Hybrid Variational Classical-Quantum computing

The Machine Learning way.

Computational Quantum Science Lab.

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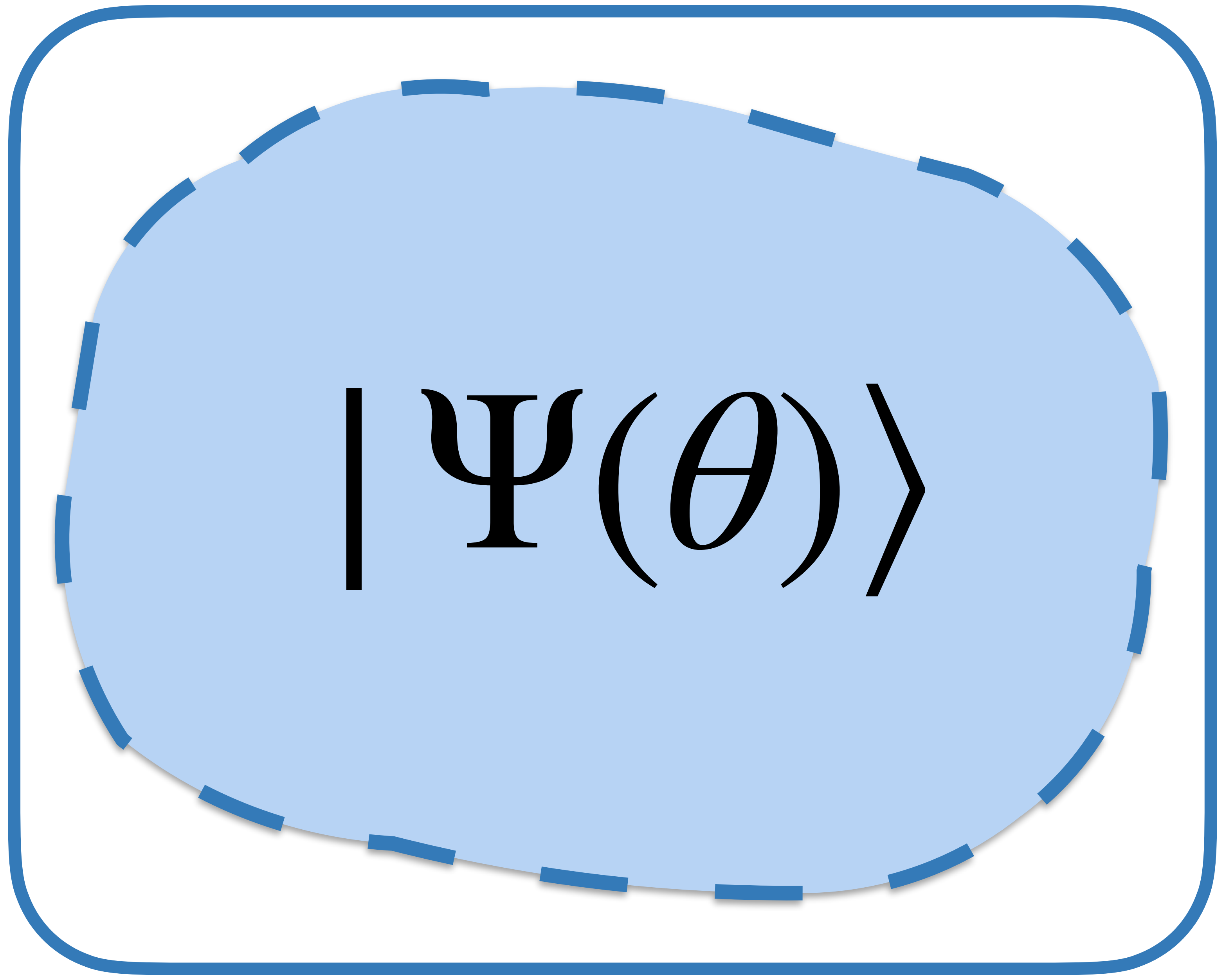
01.

Variational Representations and Methods.

01.1 - Variational Representations of Quantum States

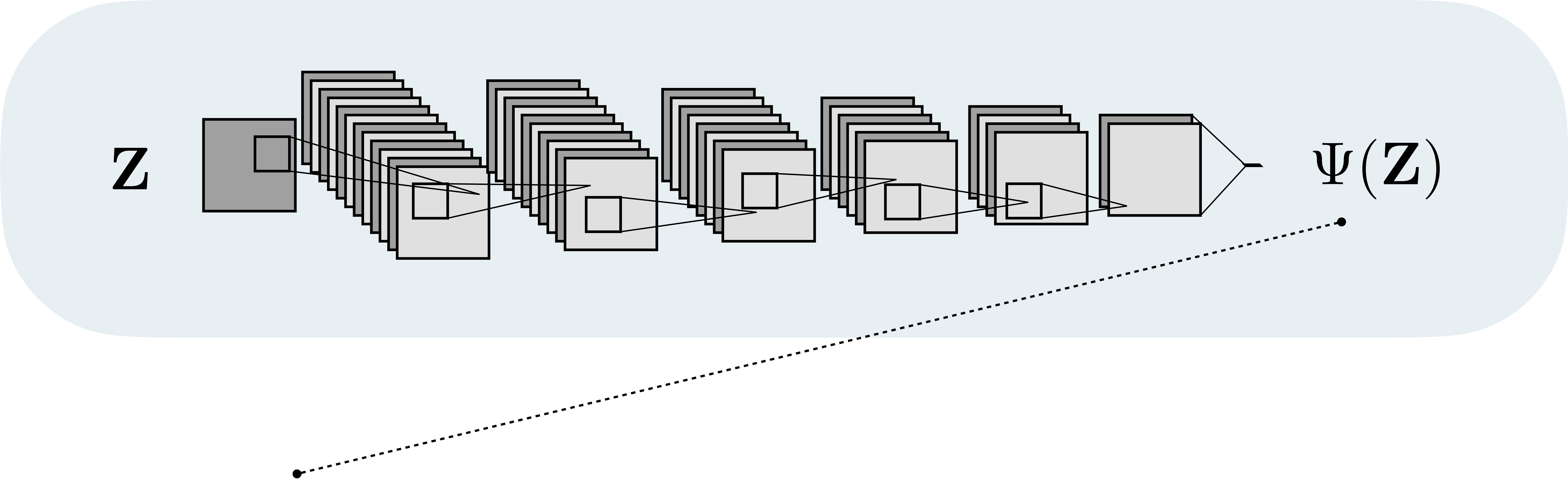


Classical Representations

Quantum Representations

01.2 - Personal Favorite: Neural Quantum States

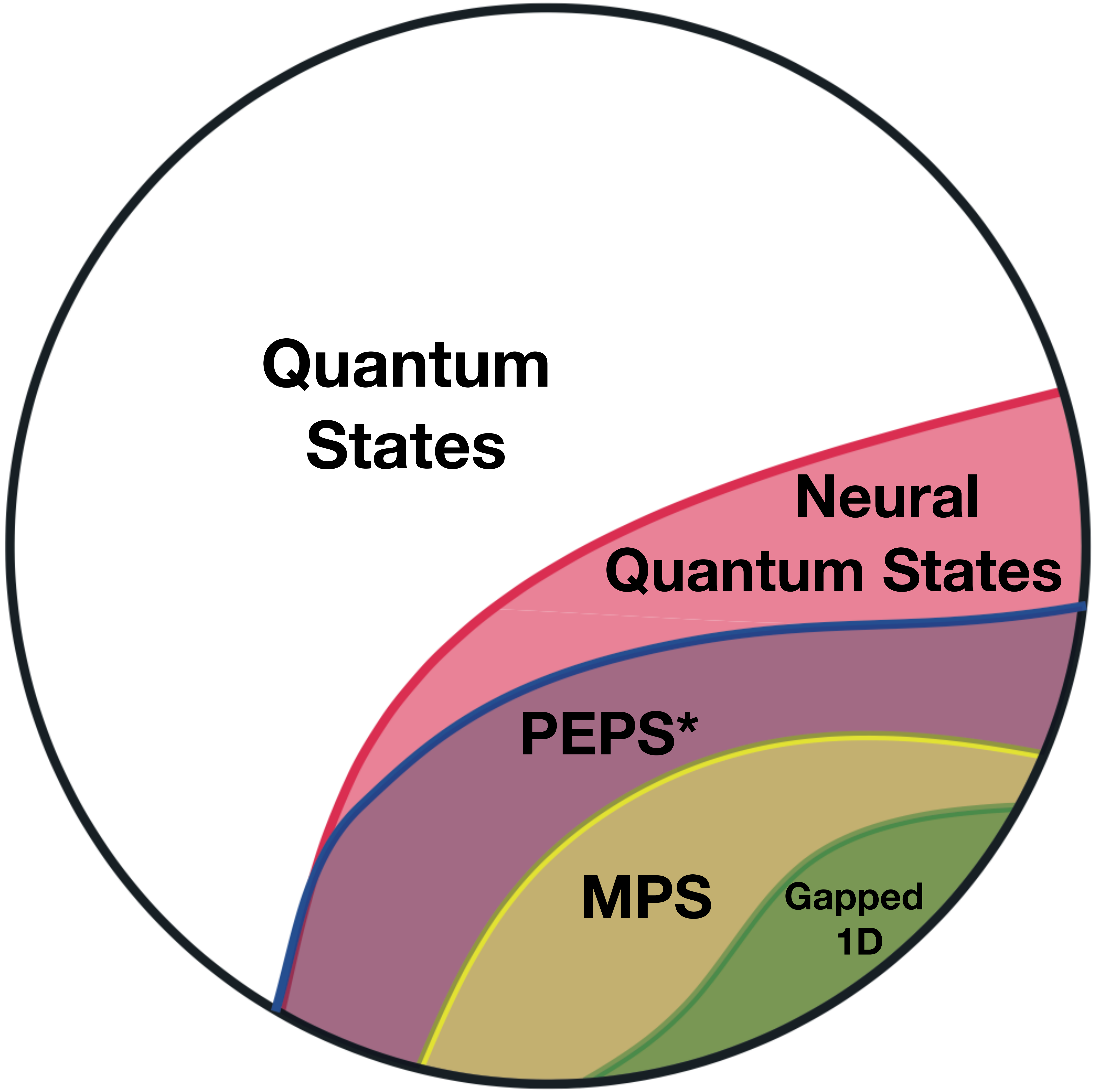
Carleo, and Troyer
Science 355, 602 (2017)



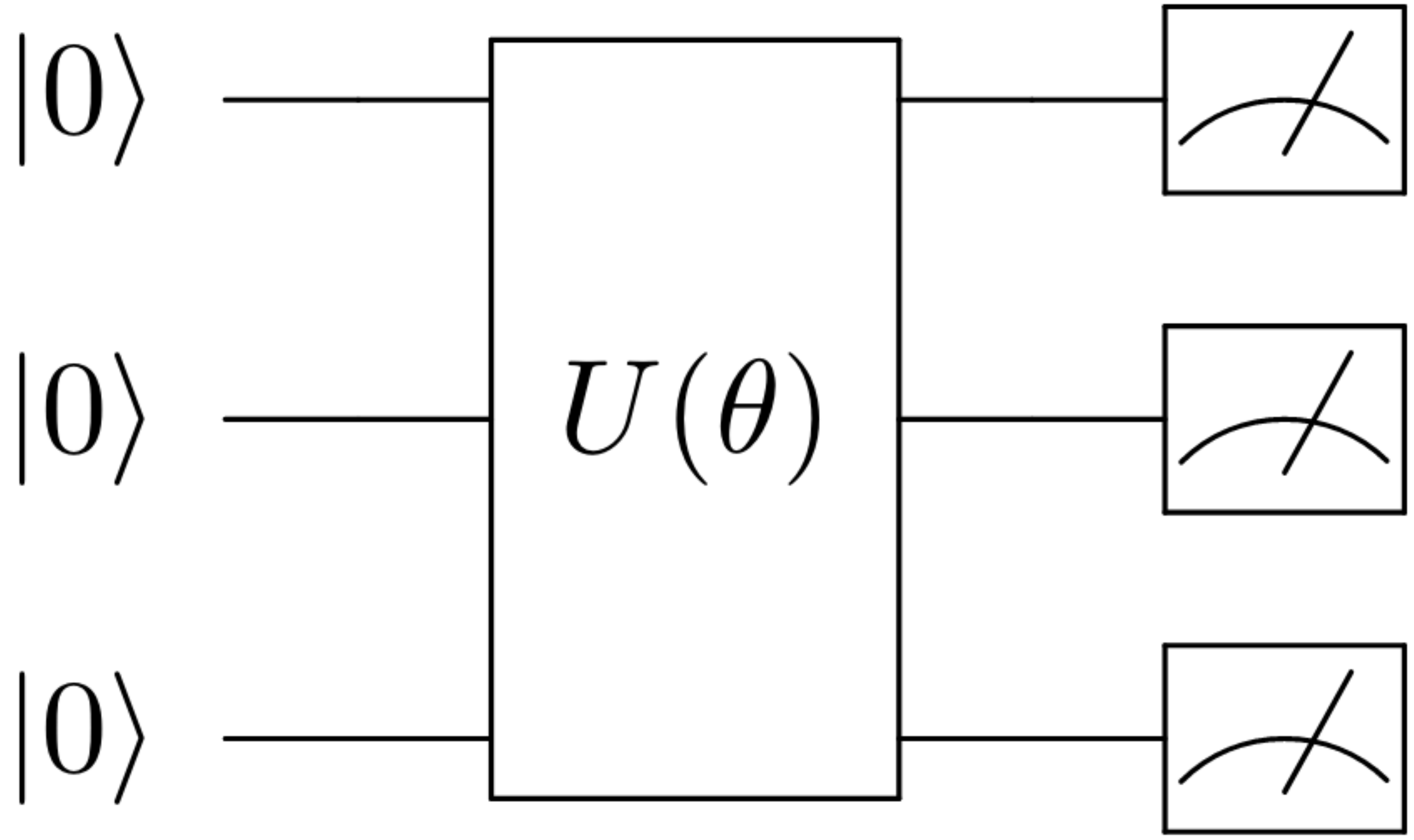
$$\langle Z_1 Z_2 \ldots Z_N | \Psi \rangle = g^{(L)} \circ W^{(L)} \ldots g^{(2)} \circ W^{(2)} g^{(1)} \circ W^{(1)} \mathbf{Z}$$

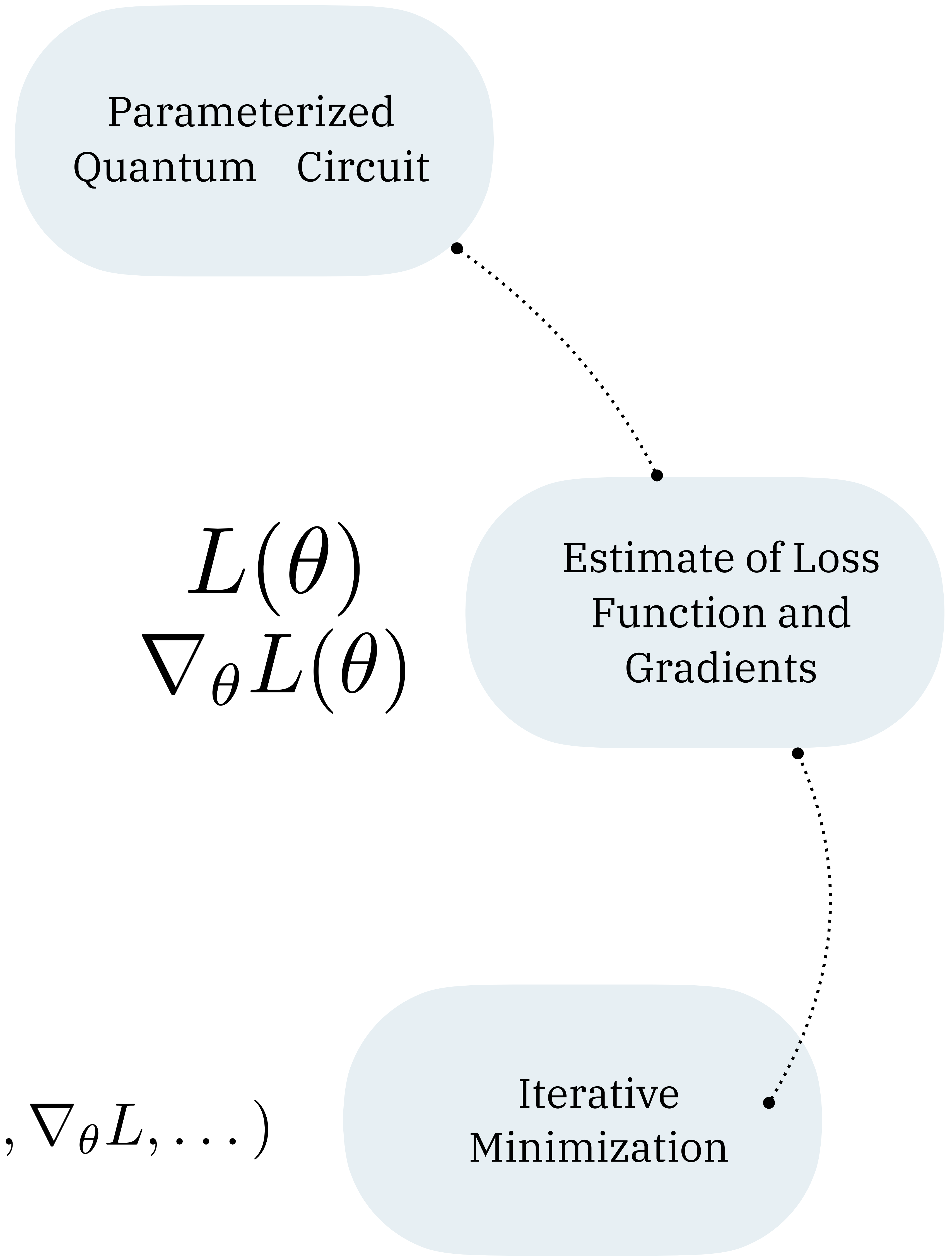
01.3 - Classical Representability Diagram

Sharir, Shashua, and Carleo
arXiv:2103, 10293 (2021)



01.4 - Second Personal Favorite: Parameterized Quantum Circuits





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

$$\theta^{(n+1)} = \theta^{(n)} + \Delta_\theta(\theta^{(n)}, L, \nabla_\theta L, \dots)$$

01.5 - Strong methodological interplay

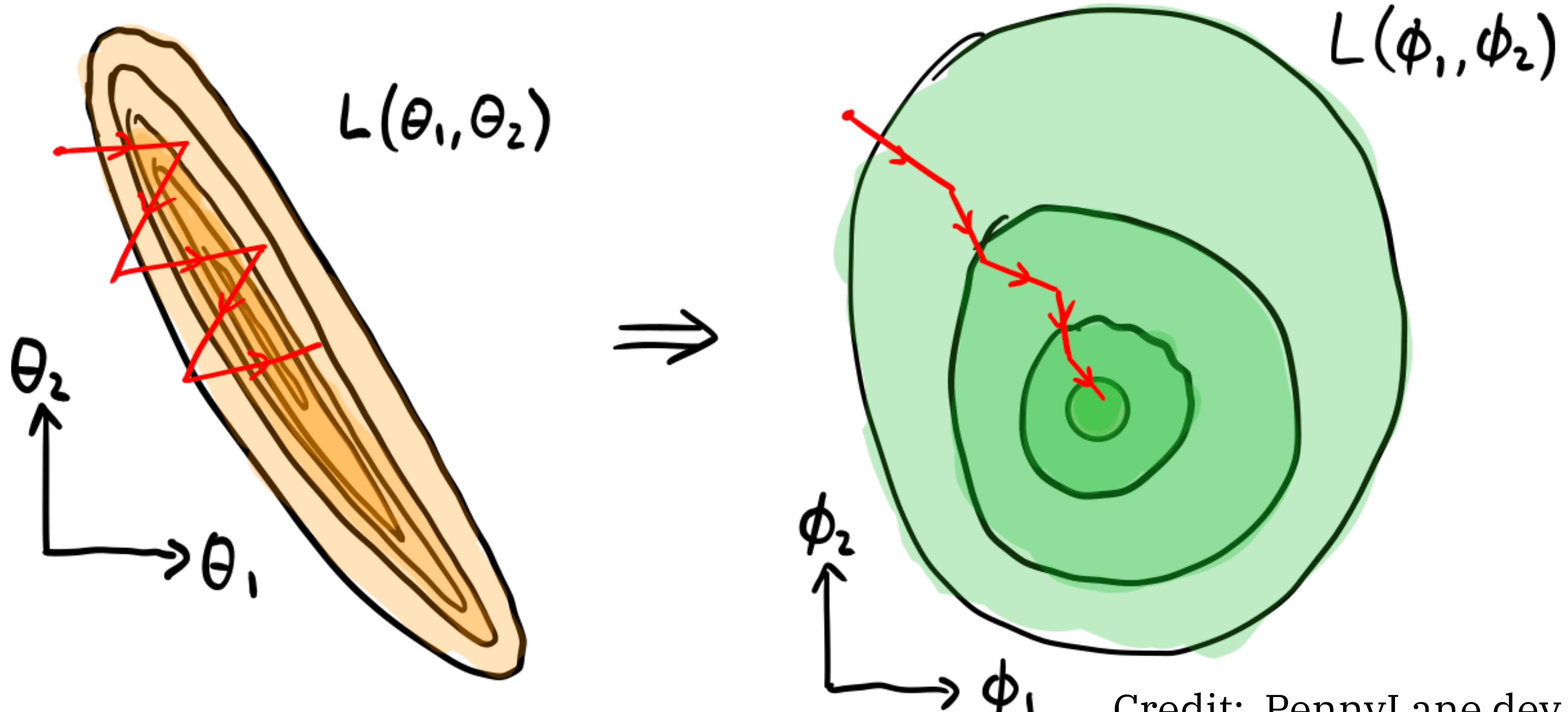
$$Z \sim |\langle Z|\Psi(\theta)\rangle|^2$$

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]

02.

Quantum Natural Gradient.

02.1 - Natural Gradient Descent



Credit: PennyLane dev

$$\theta^{(n+1)} = \theta^{(n)} - \eta g^{-1}(\theta^{(n)})\nabla L(\theta^{(n)})$$

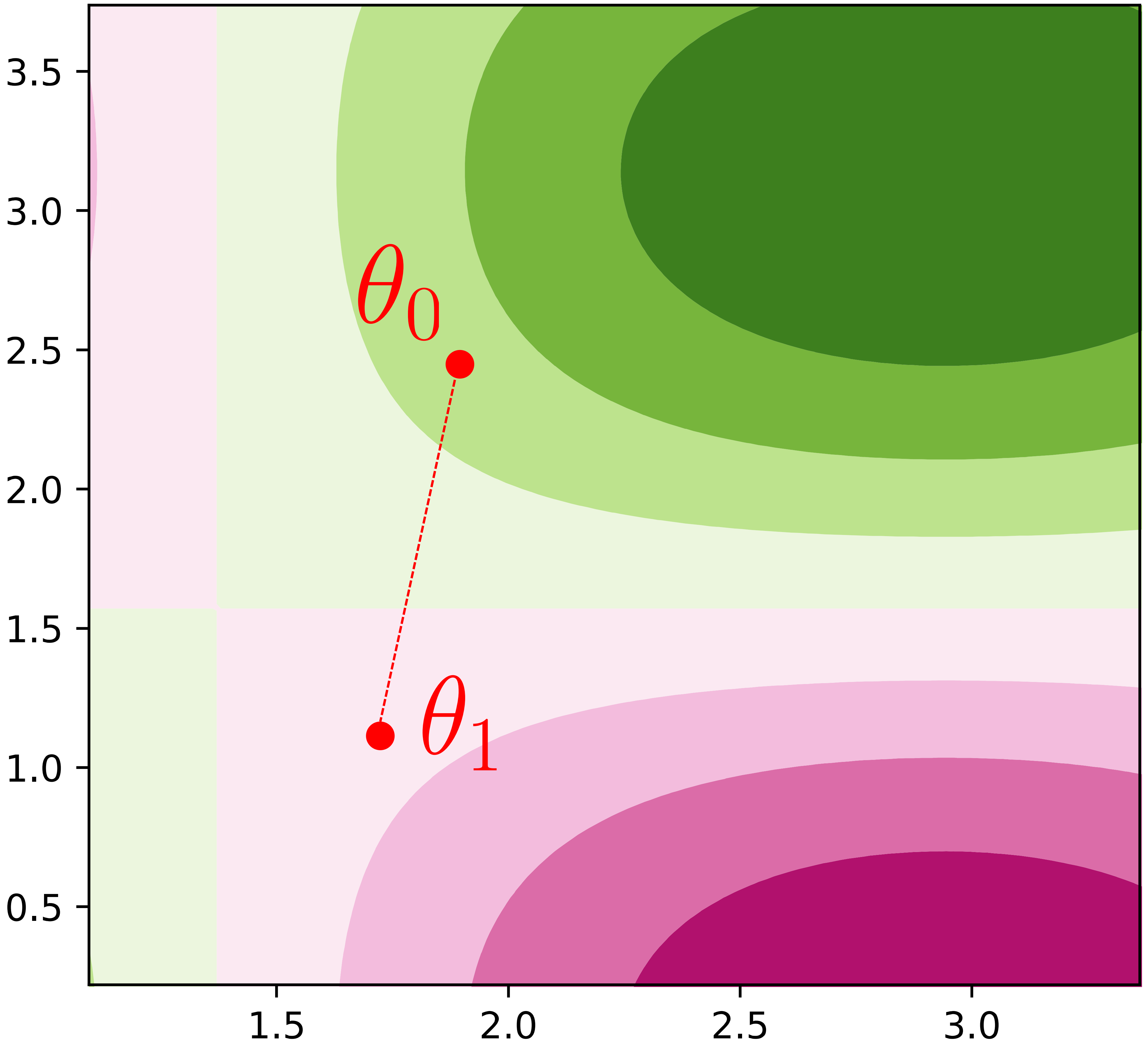
Shun-Ichi Amari
Neural Computation 10, 251 (1998)

Sandro Sorella
Physical Review Letters 80, 4558 (1998)

$$\text{argmin}_{\theta\in\mathbb{R}^d}\left[\langle\theta-\theta^{(n)},\nabla L(\theta^{(n)})\rangle + \frac{1}{2\eta}||\theta-\theta^{(n)}||^2_{g(\theta^{(n)})}\right]$$

02.2 - Quantum Natural Gradient

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



Credit: Julien Gaçon (EPFL/IBM)

Measure of closeness (fidelity)

$$d(\theta_0, \theta_1) = \left|\langle\psi(\theta_0)|\psi(\theta_1)\rangle\right|^2$$

Induced metric tensor

$$g_{ij}(\theta) = -\frac{1}{2}\partial_i\partial_j\left|\langle\psi(\theta')|\psi(\theta)\rangle\right|^2\Big|_{\theta'=\theta}$$

$$= \mathrm{Re}\left\{\langle\partial_i\psi|\partial_j\psi\rangle - \langle\partial_i\psi|\psi\rangle\langle\psi|\partial_j\psi\rangle\right\}$$

A.k.a. Quantum Fisher Information Matrix

02.3 - But: the Cost of Quantum Natural Gradient

Computing the Full Quantum Geometric Tensor Requires **Quadratic** Number of Evaluations in Parameters

An efficient variational algorithm should scale at most **linearly** with the number of variational parameters

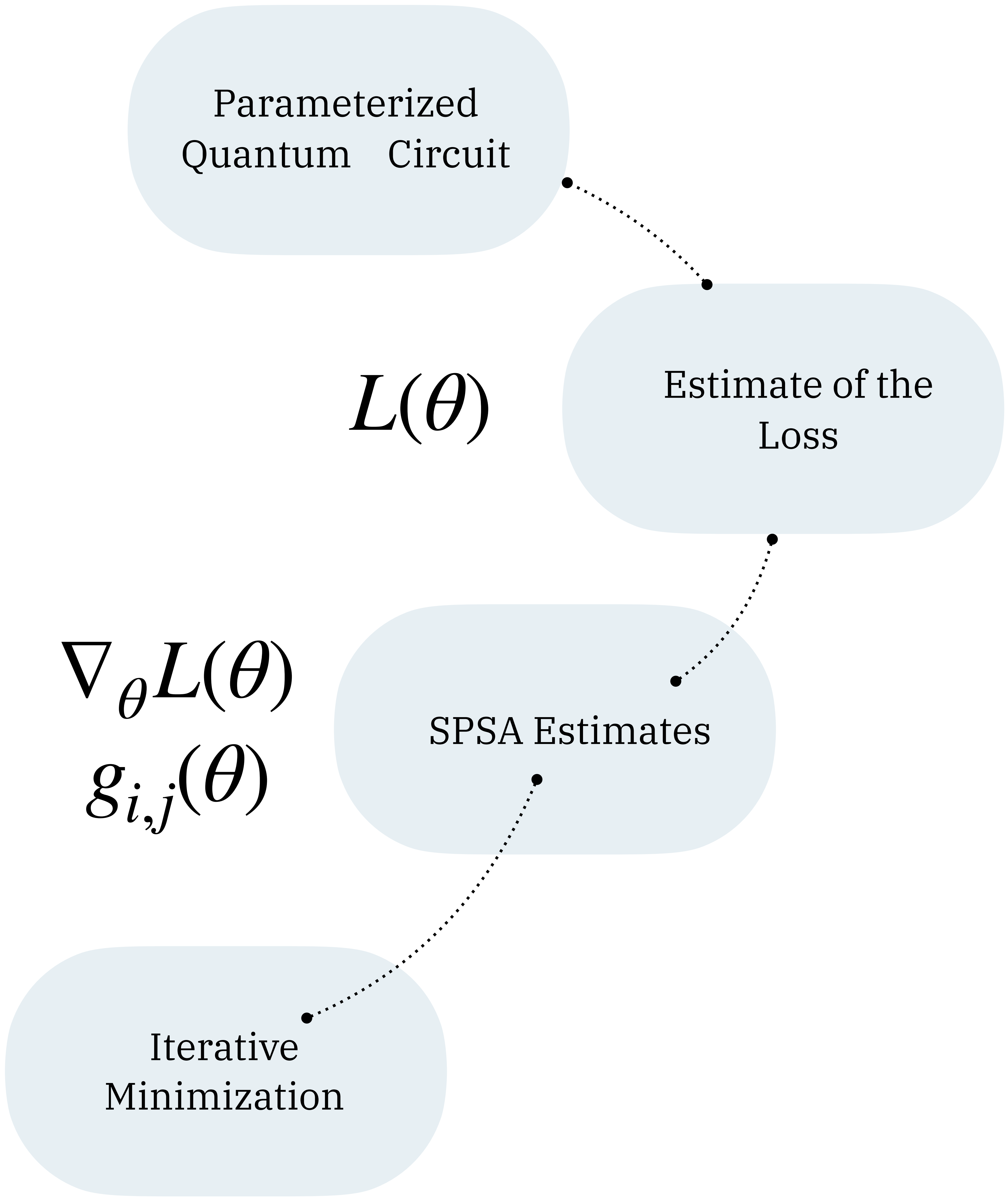
$$
\begin{aligned}
g_{j_1,j_2}(\theta) = -\tfrac{1}{8}\Big[& \left|\langle\psi(\boldsymbol{\theta})|\psi\big(\boldsymbol{\theta}+\big(\mathbf{e}_{j_1}+\mathbf{e}_{j_2}\big)\pi/2\big)\rangle\right|^2 \\
& - \left|\langle\psi(\boldsymbol{\theta})|\psi\big(\boldsymbol{\theta}+\big(\mathbf{e}_{j_1}-\mathbf{e}_{j_2}\big)\pi/2\big)\rangle\right|^2 \\
& - \left|\langle\psi(\boldsymbol{\theta})|\psi\big(\boldsymbol{\theta}+\big(-\mathbf{e}_{j_1}+\mathbf{e}_{j_2}\big)\pi/2\big)\rangle\right|^2 \\
& + \left|\langle\psi(\boldsymbol{\theta})|\psi\big(\boldsymbol{\theta}-\big(\mathbf{e}_{j_1}+\mathbf{e}_{j_2}\big)\pi/2\big)\rangle\right|^2 \Big].
\end{aligned}
$$

Mari, Bromley, and Killoran
Phys. Rev. A 103, 012405 (2021)

O2.4 - Faster Version: SPSA Quantum Natural Gradient

Gacon, Zoufal, Carleo, and Woerner
Quantum 5, 567 (2021)

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



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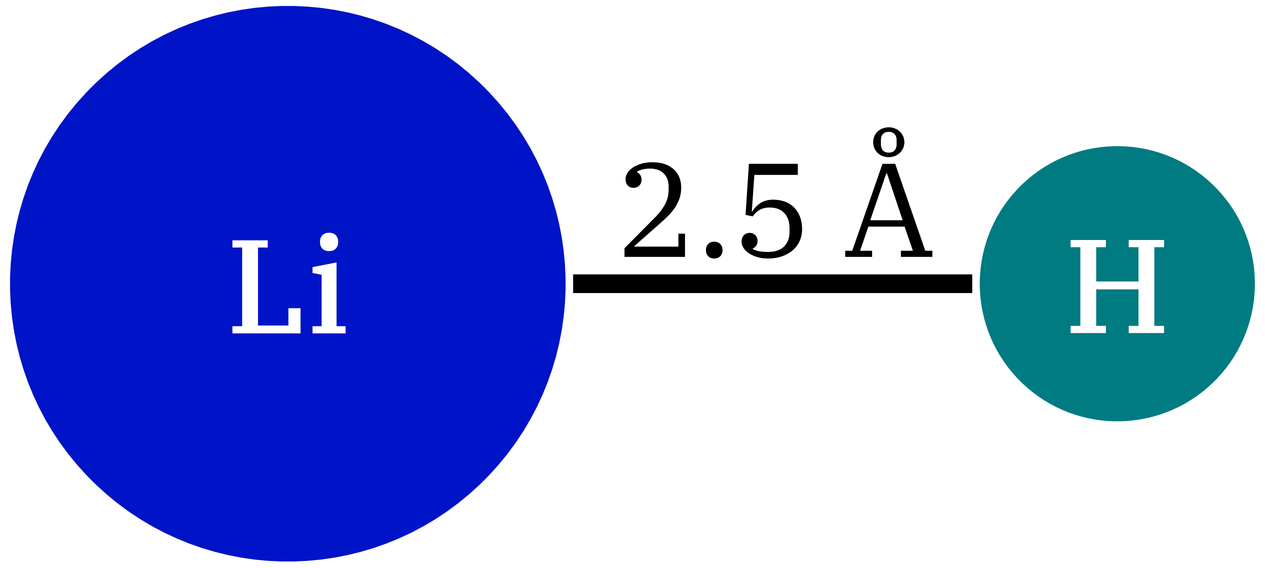
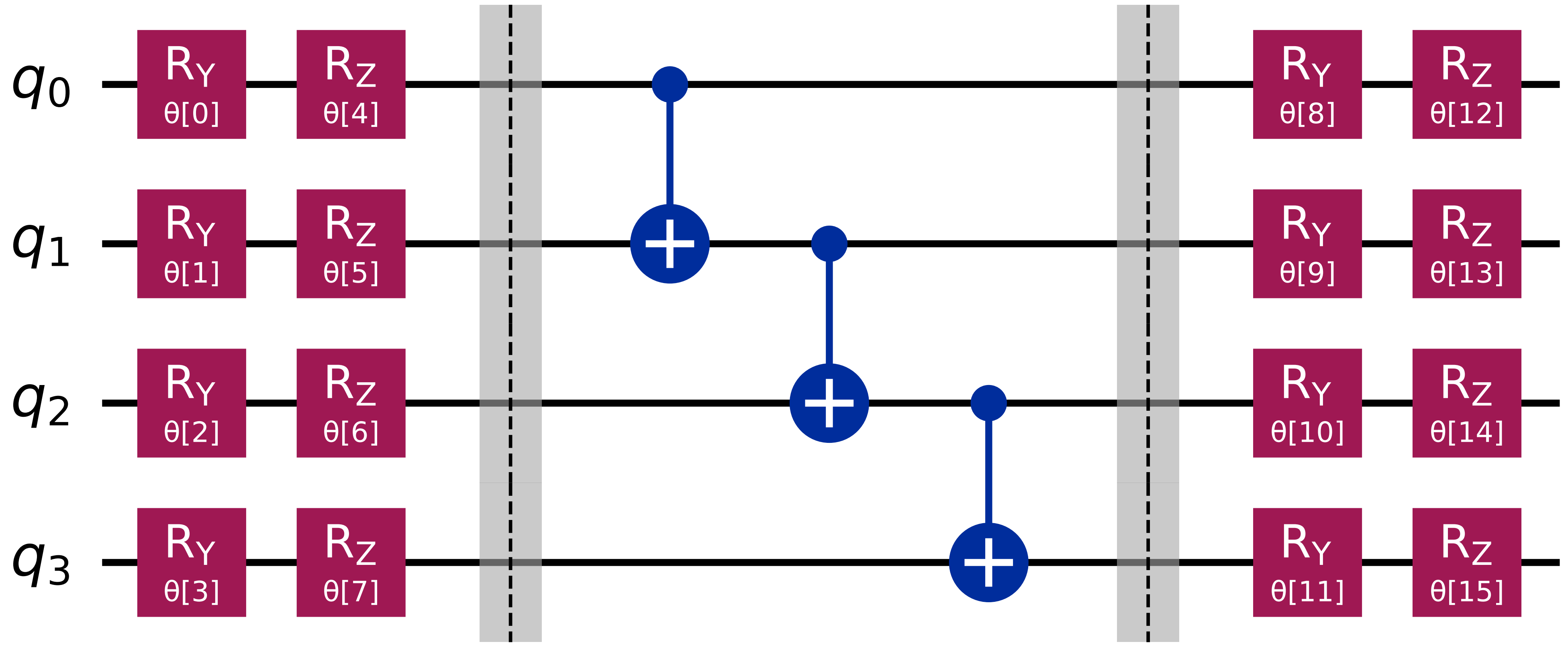
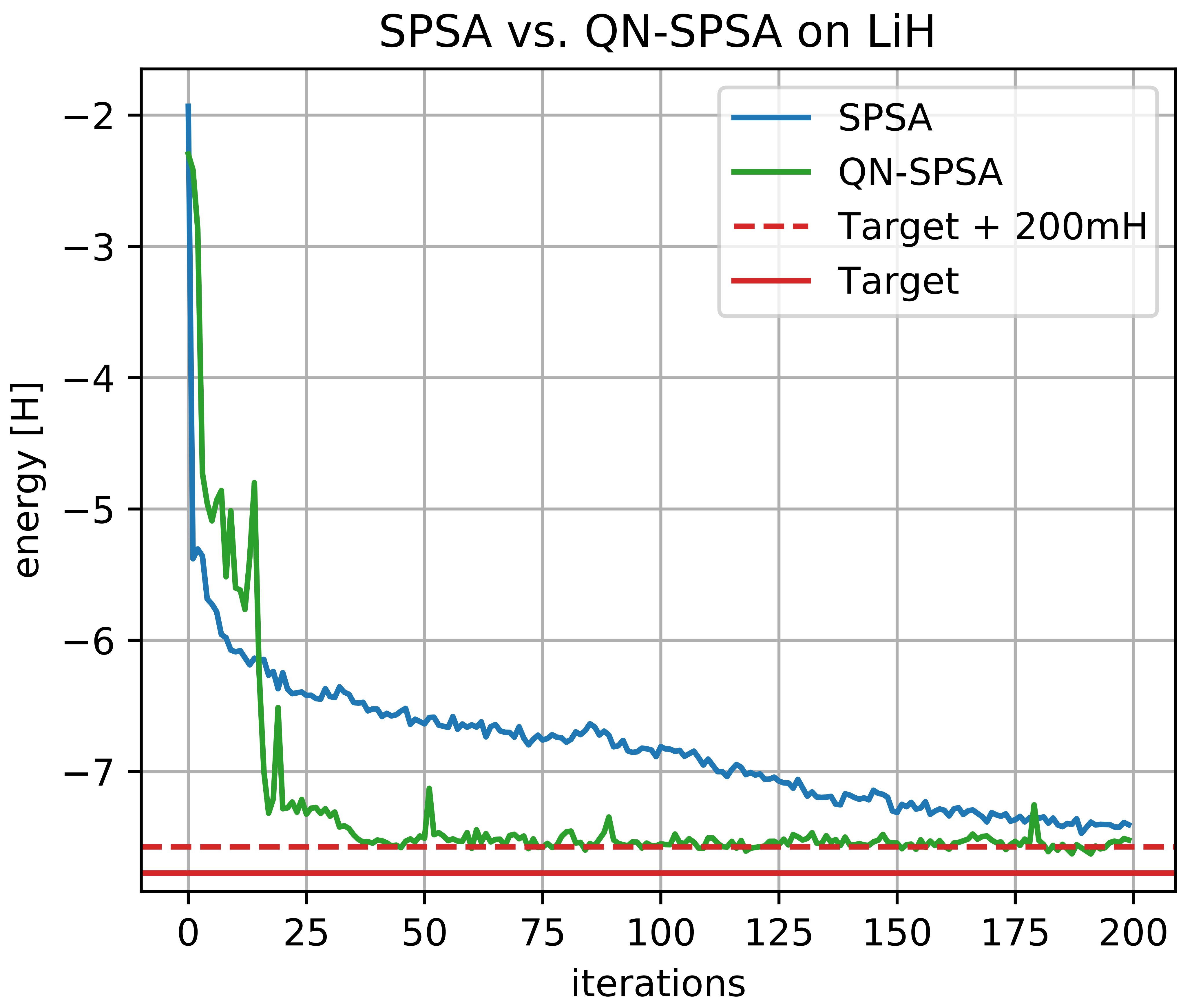
$$g(\theta)\Delta\theta = \nabla_\theta L(\theta)$$

02.5 - Application to LiH on IBMQ Montreal

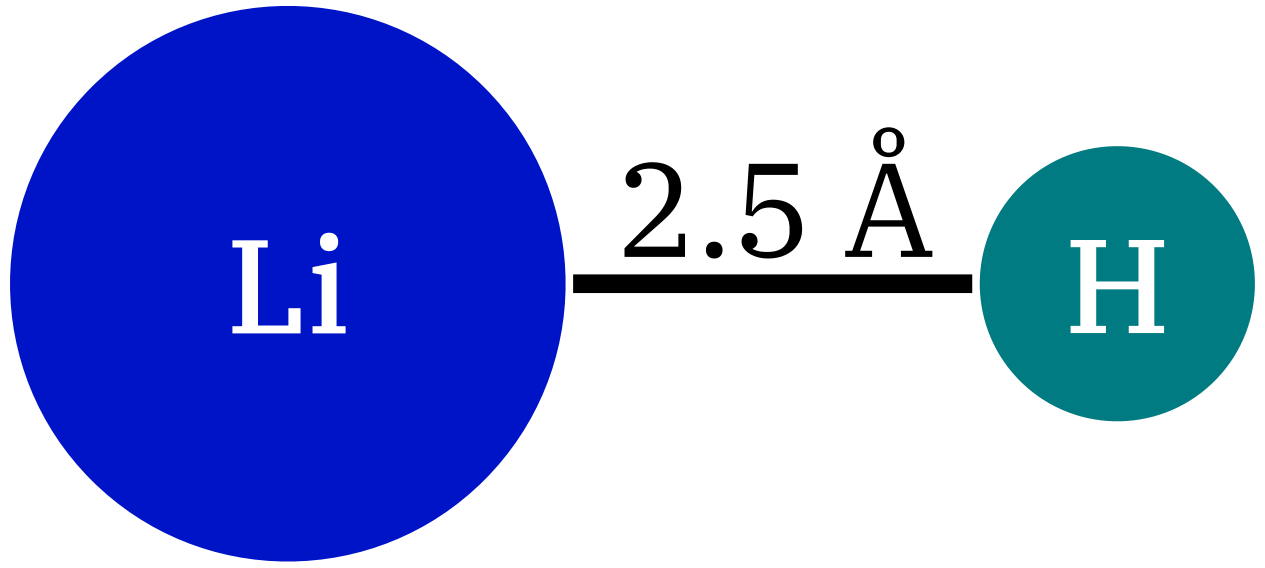


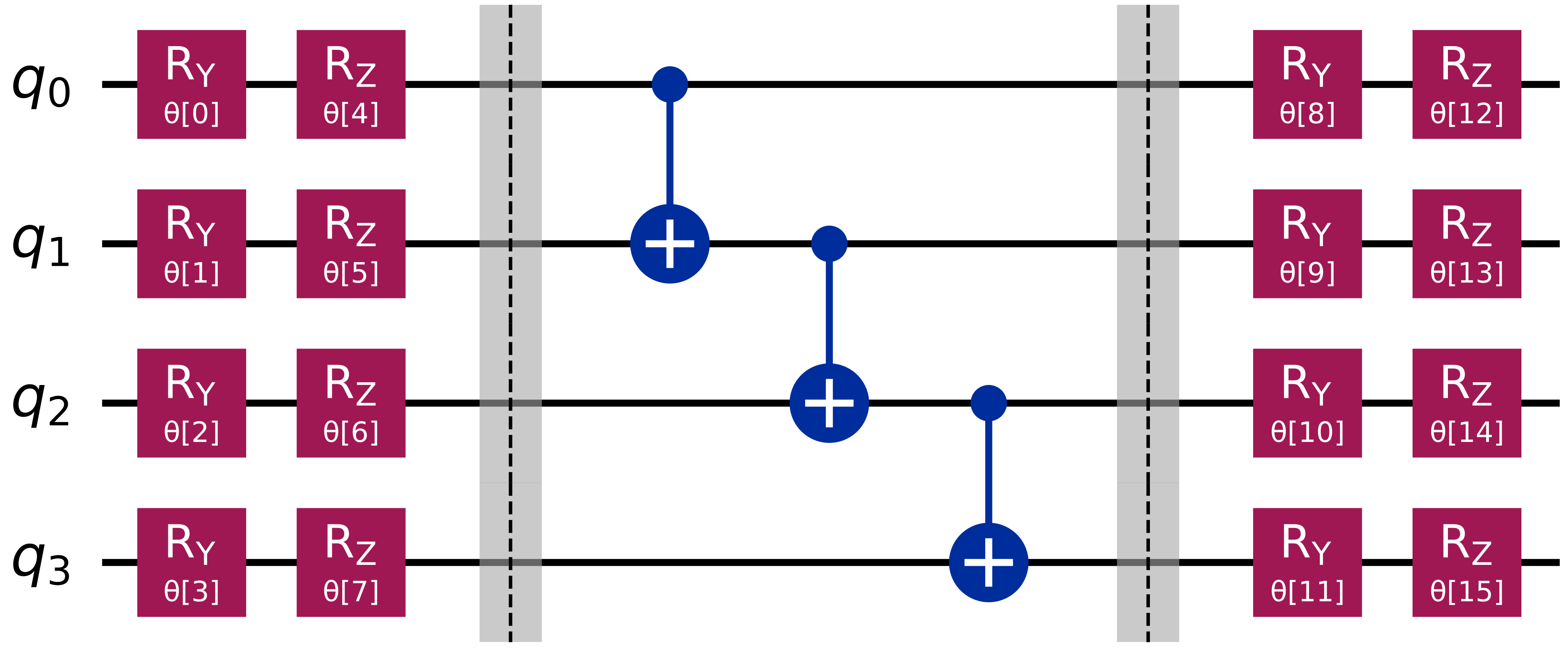


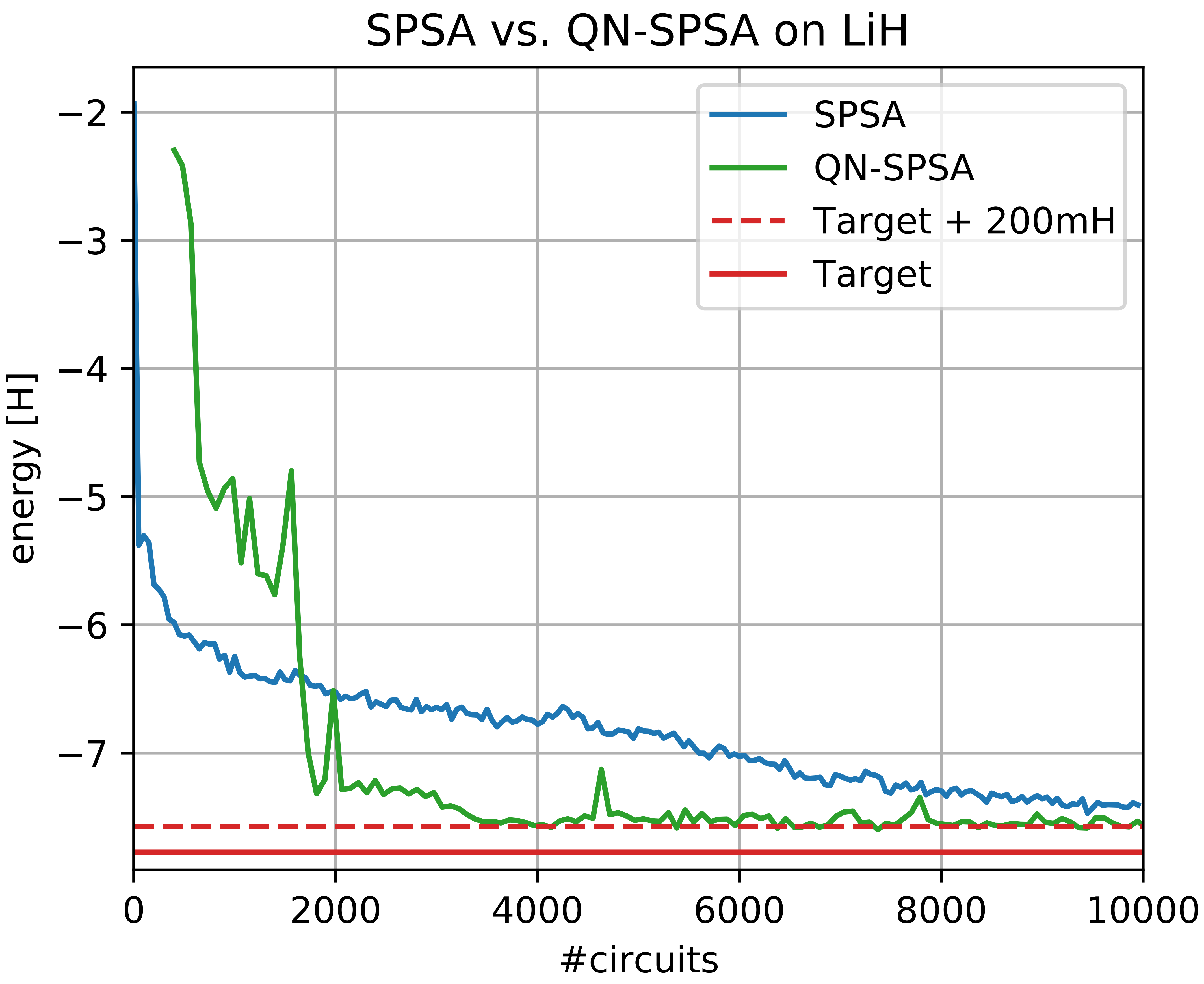


Data: IBM Quantum / Julien Gacon, Stefan Woerner

02.6 - Application to LiH on IBMQ Montreal







Data: IBM Quantum / Julien Gacon, Stefan Woerner

03.

Projected Variational Quantum Dynamics.

O3.1 - Approximate Hamiltonian Dynamics with Fixed-Depth Circuit

Barison, Vicentini, and Carleo
Quantum 5, 512 (2021)

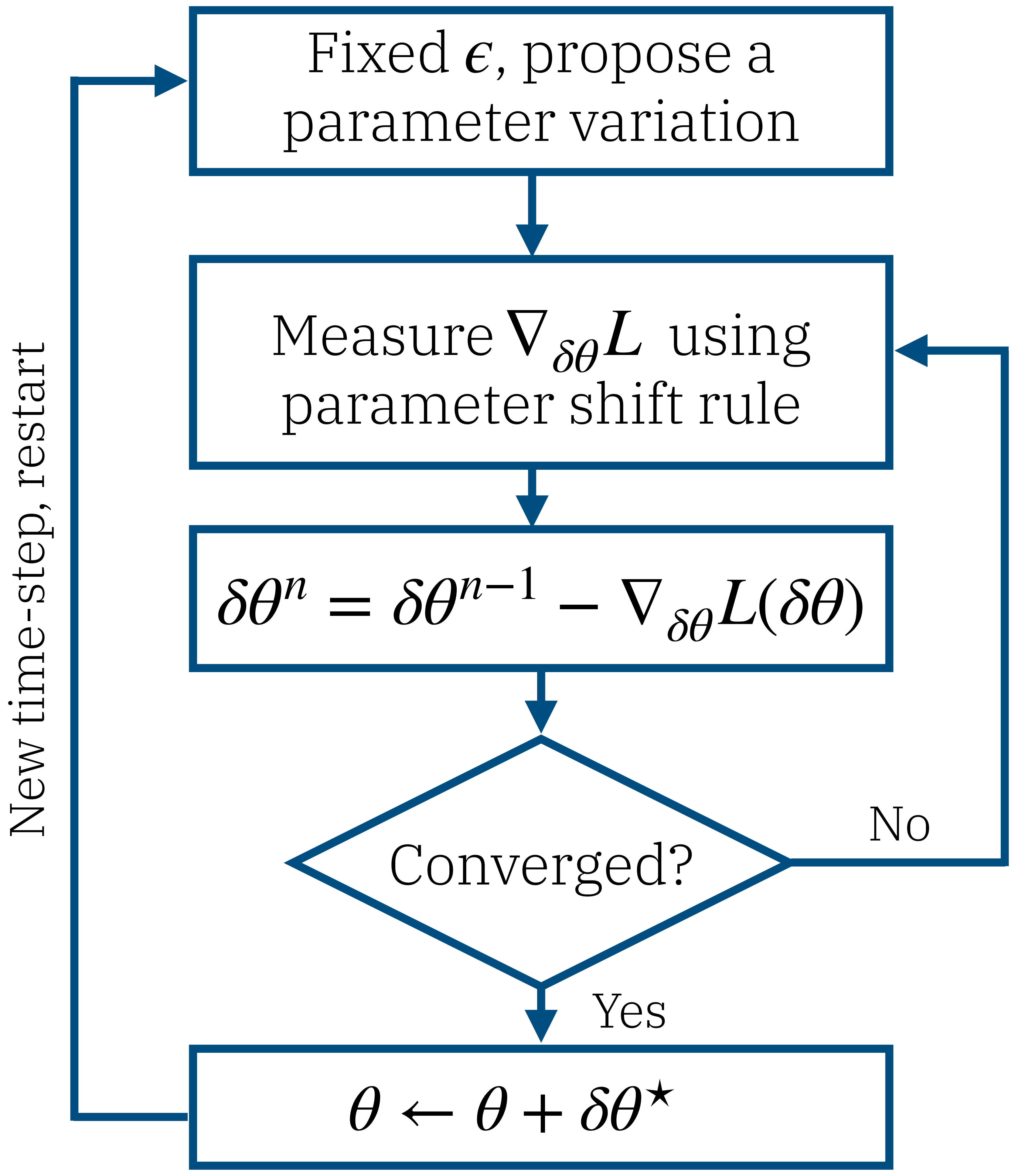
Maximize the overlap

$$|\langle \phi(\theta + \delta\theta)|e^{-i\epsilon H}|\phi(\theta)\rangle|^2$$

or minimize the cost function

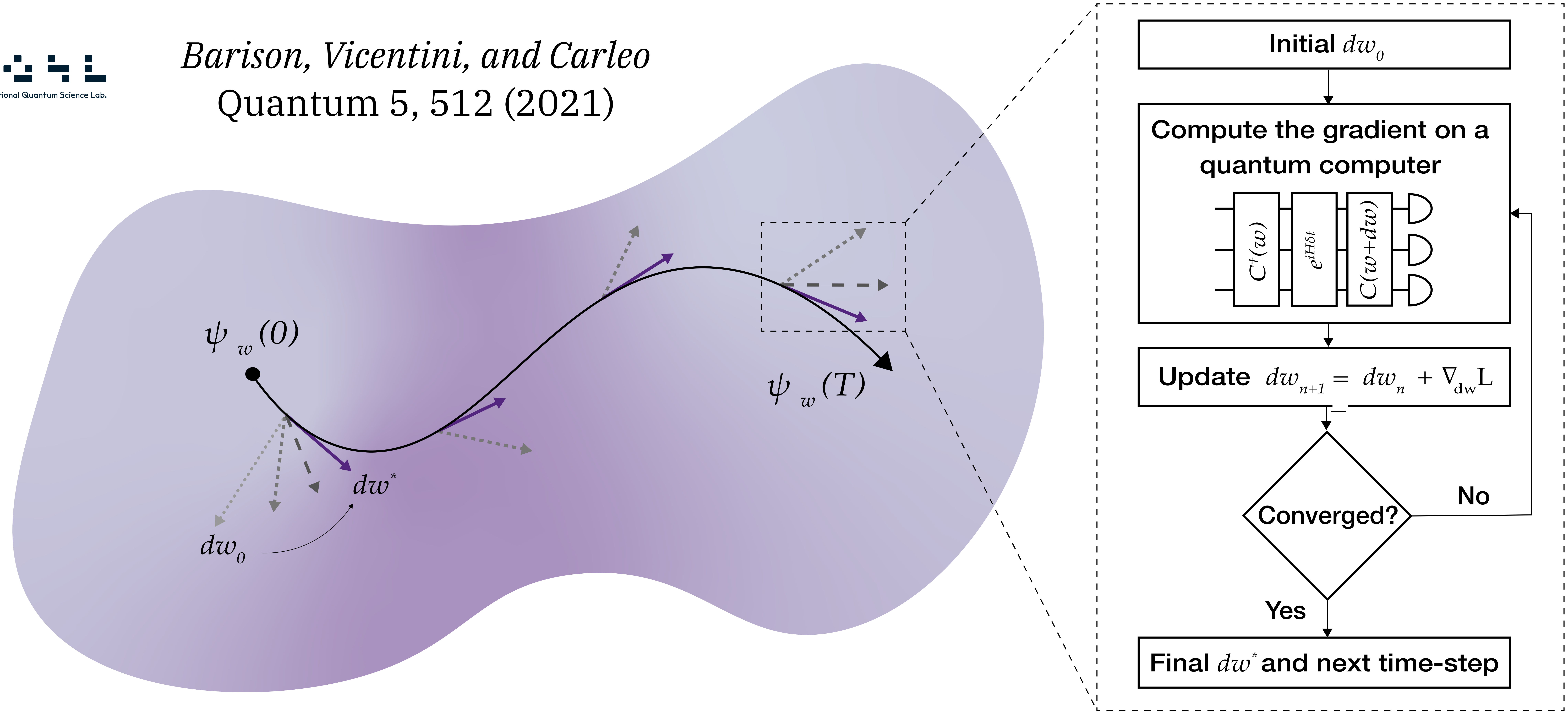
$$L(\delta\theta) = \frac{1 - |\langle \phi(\theta + \delta\theta)|e^{-i\epsilon H}|\phi(\theta)\rangle|^2}{\epsilon^2}$$

Independent from the time-step in the limit $\epsilon \to 0$

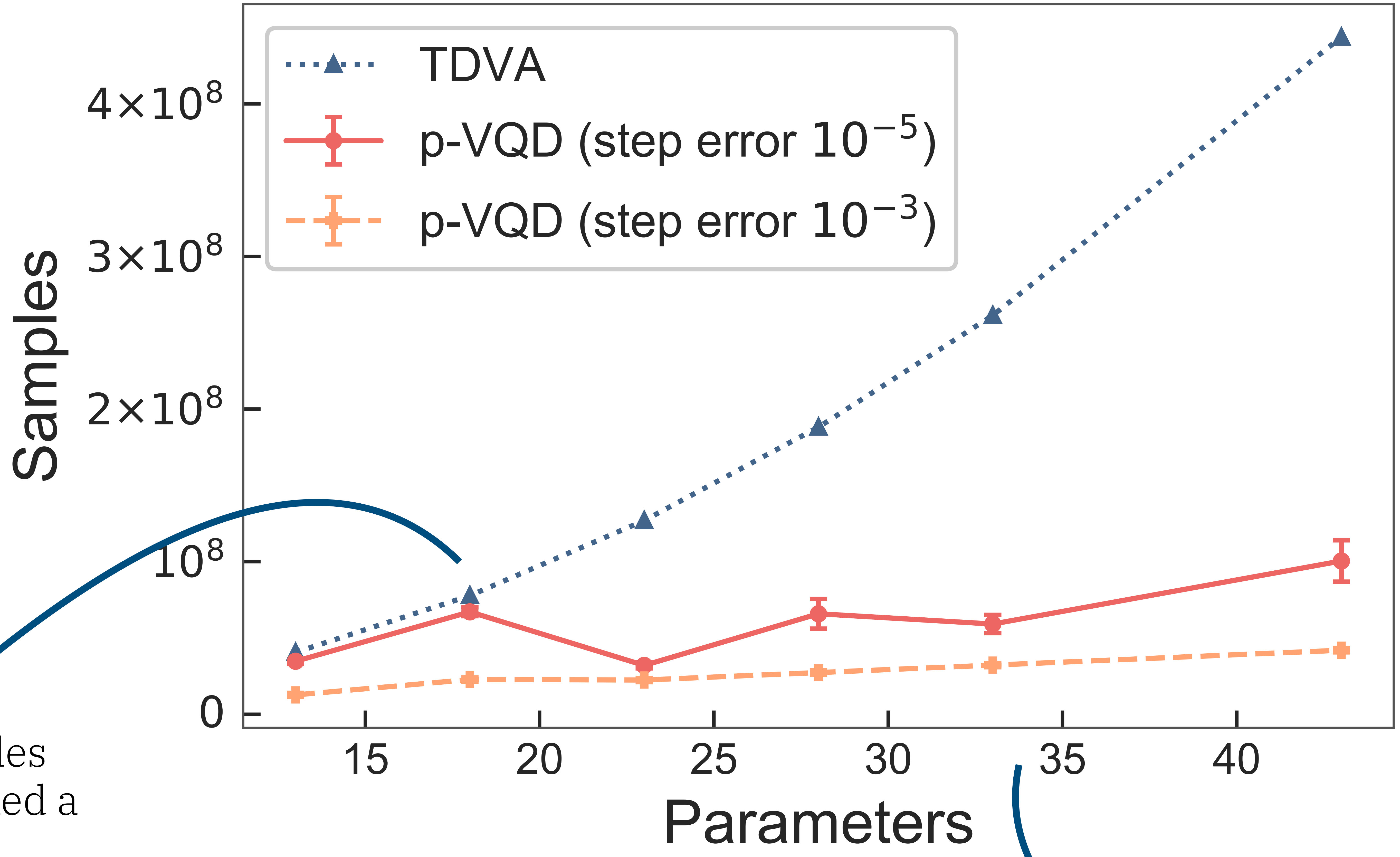


03.2 - PVQD

Barison, Vicentini, and Carleo
Quantum 5, 512 (2021)



O3.3 - Favorable Scaling with Number of Parameters



The number of samples required by TDVA is fixed a priori

For p-VQD we made multiple run and considered the mean value for different step errors

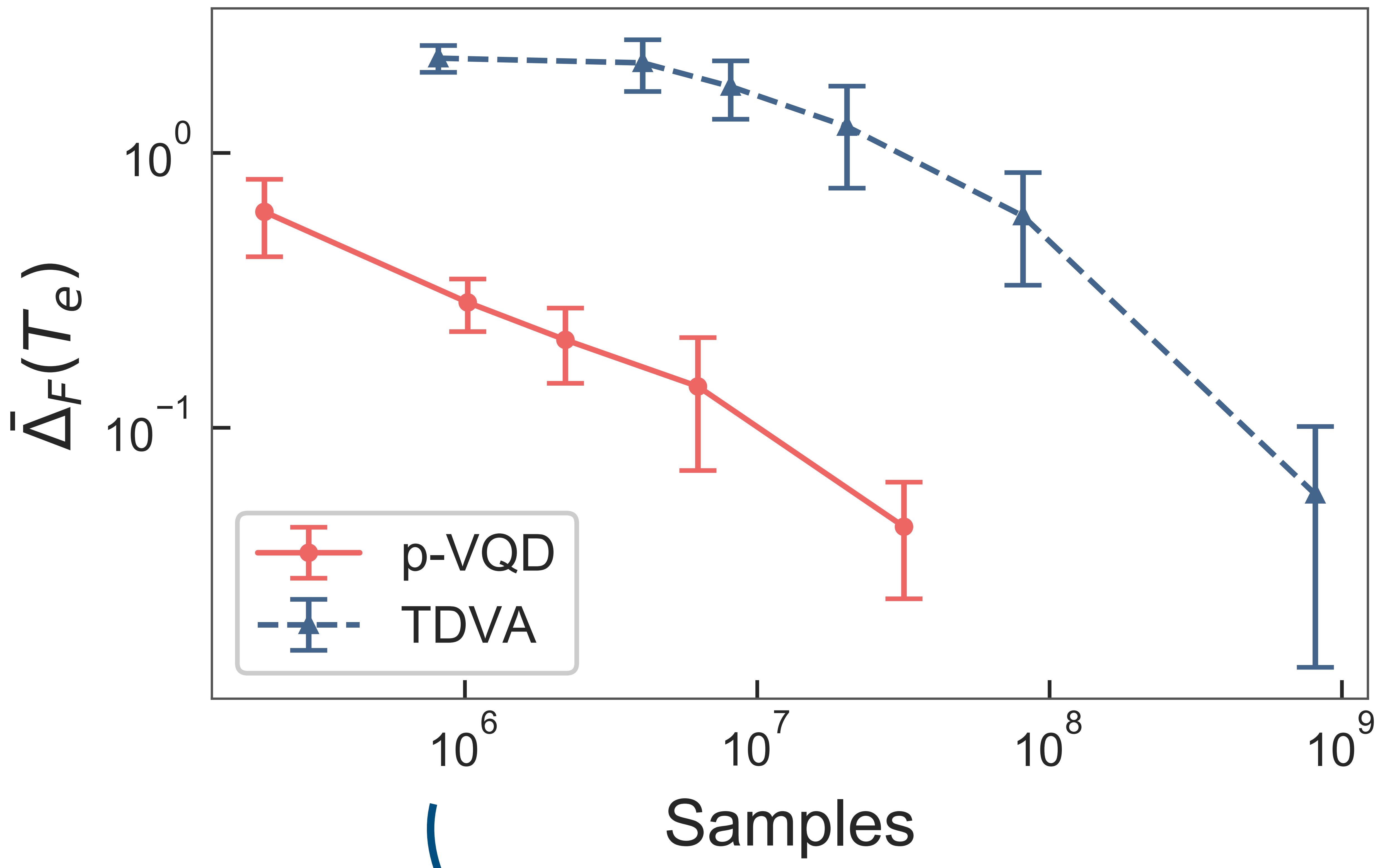
Li, and Benjamin
Phys. Rev. X 7, 021050 (2017)

03.4 - Fidelity and Number of Samples

Integrated infidelity

$$\Delta_F(T) = \int_0^T \left(1 - |\langle \Psi(t) | \phi(\theta) \rangle|^2\right) dt$$

State from exact simulation



The total number of samples required includes the number of time-steps, of parameters, of optimisation steps and of shots per circuit evaluation

04.

Neural Entanglement Forging.

04.1 - Goal: use half of the qubits

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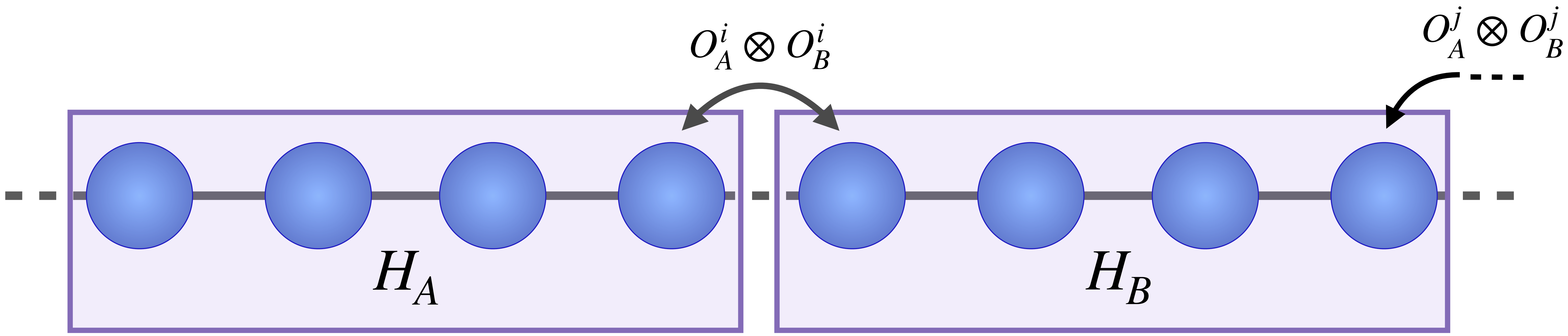


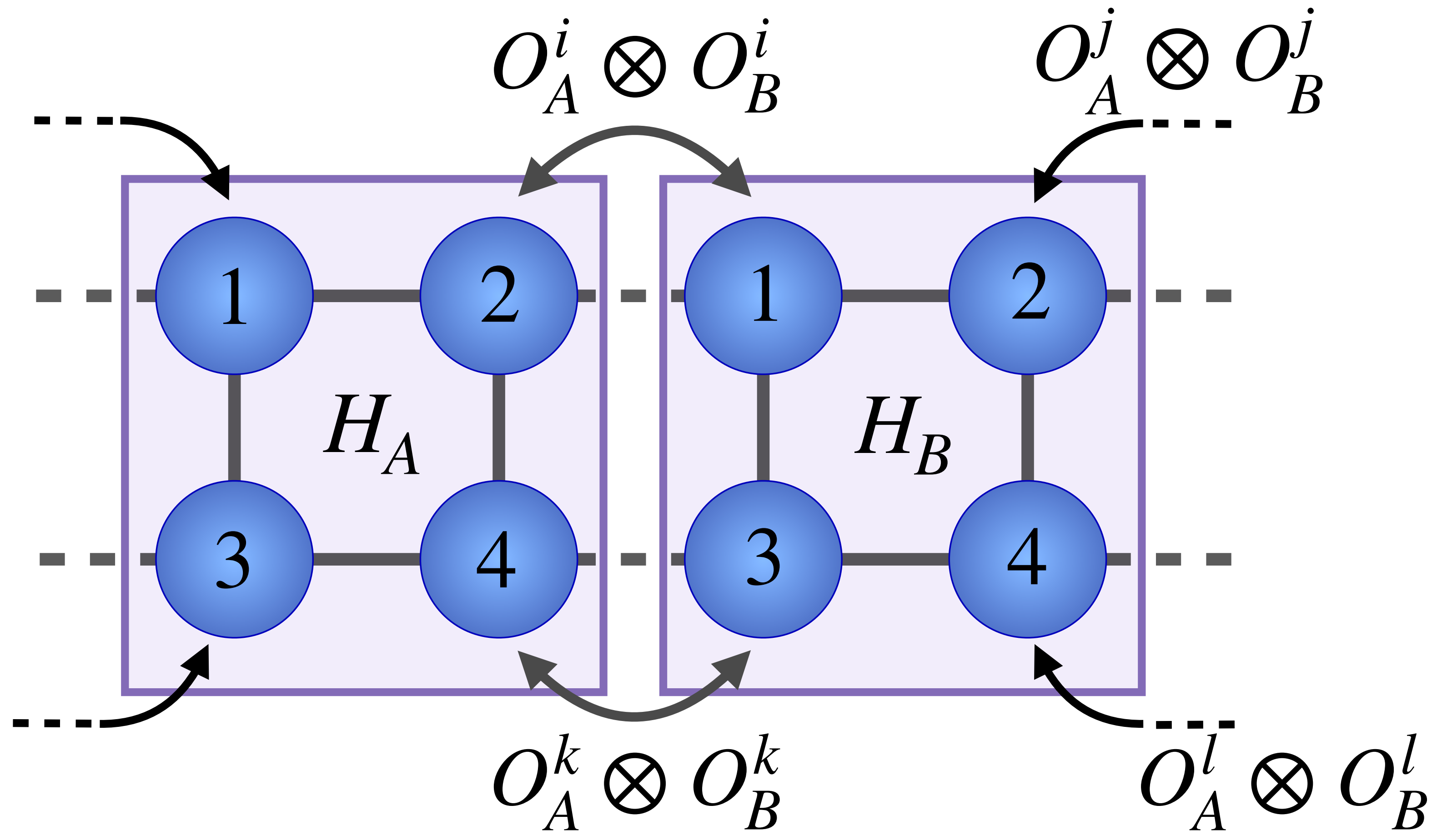
$$|\psi\rangle = U \otimes U \sum_{\boldsymbol{\sigma}} \lambda_{\boldsymbol{\sigma}} \, |\boldsymbol{\sigma}\rangle_A \, |\boldsymbol{\sigma}\rangle_B$$

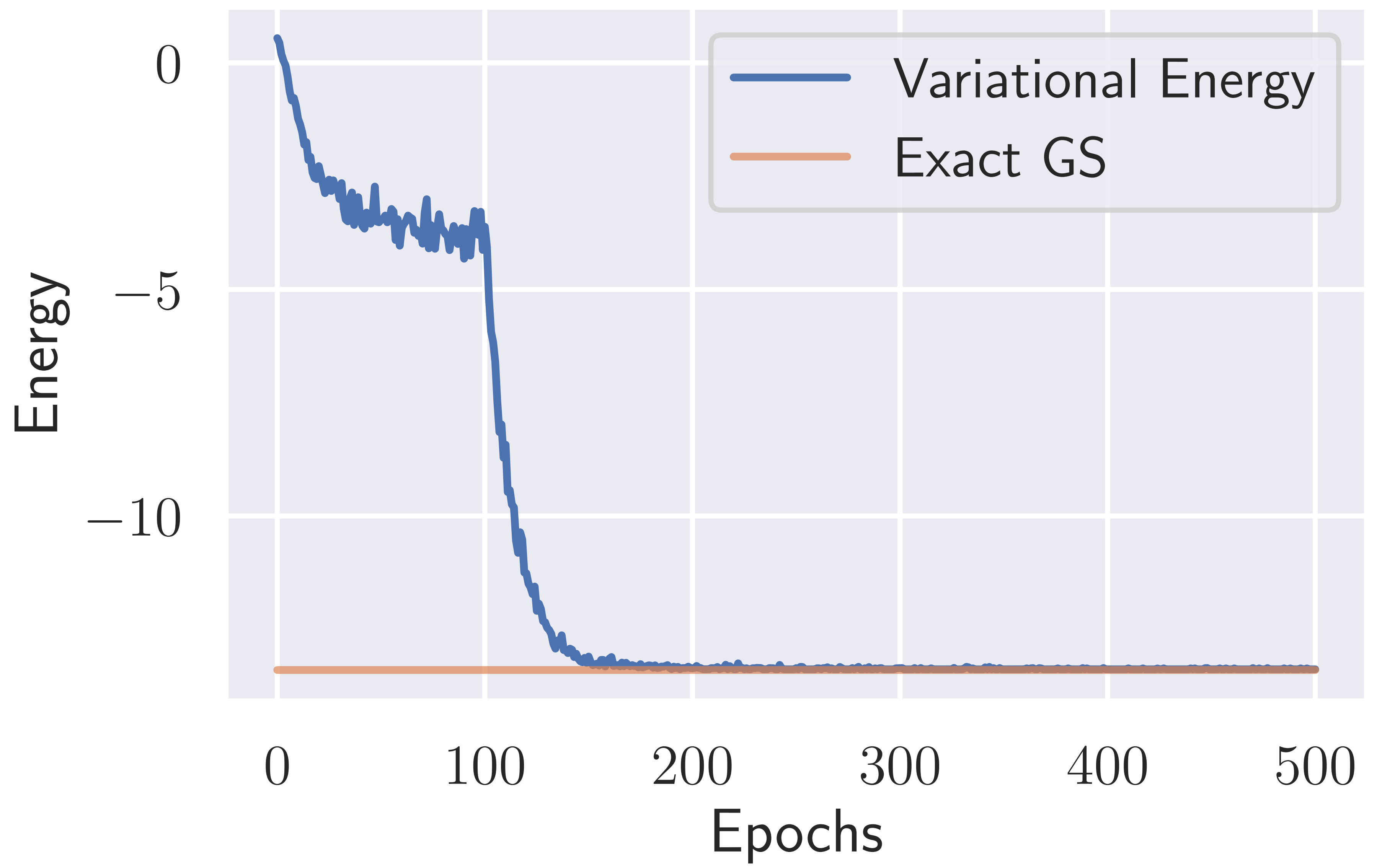
Generative Neural Network

Parameterized unitary

Huembeli, Carleo, and Mezzacapo
arXiv:2205.00933 (2022)

04.2 - Application: ground-state of 2D Transverse-Field Ising Model





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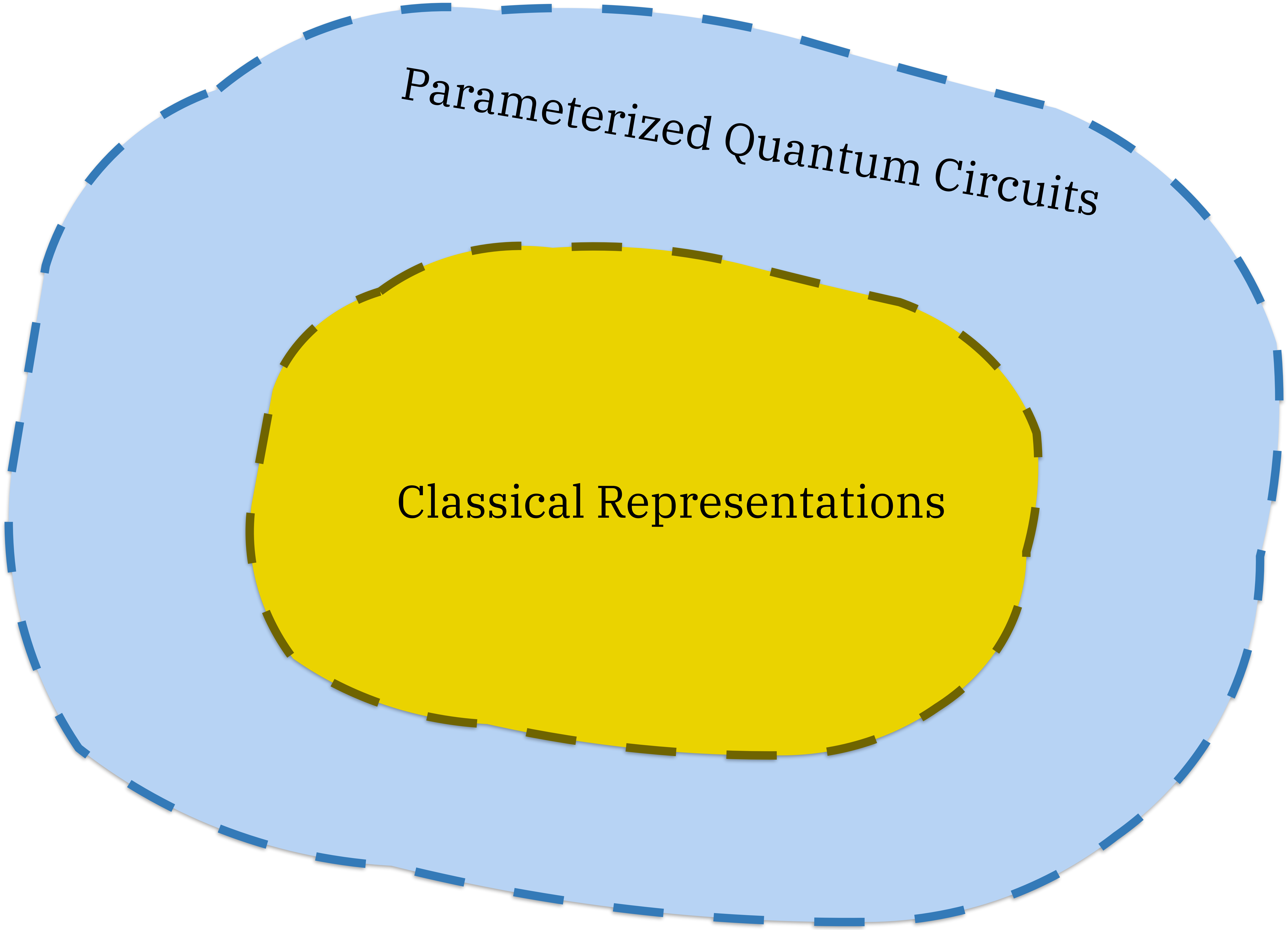
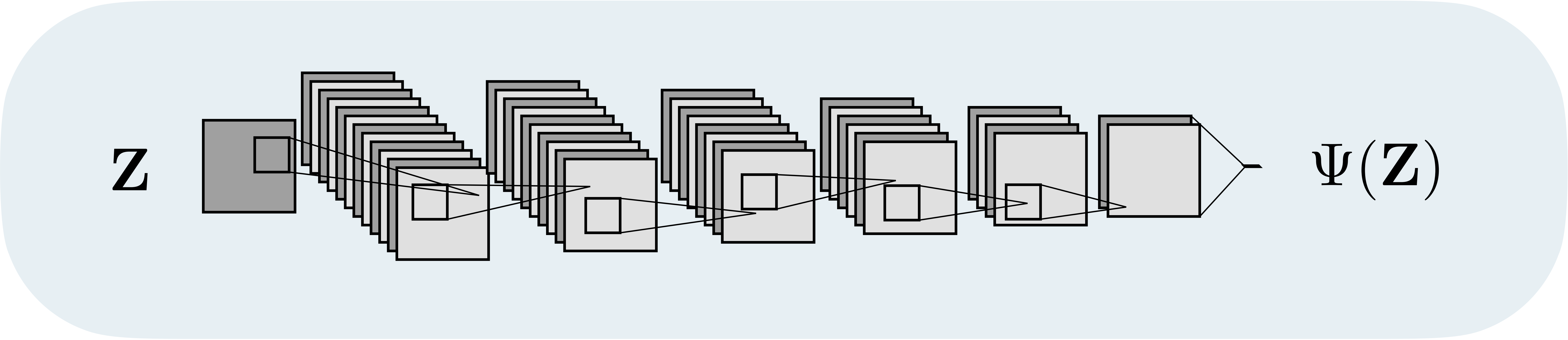
05.

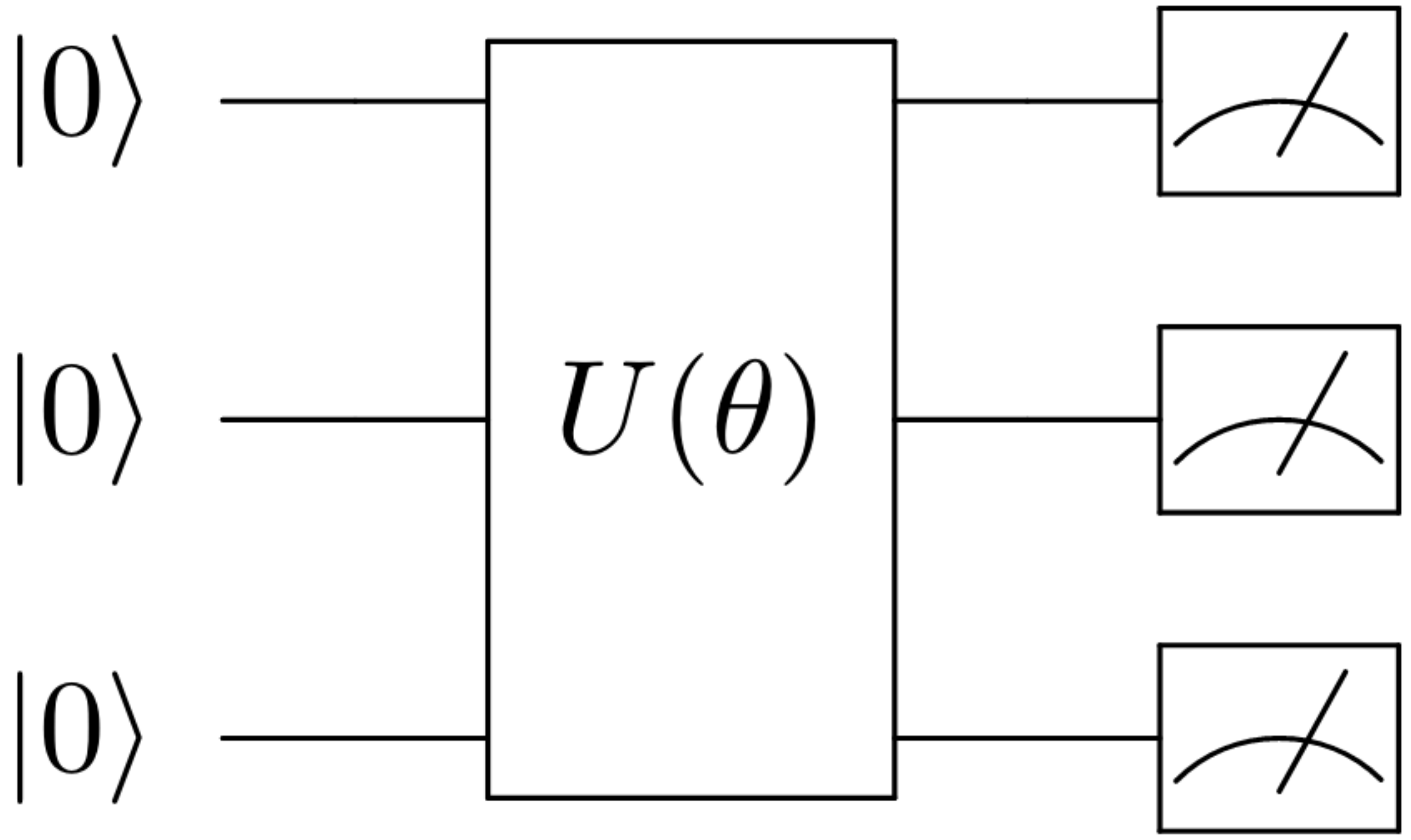
Two concluding questions.

Q5.1 - Relative representation power for useful apps?



O5.2 - Can we combine optimally classical and quantum representations?





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