Quantum Computing the Climate?

Preliminary explorations using noisy intermediate-scale quantum hardware

BROWN

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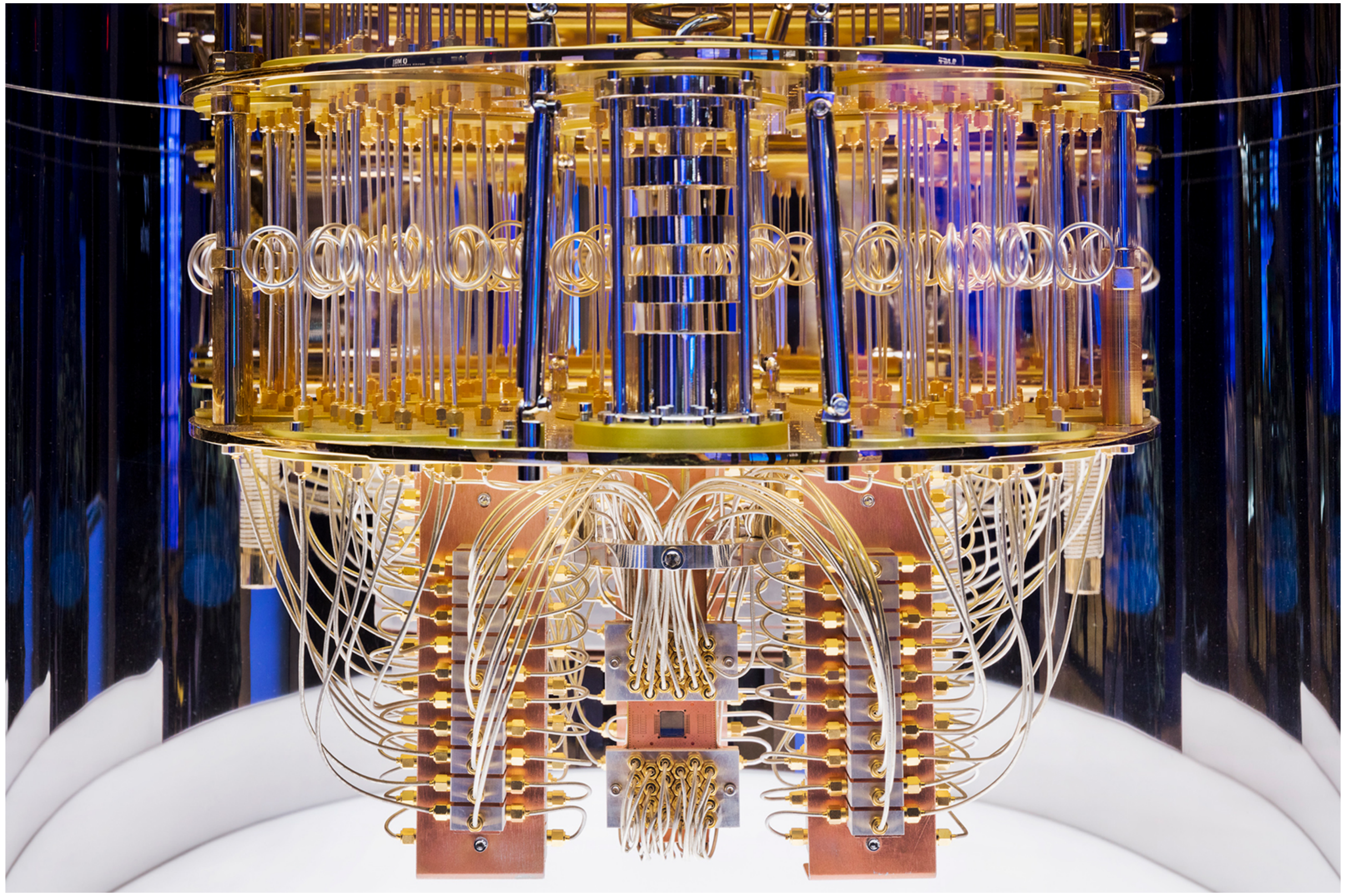
arXiv:2409.06036

IBM Superconducting Qubit Quantum Computer



Direct Statistical Simulation
of Dynamical Systems

$$\frac{d\vec{x}}{dt} = \vec{u}(\vec{x}) + \vec{\eta}(t)$$

Key idea: Quantum mechanics is linear so transform non-linear ODEs into linear PDEs. Quantum computers with exponentially large Hilbert spaces may be able to help with vastly increased dimension. The approach differs from attempts to use quantum computers to speed up non-linear dynamics.

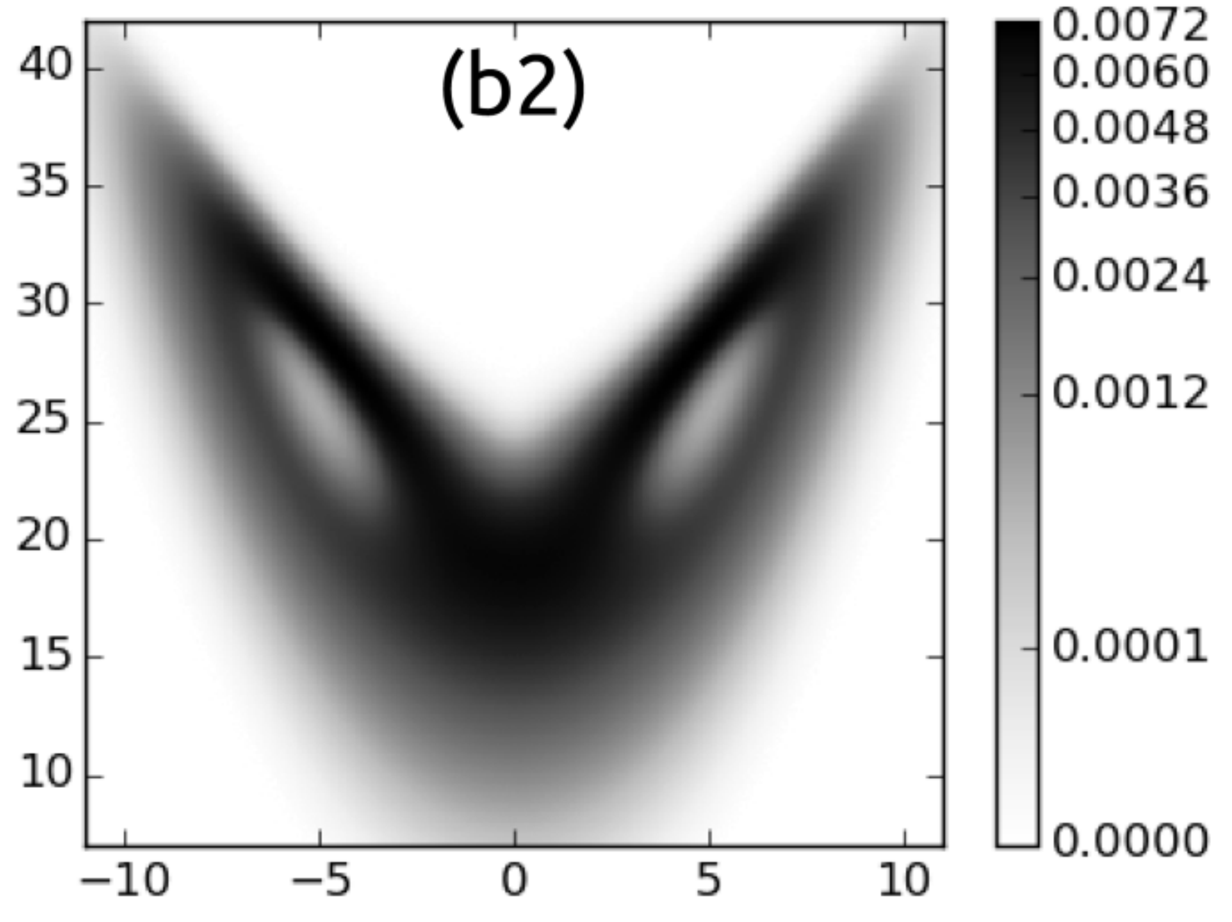
Conservation of Probability:
Flux-Form of the Fokker-Planck Equation

$$\frac{\partial P(\vec{x},t)}{\partial t} = -\hat{L}_{\mathrm{FPE}}\ P(\vec{x},t)$$

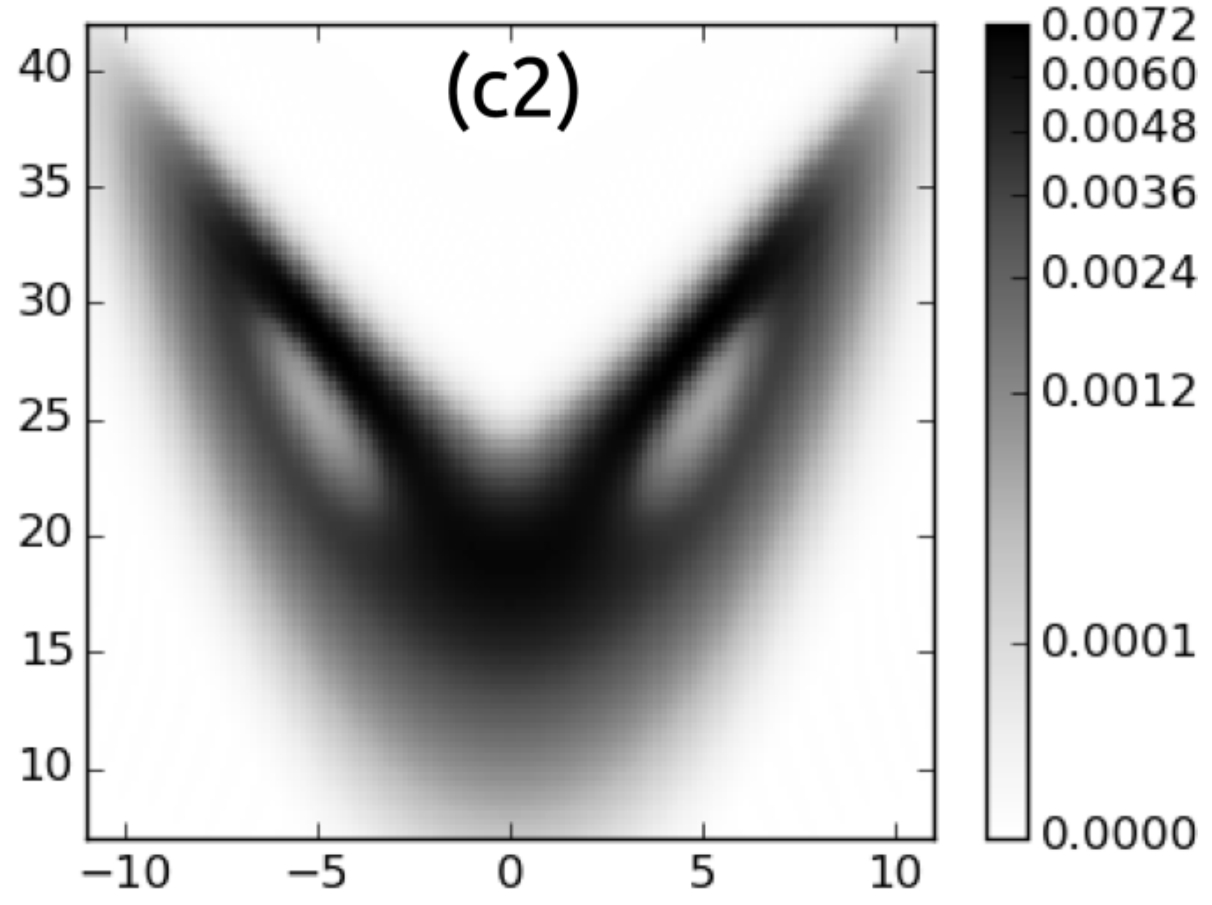
$$\hat{L}_{\mathrm{FPE}}\ P = \nabla_x \cdot \left(\vec{u}\ P - D\vec{\nabla}_x P\right)$$

Statistical Steady State: $\hat{L}_{\mathrm{FPE}}\ P(x) = 0$

By Accumulation



FPE



A. Allawala & J.B. Marston, "Statistics of the Stochastically-Forced Lorenz Attractor by the Fokker-Planck Equation and Cumulant Expansions," *PRE* 052218 (2016).

Non-Linear Ornstein-Uhlenbeck Problem

$$u(x) = -ax - bx^3$$

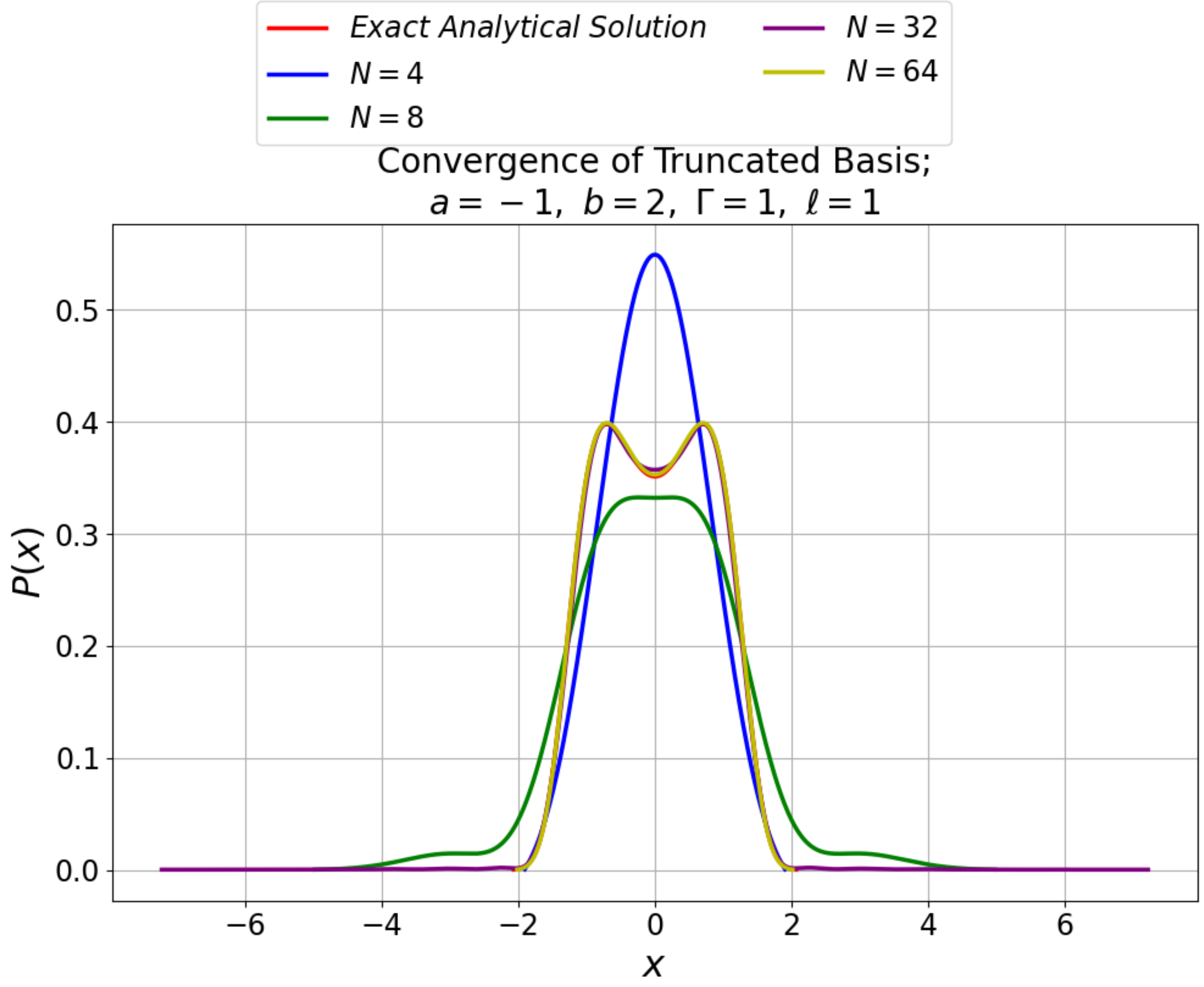
$$P(x) = N\ \exp\left(-\frac{ax^2}{2\Gamma} - \frac{bx^4}{4\Gamma}\right)$$

Finite Basis & Hermitian Operator

$$|n\rangle = \frac{\sqrt{\ell}}{\pi^{1/4}\sqrt{2^n n!}}\ H_n(\ell x)\ e^{-\ell^2 x^2/2}$$

$$L_{mn} = \langle m|\,\hat{L}_{\mathrm{FPE}}\,|n\rangle$$

$$H_{mn} = \sum_{p=0,2,4,\ldots}^{N\ \text{states}} L^*_{pm} L_{pn}$$



Ladder Operator Representation of FPE Operator

Idea: Represent the FPE Operator using ladder operators from the quantum harmonic oscillator to enable mapping to qubit space.

Ladder Operators:

$$\hat{a} = \frac{1}{\sqrt{2}}(Lx + \frac{1}{L}\frac{\partial}{\partial x}),\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}(Lx - \frac{1}{L}\frac{\partial}{\partial x})$$

$$\downarrow$$

$$x = \frac{1}{L\sqrt{2}}(\hat{a} + \hat{a}^\dagger),\ \frac{\partial}{\partial x} = \frac{L}{\sqrt{2}}(\hat{a} - \hat{a}^\dagger)$$

FPE Operator:

$$\hat{L}_{FPE} = \frac{a}{2}(\hat{a} - \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) + \frac{b}{4L^2}(\hat{a} - \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger)^3 + \frac{\Gamma L^2}{2}(\hat{a} - \hat{a}^\dagger)^2$$

Mapping Hermite Polynomial Basis to Qubit Basis

Hermite Basis | **Qubit Basis**

Basis States

$$|0\rangle\,,\ |1\rangle\,,\ |2\rangle\,,\ldots,\ |n-1\rangle\,,$$
$$\text{for } n \in \{2^k | k \in \mathbb{Z}\}$$

$\rightarrow$

$$|0\ldots00\rangle\,,\ |0\ldots01\rangle\,,$$
$$|0\ldots10\rangle\,,\ldots,\ |1\ldots11\rangle$$

Ladder Operators (let $n = 4$ for illustration)

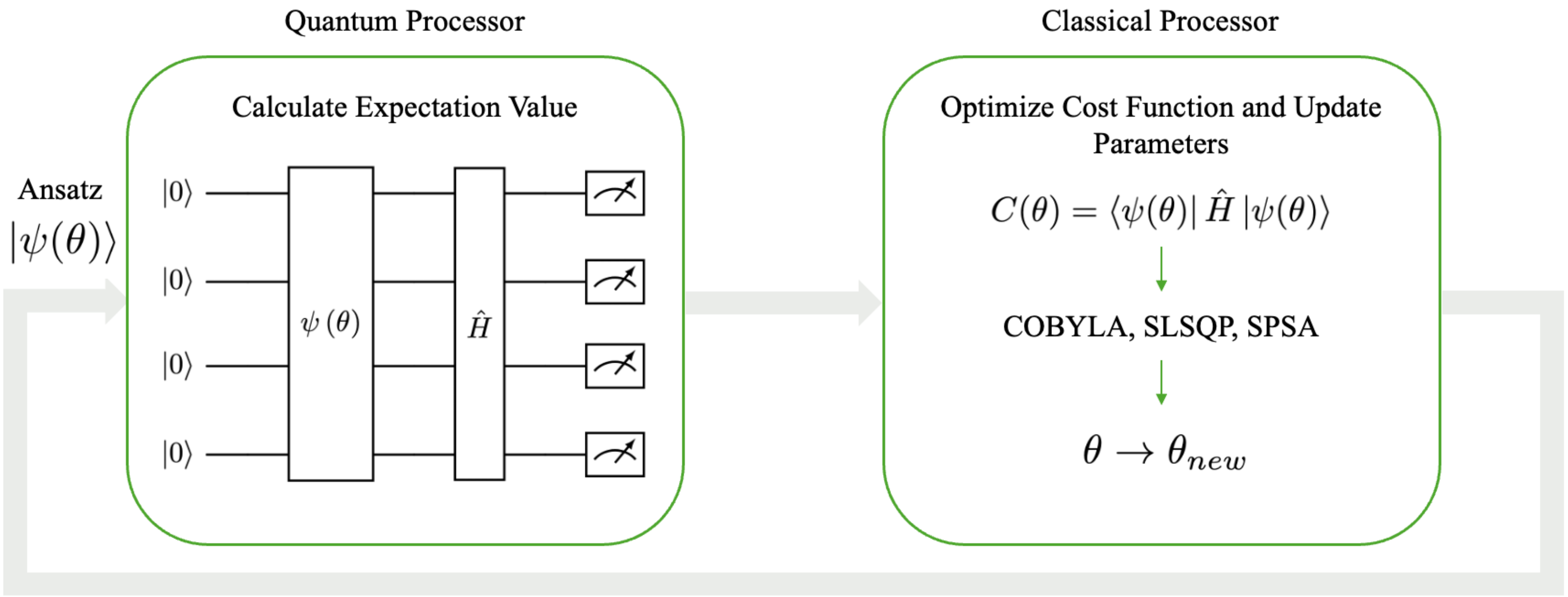
$$\hat{a}\,|3\rangle = \sqrt{3}\,|2\rangle\,,$$
$$\hat{a}\,|2\rangle = \sqrt{2}\,|1\rangle\,,$$
$$\hat{a}\,|1\rangle = |0\rangle$$

$\rightarrow$

$$\hat{a}_{|3\rangle\rightarrow|2\rangle}\,|11\rangle = \sqrt{3}(\frac{1}{2}(I-Z)\otimes\frac{1}{2}(X+iY))\,|11\rangle = \sqrt{3}\,|10\rangle\,,$$
$$\hat{a}_{|2\rangle\rightarrow|1\rangle}\,|10\rangle = \sqrt{2}(\frac{1}{2}(X+iY)\otimes\frac{1}{2}(X-iY))\,|10\rangle = \sqrt{2}\,|01\rangle\,,$$
$$\hat{a}_{|1\rangle\rightarrow|0\rangle}\,|01\rangle = \frac{1}{2}(I+Z)\otimes\frac{1}{2}(X+iY)\,|01\rangle = |00\rangle\,,$$
$$\hat{a} = \hat{a}_{|3\rangle\rightarrow|2\rangle} + \hat{a}_{|2\rangle\rightarrow|1\rangle} + \hat{a}_{|1\rangle\rightarrow|0\rangle}$$

Qubit ladder operator can be generalized to arbitrary *n* following the same pattern.

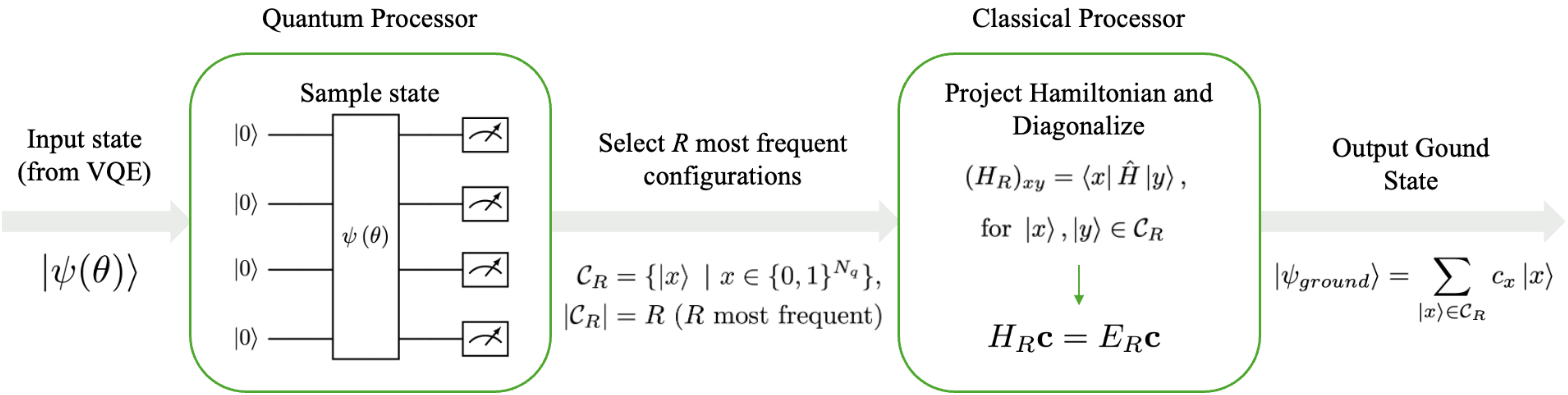
Variational Quantum Eigensolver (VQE)



Quantum chemists focus on finding eigenvalues.
Here, we know the target eigenvalue is 0. We are more interested in eigenvectors.

A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, A variational eigenvalue solver on a photonic quantum processor, Nat. Commun. **5**, 4213 (2014).

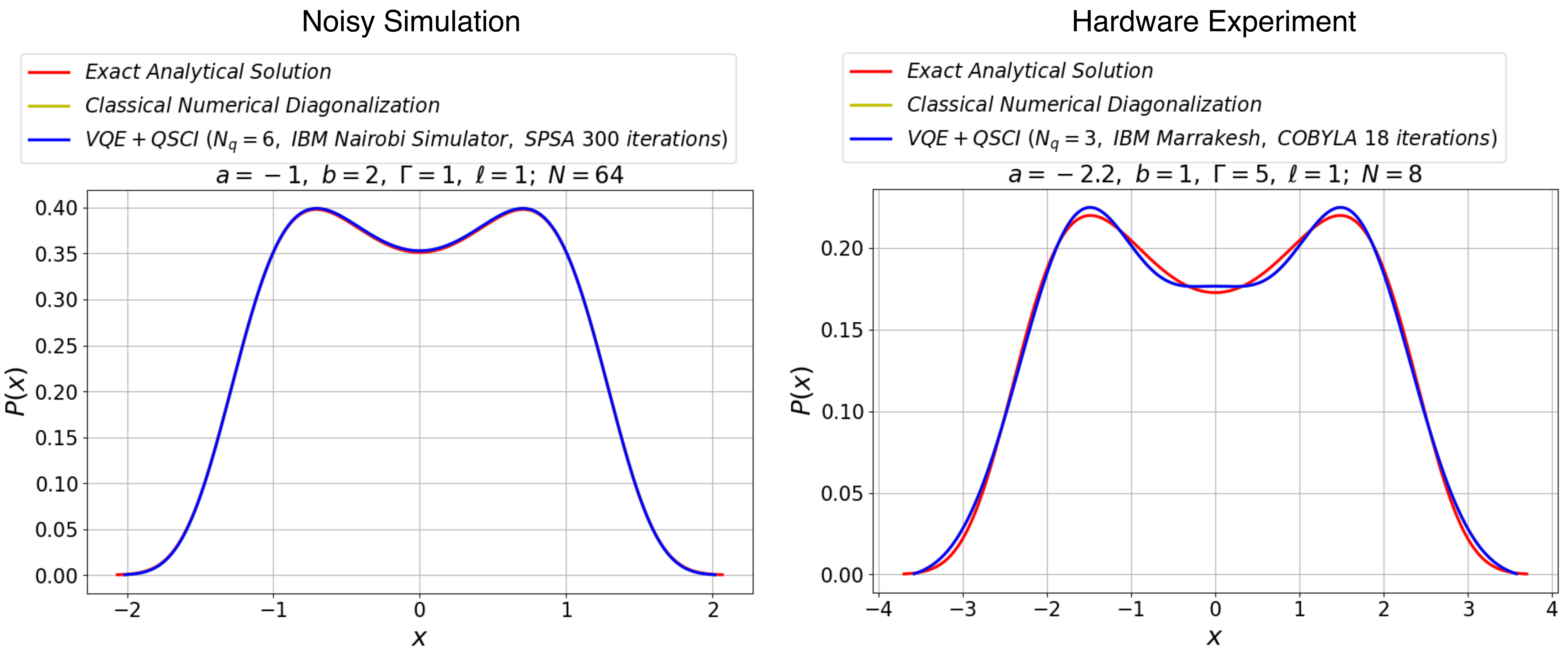
Quantum-Selected Configuration Interaction (QSCI)



Importantly, the projected Hamiltonian is of smaller dimension than the original Hamiltonian.

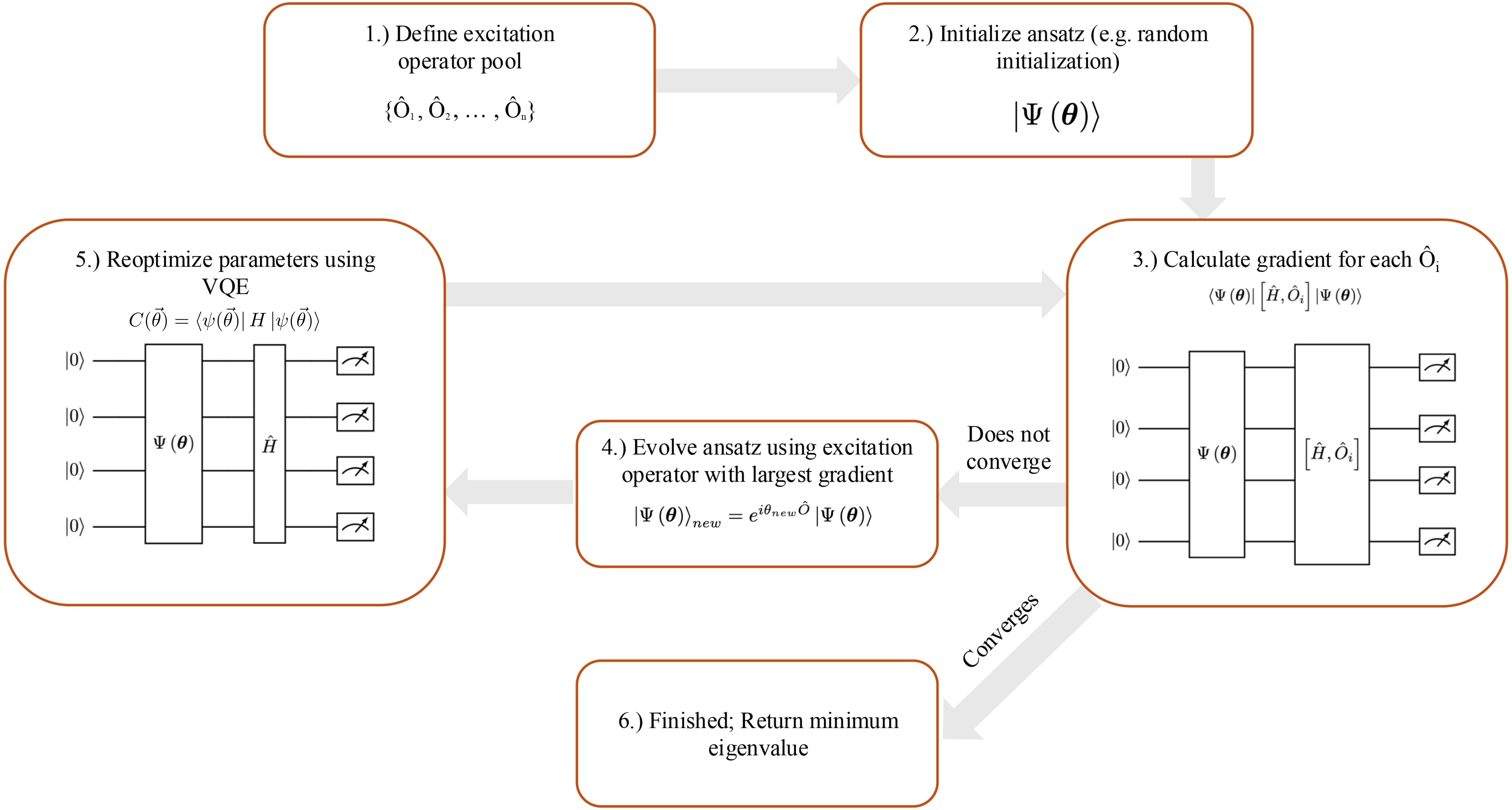
K. Kanno, M. Kohda, R. Imai, S. Koh, K. Mitarai, W. Mizukami, Y.O. Nakagawa, "Quantum-selected configuration interaction: Classical diagonalization of Hamiltonians in subspaces selected by quantum computers," *Phys. Rev. Research* **8,** 023268 (2023).

VQE Results



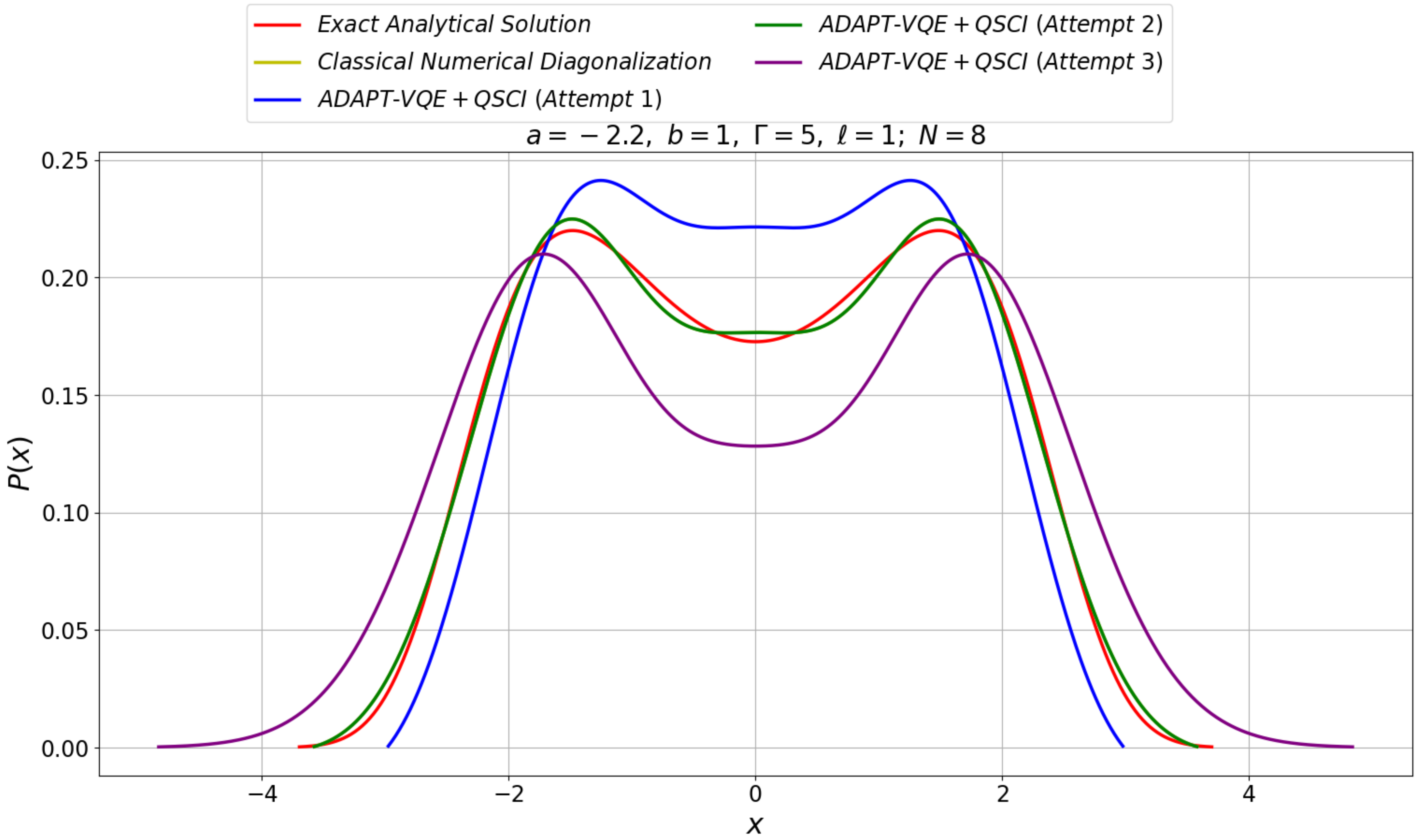
Noisy Simulation
Exact Analytical Solution
Classical Numerical Diagonalization
VQE + QSCI ($N_q = 6$, IBM Nairobi Simulator, SPSA 300 iterations)
$a = -1,\ b = 2,\ \Gamma = 1,\ \ell = 1;\ N = 64$
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$P(x)$
−2
−1
0
1
2
x
Hardware Experiment
Exact Analytical Solution
Classical Numerical Diagonalization
VQE + QSCI ($N_q = 3$, IBM Marrakesh, COBYLA 18 iterations)
$a = -2.2,\ b = 1,\ \Gamma = 5,\ \ell = 1;\ N = 8$
0.20
0.15
0.10
0.05
0.00
$P(x)$
−4
−3
−2
−1
0
1
2
3
4
x

ADAPT Variational Quantum Eigensolver (ADAPT-VQE)



H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, An adaptive variational algorithm for exact molecular simulations on a quantum computer, Nat. Commun. **10**, 3007 (2019).

ADAPT-VQE Results



ADAPT-VQE shows variations in results from simulation to simulation, unlike VQE.

Key Question To Be Answered

Can quantum computers offer an **advantage** over classical computers in finding the statistics of high-dimensional dynamical systems such as the fluid Earth system?

Next steps: Further investigate the efficacy of VQE on modern NISQ hardware. Also investigate the extent of the dimensionality reduction of QSCI.

Long term: Can a quantum algorithm be developed such that it can recover eigenvectors without the need for classical diagonalization? Are there other approaches that don't require diagonalization?

Further reading: S. Bravyi, A. Byrne, M. Zayats, S. Zhuk, "Quantum algorithms for stochastic nonlinear differential equations", https://doi.org/10.48550/arXiv.2606.08349 (2026).

- This paper discusses methods to map observables of nonlinear dynamical systems to a quantum computer using the Hermite polynomial basis and then simulate time-evolution on the quantum computer to recover the desired expected values of the observables.