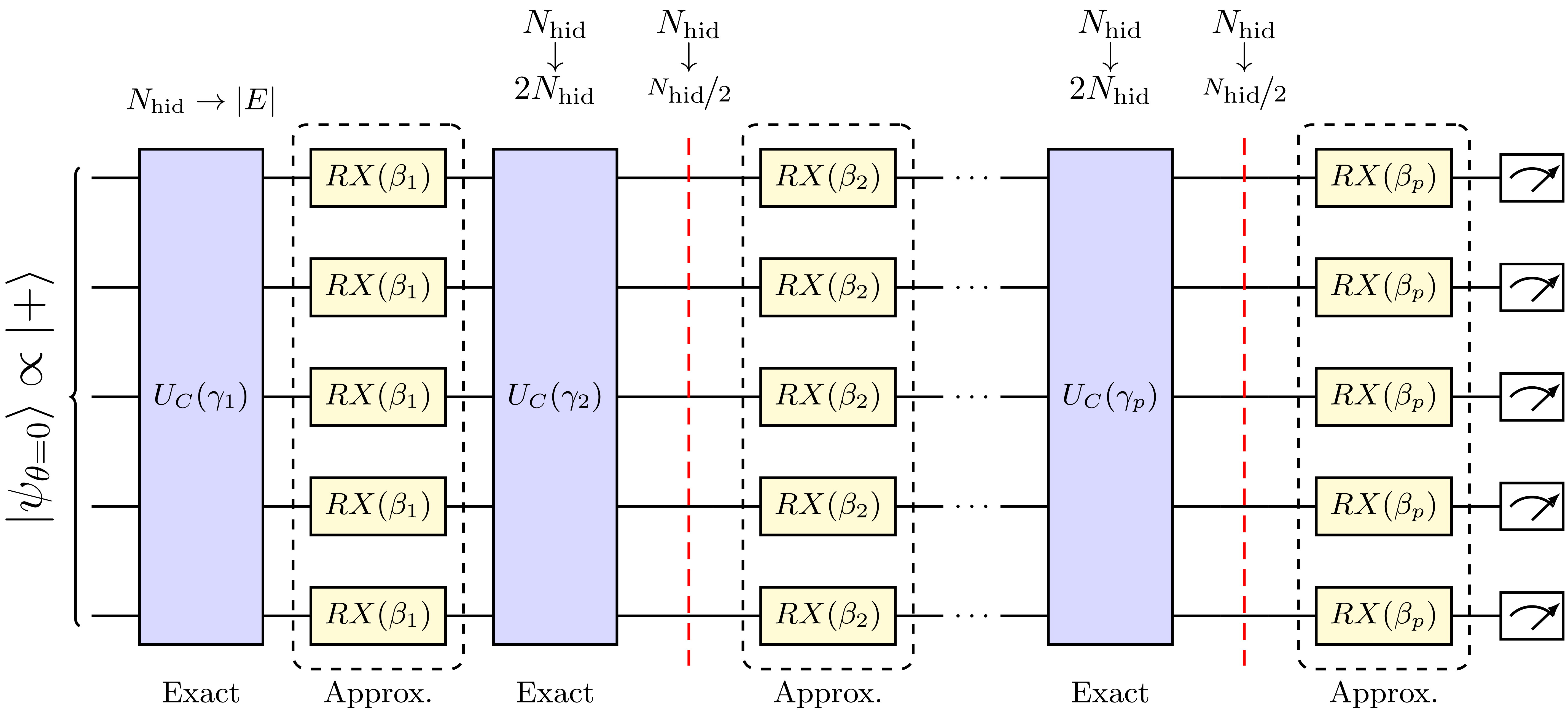


Comparing Variational Error with Depolarization Noise

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

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

03.6 - Simulating QAOA

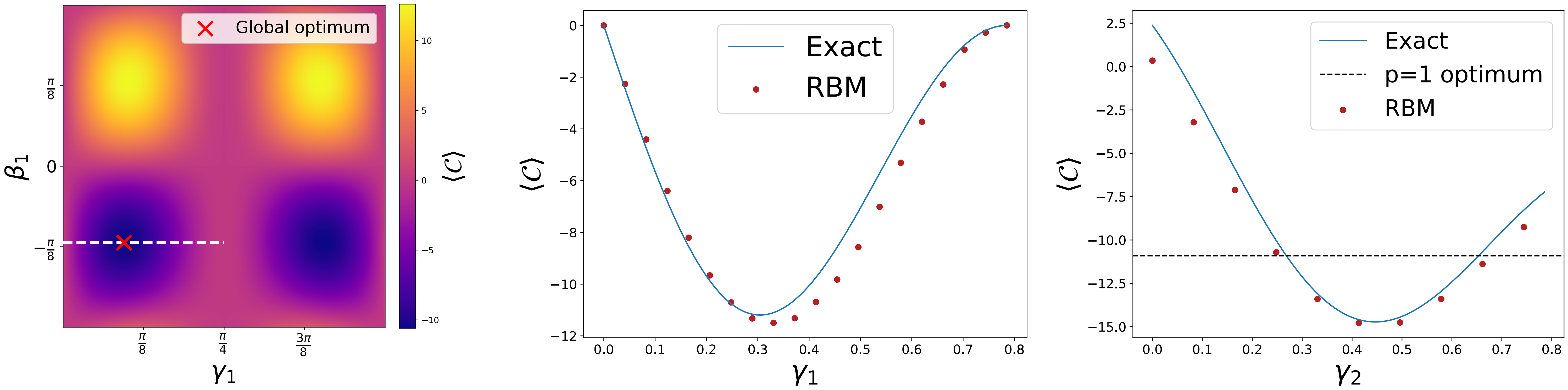


$$U_C(\gamma) = e^{-i\gamma\mathcal{C}} = \prod_{i,j\in E(G)} e^{-i\gamma w_{ij} Z_i Z_j}$$

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

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

O3.7 - Benchmark of Small Circuits

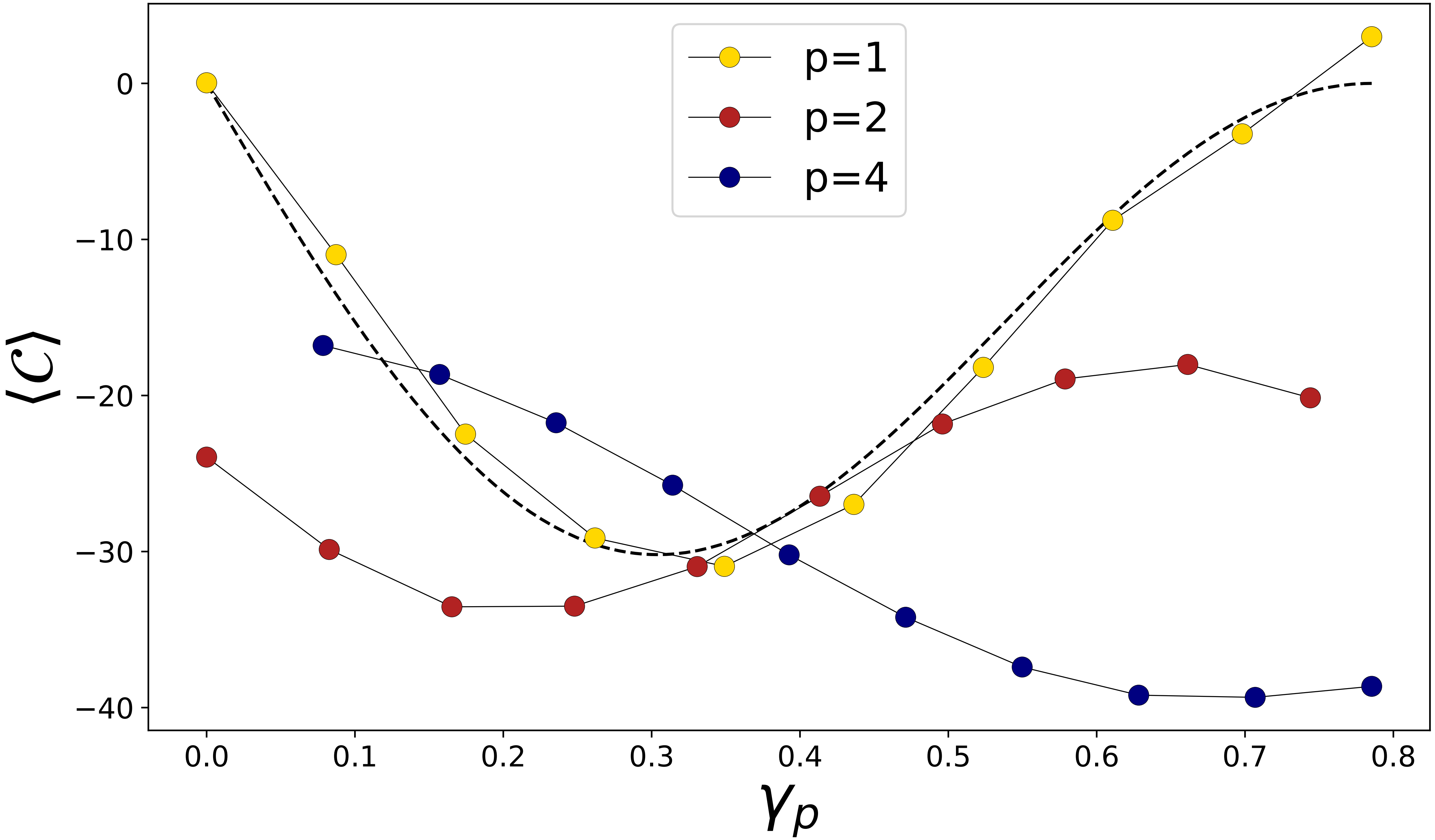


20 Qubits

3-Random Regular Graph

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

O3.8 - Simulating 54 Qubits



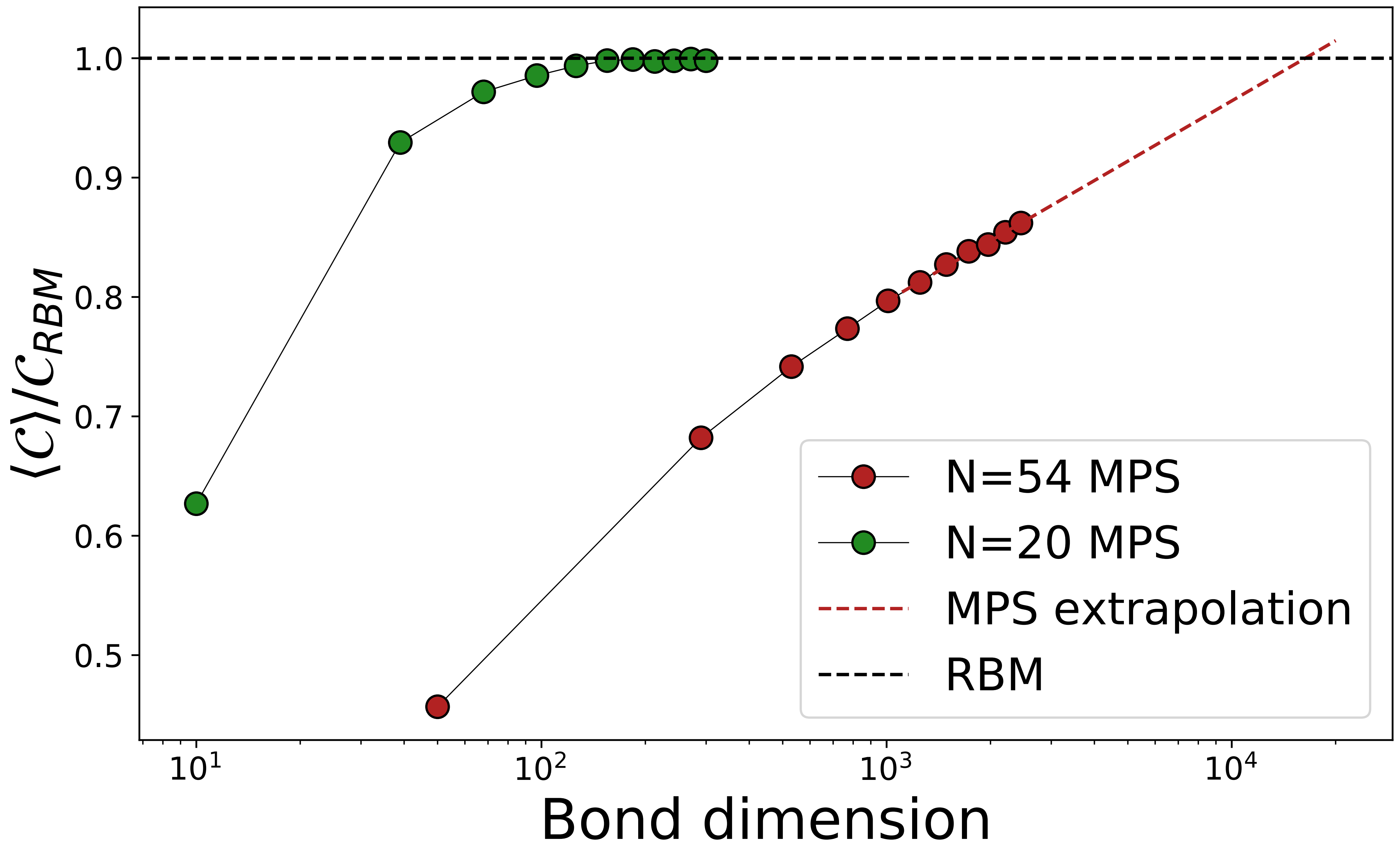
4 Layers

324 RZZ Gates

216 RX Gates

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

O3.9 - Comparing with tensor networks



Estimated Bond Dimension of ~10^4 for similar accuracy

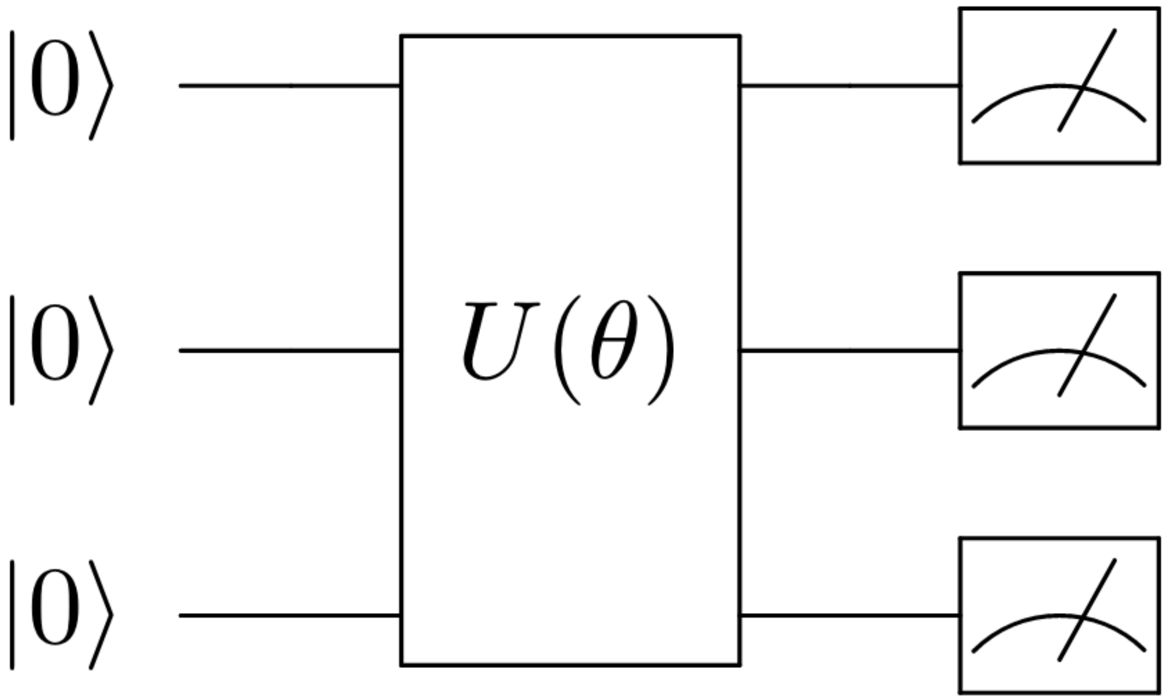
Remark: competitive tensor contraction schemes on similar problems yield only cost function not samples/ wave functions like for MPS/NQS

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

04.

Quantum Variational Representations.

04.1 - General Setup



Parameterized Quantum Circuit

$$L(\theta)$$
$$\nabla_\theta L(\theta)$$

Stochastic Estimate of Loss Function and Gradients

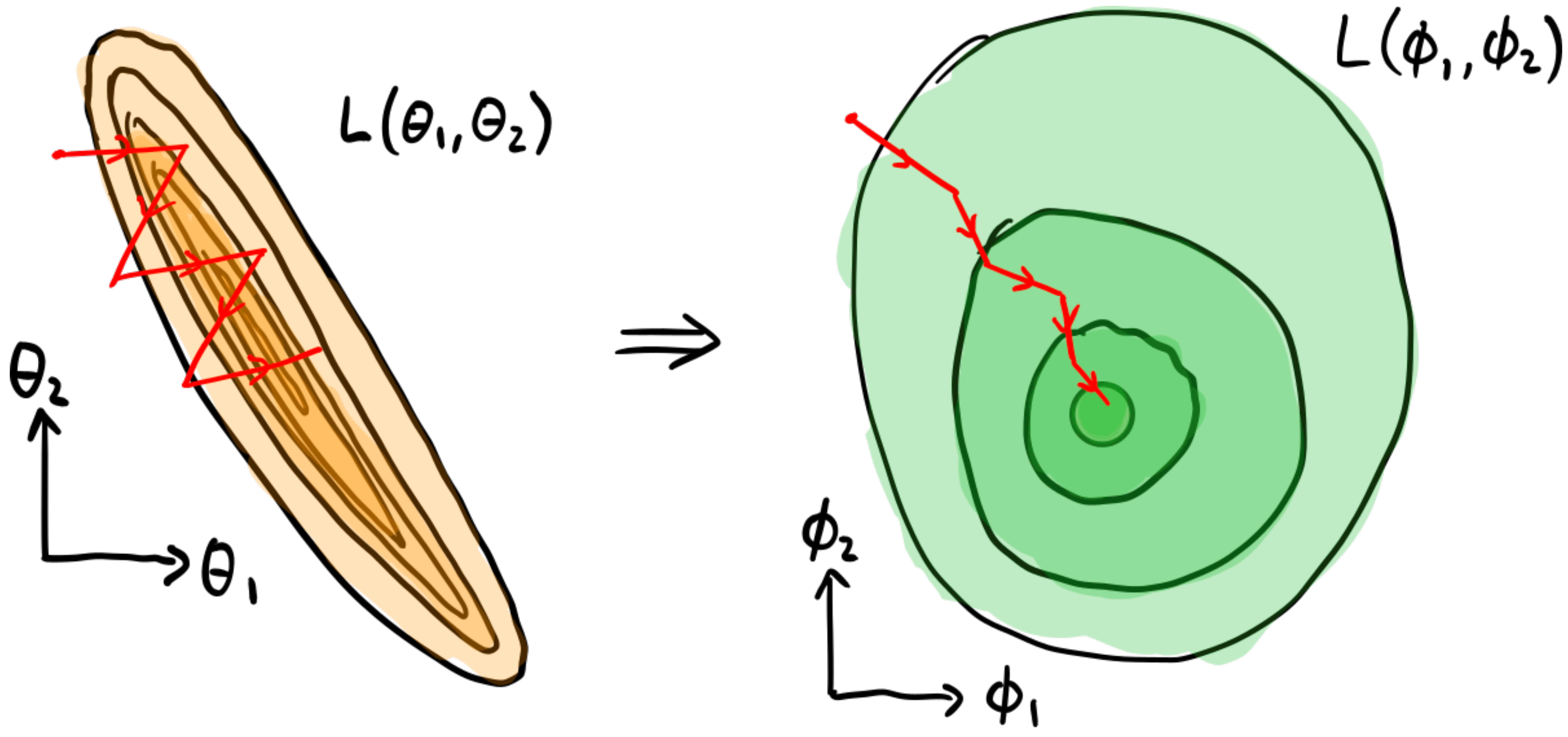
$$\theta^{(k+1)} = \theta^k - \eta \nabla_\theta L(\theta)$$

Iterative Minimization

04.2 - Quantum Natural Gradient

$$\theta^{(k+1)} = \theta^k - \eta g^{-1}(\theta^k)\nabla_\theta L(\theta)$$

Shun-Ichi Amari
Neural Computation 10, 251 (1998)



Stokes, Izaac, Killoran, and Carleo
Quantum 4, 269 (2020)

$$g_{ij}(\theta) = \mathrm{Re}\left[\left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \Psi \right\rangle \left\langle \Psi \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle\right]$$

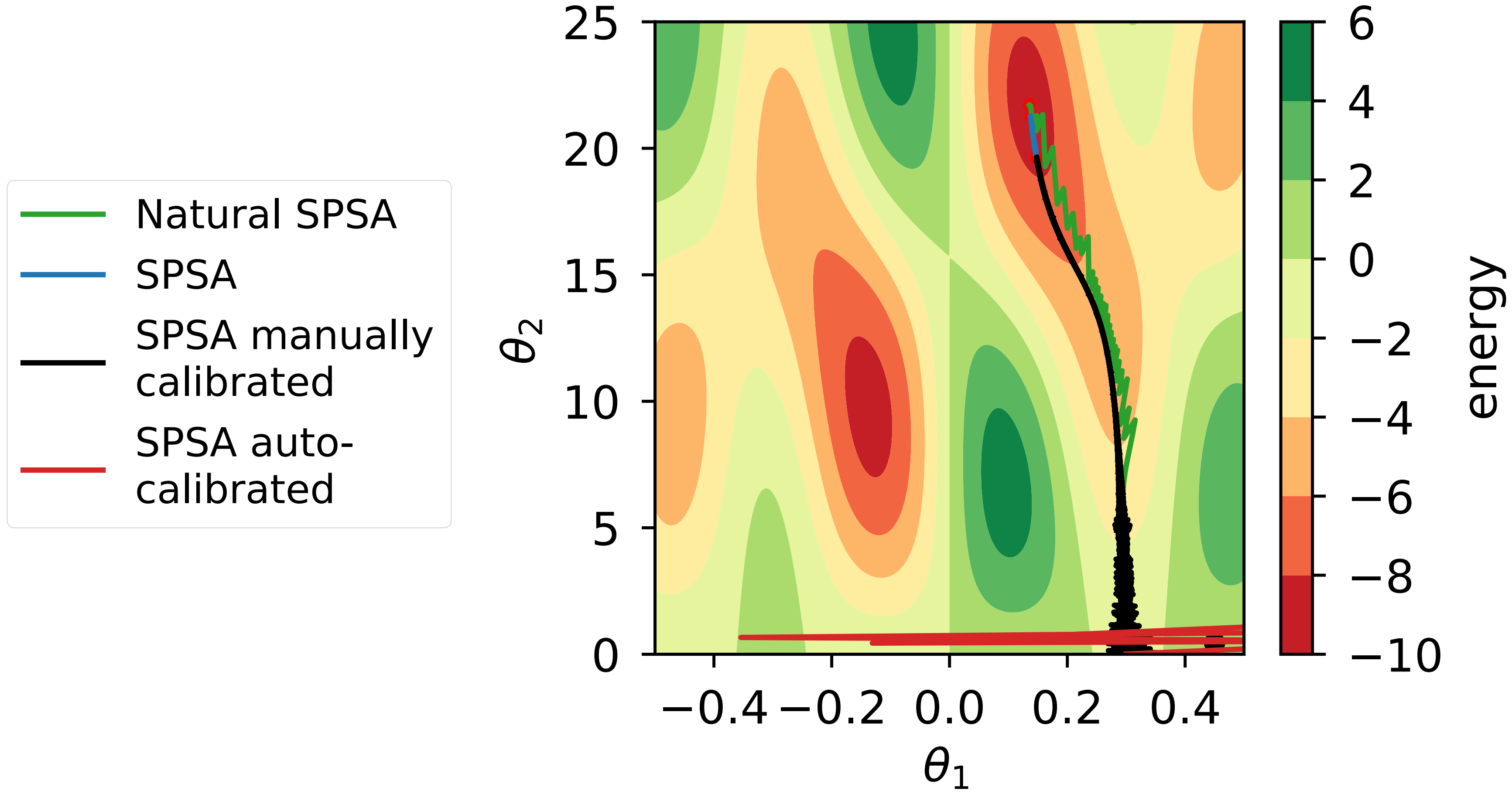
04.3 - Strong Interplay With Classical Methods

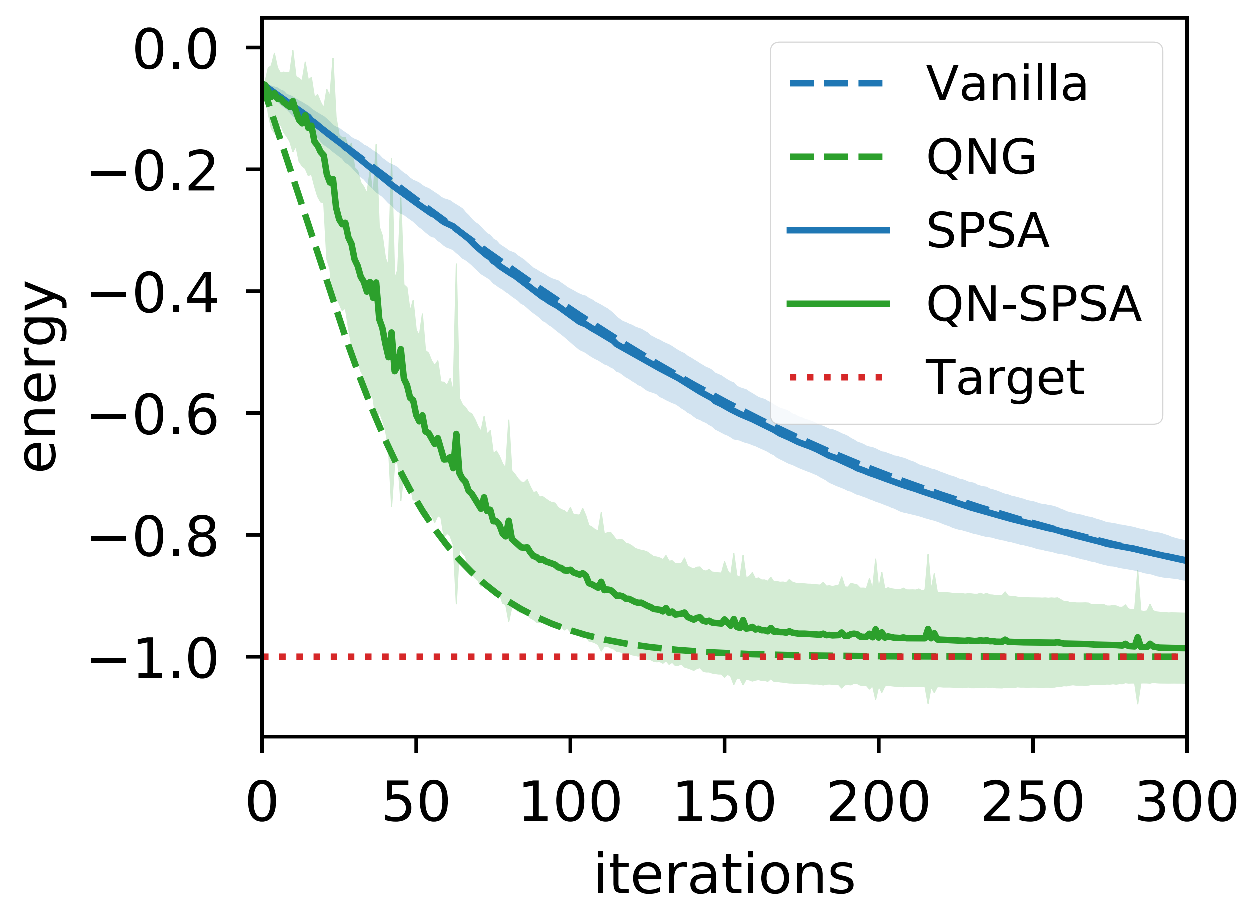
Problem	**Classical Stochastic**	**Quantum**
Variational Minimization	Variational Monte Carlo [*McMillan*, 1965]	Variational Quantum Eigensolver [*Peruzzo et al*, 2014]
Variational Imaginary Time Evolution	Stochastic Reconfiguration [*Sorella*, 1998]	[*McArdle et al*, 2019]
Variational Real Time Evolution	Time-Dependent Variational Monte Carlo [*Carleo et al*, 2012]	TDVA [*Lee and Benjamin*, 2017]
Machine Learning	Natural Gradient Descent [*Amari*, 1998]	Quantum Natural Gradient Descent [*Stokes et al*, 2020]

04.4 - Fast Quantum Natural Gradient: QN-SPSA

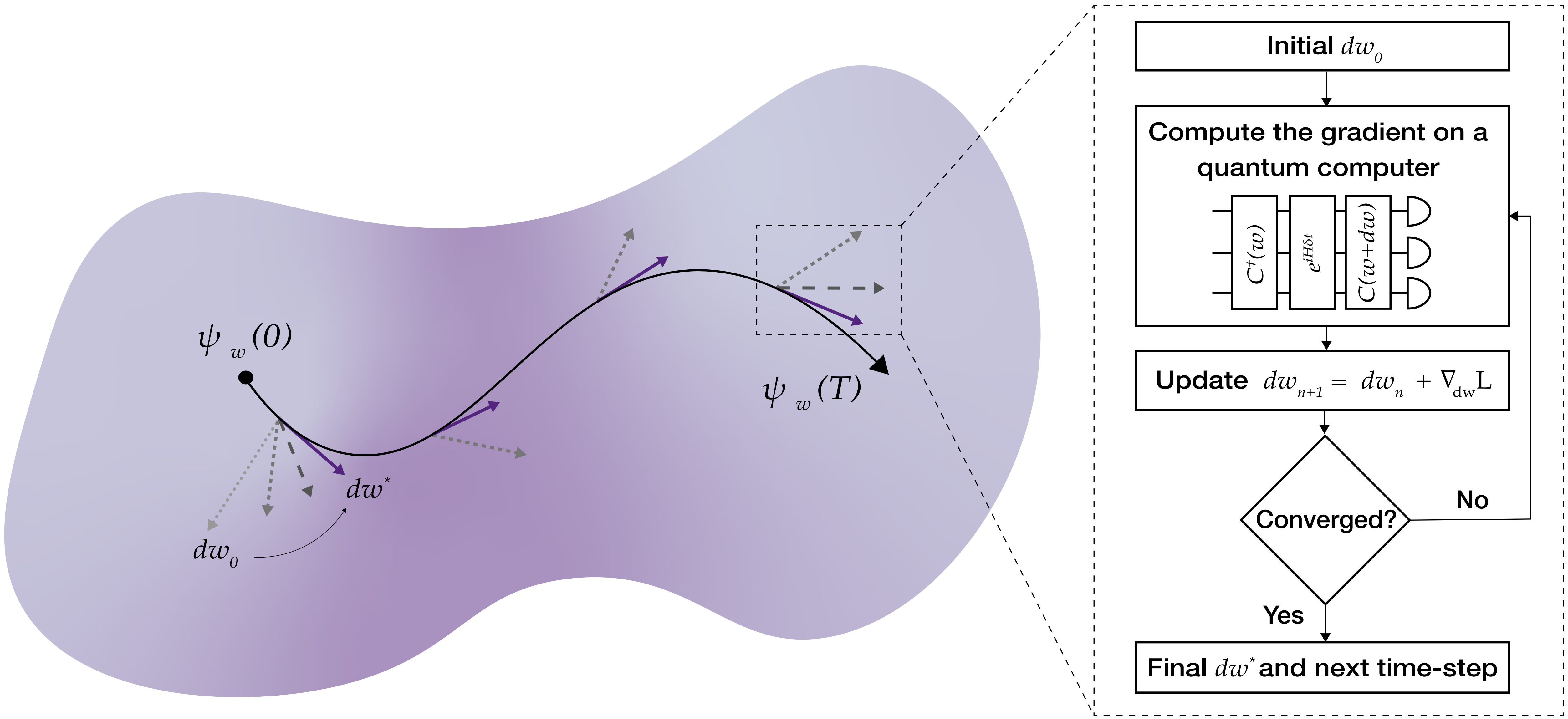
$$g_{ij}(\theta) = -\frac{1}{2}\frac{\partial}{\partial\theta_i}\frac{\partial}{\partial\theta_j}\left|\langle\psi_{\theta'}|\psi_\theta\rangle\right|^2\Big|_{\theta'=\theta}$$

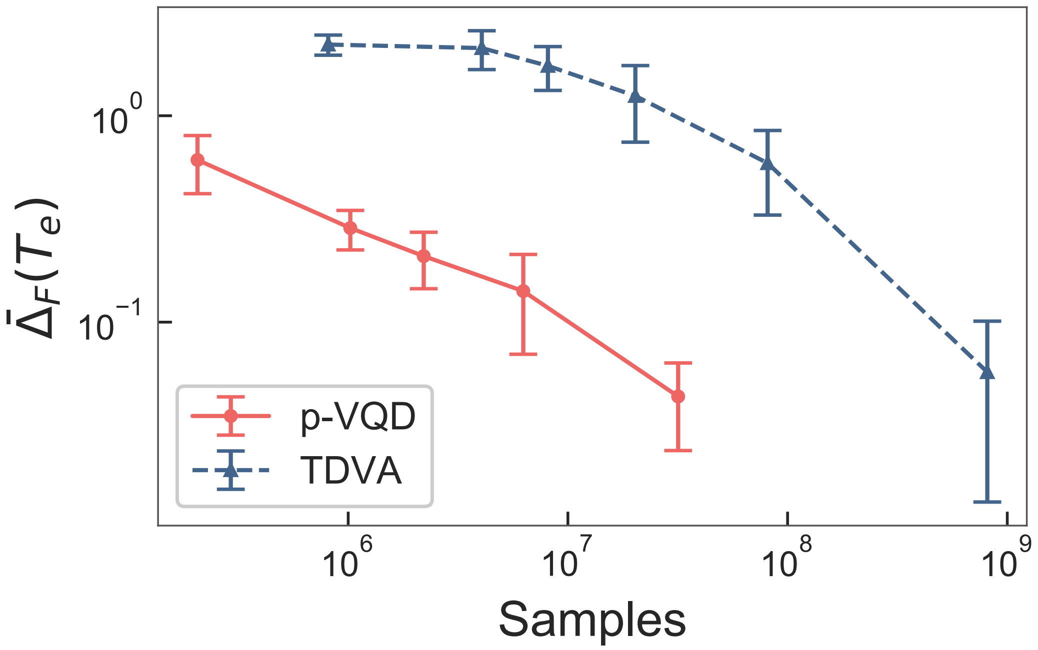
Gacon, Zoufal, Carleo, and Woerner
arXiv:2103.09232, (2021)





04.5 - Fast Variational Real-Time Evolution: p-VQD





Barison, Vicentini, and Carleo
arXiv:2101.04579, (2021)

05.

“Shot" Noise Reduction.

05.1 - The Problem

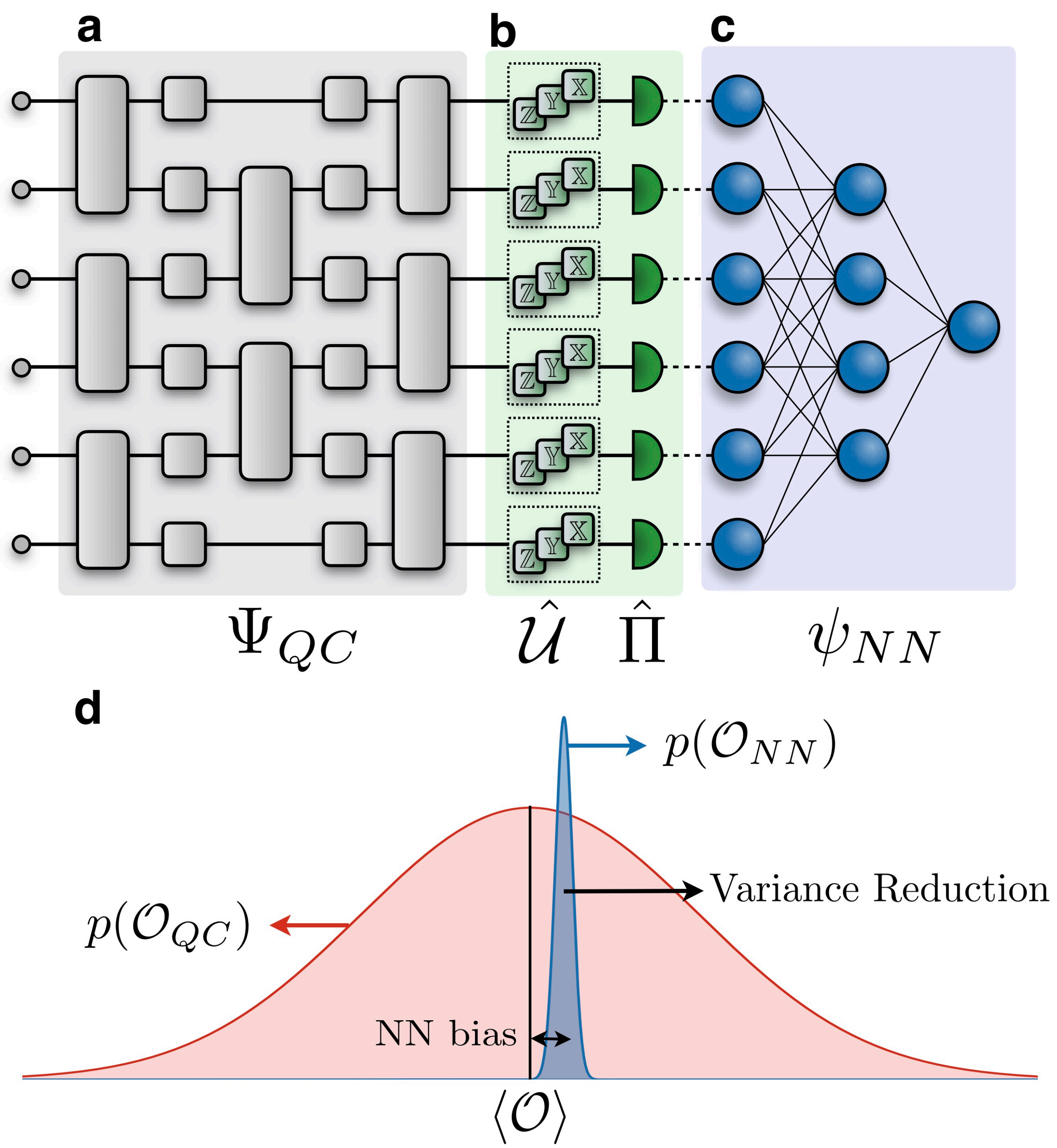
Precise Estimates of Physical Observables
typically require several millions or more of
measurements even on very small systems

Examples: Estimate Energy Using Measurements in Pauli Basis;
Estimate Entanglement Entropy...

$$\mathcal{H} = \sum_k c_k \sigma_1^{(x,y,z)} \ldots \sigma_N^{(x,y,z)}$$

05.2 - Trade Variance With (Small) Bias

Torlai, Mazzola, Carleo, and Mezzacapo
Phys. Rev. Research 2, 022060 (2020)



Prepare Quantum State

Do “Standard” Pauli Measurements

Learn an approximate Classical State

Enjoy “Zero-Variance”

Property

of Classical State

O5.3 - Neural-Network Quantum State Tomography

Torlai, Mazzola, Carrasquilla, Troyer, Melko, and Carleo
Nature Physics (2018)

Neural-Network Training: find $\mathbf{W}$ such that

$|\Psi_b(\mathbf{s}, \mathbf{W})|^2 \simeq P_b(\mathbf{s})$ in all given bases

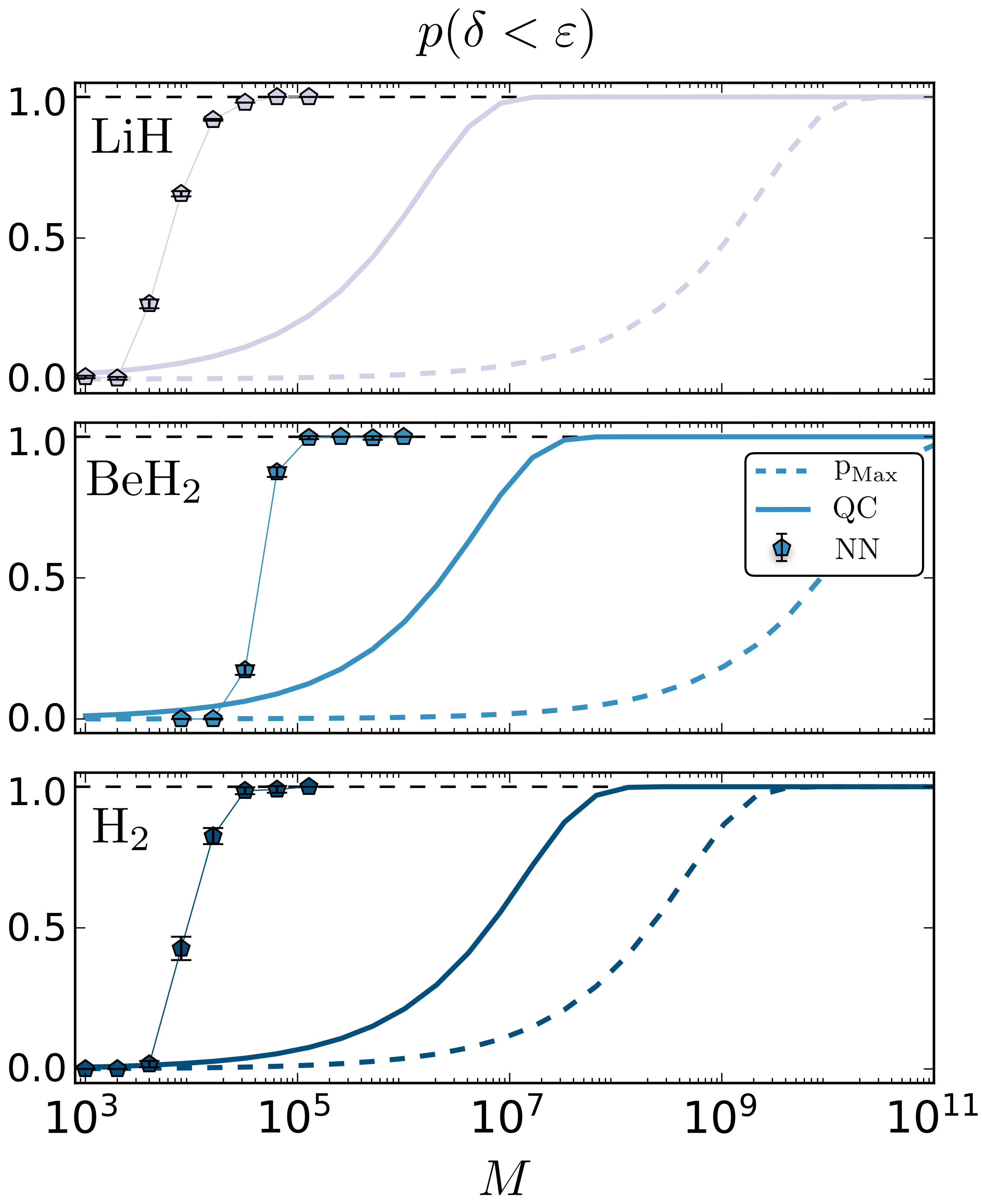
$$\Psi_b(\mathbf{s}, \mathbf{W}) = \sum_{\mathbf{s}'} \Psi(\mathbf{s}, \mathbf{W}) U^b_{s,s'}$$

Sparse Unitary Matrices

$$\mathcal{L}(\mathbf{W}) = \sum_b \sum_{\mathbf{s}} P_b(\mathbf{s}) \log \frac{P_b(\mathbf{s})}{|\Psi_b(\mathbf{s}, \mathbf{W})|^2}$$

Minimise Sum of Kullback-Leibler Divergences

O5.4 - Probability of "Chemical Accuracy"



Reduce number of measurements by few orders of magnitude

Torlai, Mazzola, Carleo, and Mezzacapo
Phys. Rev. Research 2, 022060 (2020)

06.

Outlook.

Classical Variational Simulation

Highly Entangled State

Exact Sampling [Autoregressive]

Heuristic Approach

Need to approximate some gates

Quantum Variational Simulation

Potentially More Expressive

“Arbitrary” Unitaries

Noise

Shallow Circuits

Medvidovic, and Carleo
arXiv:2009.01769 (2020)

Sharir, Shashua, and Carleo
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