Variational quantum algorithm for eigenvalue problems of a class of Schrödinger-type partial differential equations

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MINISTERIO DE CIENCIA E INNOVACIÓN

INSTITUTO DE FÍSICA FUNDAMENTAL

CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Quantum numerical analysis

- Systems of equations → HHL algorithm
  A. W. Harrow, A. Hassidim, and S. Lloyd, Phys. Rev. Let. 103(15) (2009).
- Ordinary differential equations (ODE's)
  D. W. Berry, Journal of Physics A 47(10):105301 (2014).
  D. W. Berry, A. M. Childs, A. Ostrander, and G. Wang, Comm. In Math. Phys. 356(3):1057-1081 (2017).
- Partial differential equations (PDE's)
  P. C. S. Costa, S. Jordan, and A. Ostrander, Phys. Rev. A. 99(1) (2019).
  A. M. Childs, J. Liu, and A. Ostrander, arXiv:2002.07868 (2020).
  N. Linden, A. Montanaro, and C. Shao, arXiv:2004.06516 (2020).
  A. Suau, G. Staffelbach, and H. Calandra, ACM Transactions on Quantum Computing 2(1):1–35 (2021).

HLL-based methods are fault-tolerant algorithms!

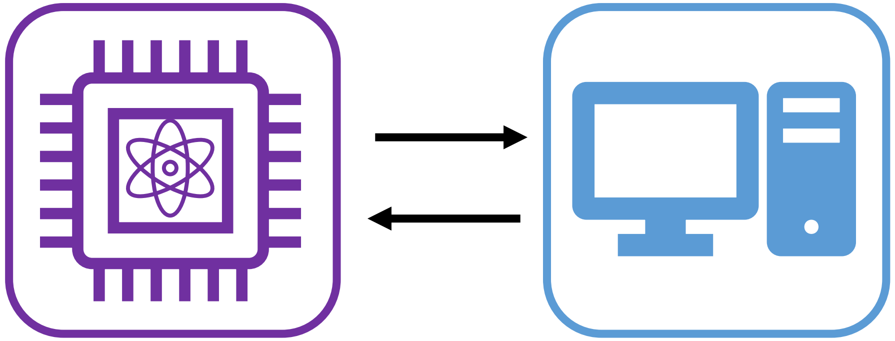
Noisy Intermediate-Scale Quantum era (NISQ era)

J. Preskill, Quantum, 2:79 (2018).

Limitations of current quantum computers

- Limited number of qubits.
- Noise sources limit the number of operations.
- ...

Solution:
Variational hybrid quantum-classical algorithms



Peruzzo, Alberto, et al., Nature communications 5: 4213 (2014).
J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, New Journal of Physics 18(2):023023 (2016).
M. Lubasch, J. Joo, P. Moinier, M. Kiffner, and D. Jaksch, Phys. Rev. A 101(1) (2020).
K. Sharma, S. Khatri, M. Cerezo, and P. J. Coles, New Journal of Physics 22(4):043006 (2020).

Partial differential equations (PDE's) of the form

$$[D(-i\nabla) + V(\mathbf{x})]f(\mathbf{x}) = Ef(\mathbf{x}),$$

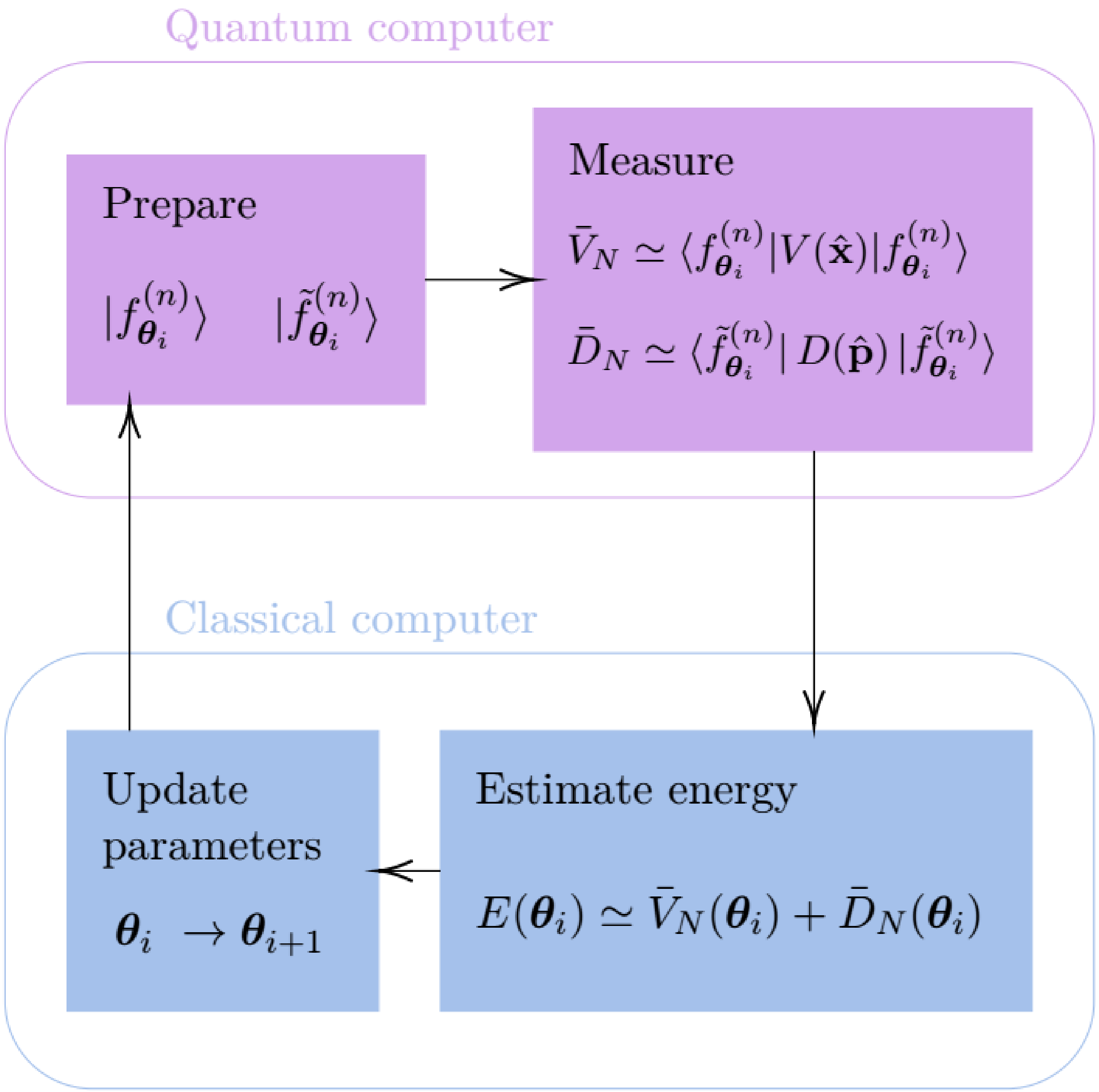
with $x_i \in [a_i, b_i)$, $f(\mathbf{x} + (b_i - a_i)\mathbf{e_i}) = f(\mathbf{x})$,
$f(\mathbf{x})$ bandwith − limited and $D(\mathbf{p}), V(\mathbf{x}) \in \mathbb{R}$.

We assume that the PDE is a lower bounded Hamiltonian operator

$$H = D(-i\nabla) + V(\mathbf{x}) \geq E_{\min}.$$

Result

$$\text{argmin}_f \langle f|H|f\rangle \leq f_{\text{argmin}_{\boldsymbol{\theta}} E(\boldsymbol{\theta})}.$$



Mapping continuous functions to quantum registers

$$f(x) \quad \rightarrow \quad f(x_s) = \langle s | f^{(n)} \rangle,$$

$$x_s^{(n)} = a + s\Delta x, \quad \text{with } s \in \{0, 1, \dots, 2^n - 1\} \text{ and } \Delta x = \frac{L_x}{2^n}.$$

Quantum representation of the operators

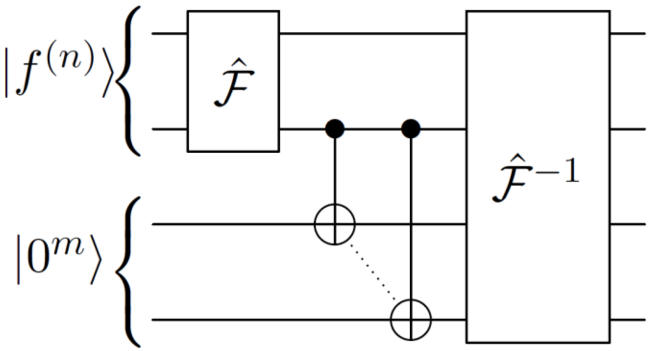
$$V\left(\hat{x}^{(n)}\right) := \sum_s V(x_s) |s\rangle\langle s|$$

$$p_s = \frac{2\pi}{\Delta x^{(n)} 2^n} \times \begin{cases} s, & 0 \leq s < 2^{n-1} \\ s - 2^n, & \text{otherwise} \end{cases}$$

$$D\left(\hat{p}^{(n)}\right) := \hat{\mathcal{F}}^{-1} \sum_s D(p_s) |s\rangle\langle s| \hat{\mathcal{F}}$$

Fourier interpolation

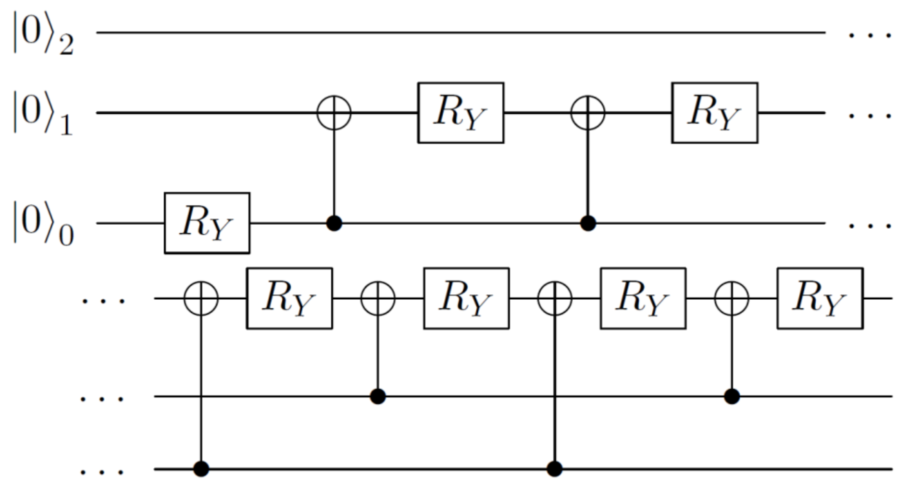
$$f(x) \propto \sum_{s=0}^{2^n - 1} e^{-i p_s x} \langle s | \hat{\mathcal{F}} | f^{(n)} \rangle$$



J. J. García-Ripoll, Quantum 5, 431 (2021).

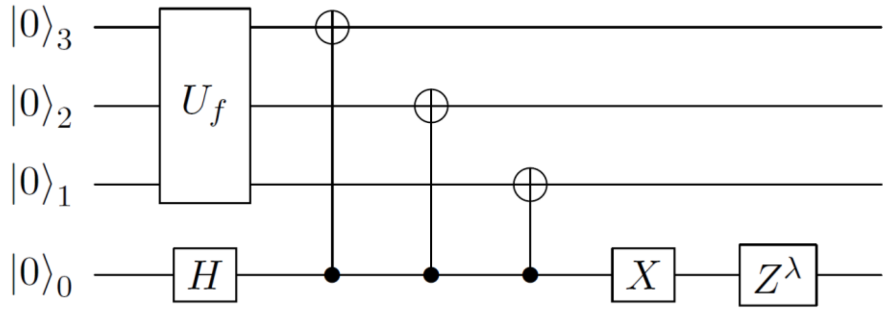
Encoding of continuous functions in a variational quantum circuit

C. Zalka, Proceedings of the Royal Society of London. Series A. 454(1969):313–322, (1998).
L. Grover and T. Rudolph, arXiv:quant-ph/0208112 (2002).



ZGR ansatz

Symmetry embedding



$$\langle 1 s_1 \dots s_{n-1} | f^\lambda \rangle = (-1)^\lambda \langle 0 \bar{s}_1 \dots \bar{s}_{n-1} | f^\lambda \rangle, \quad \lambda = 0, 1$$

Harmonic oscillator

H. Nyquist, Transactions of the American Institute of Electrical Engineers 47(2):617–644 (1928).
C.E. Shannon, Proceedings of the IRE, 37(1):10–21 (1949).

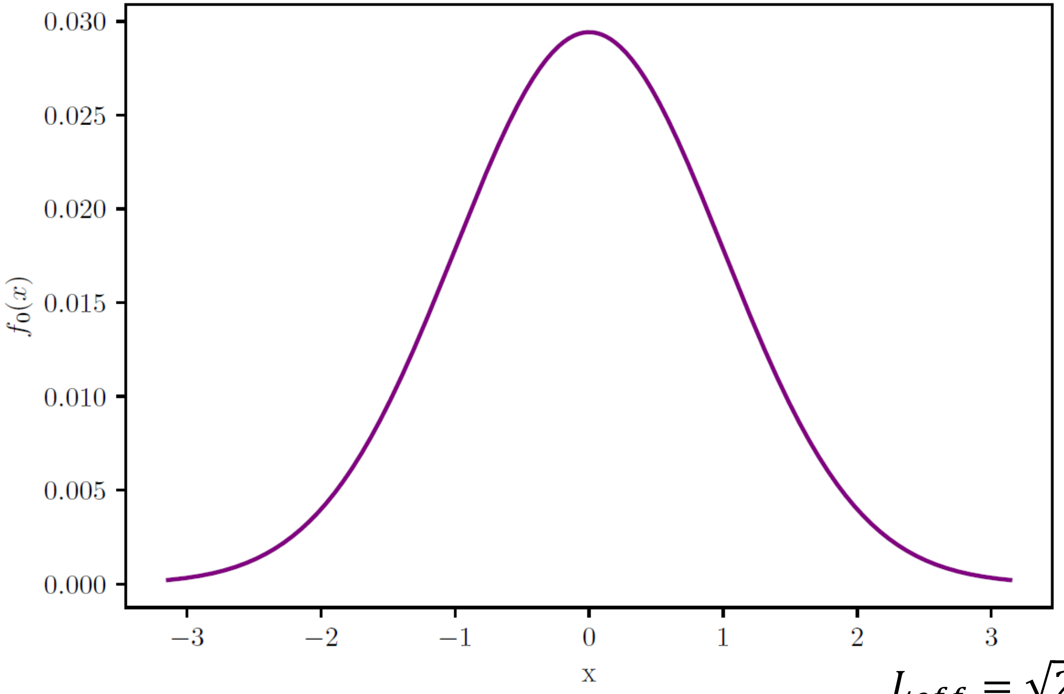
- Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2 x^2 - E\right) f(x) = 0$$

- Ground state

$m = \omega = \hbar = 1$

$$f_0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}$$



$L_{eff} = \sqrt{2\pi 2^n}$

Figures of merit

- Continuous fidelity

$$F^{\infty} := \lim_{m\to\infty} \left|\langle f^{(n+m)} \middle| U_{\text{int}}^{n,m} W(\boldsymbol{\theta}_{\text{opt}}) \middle| 0^{\otimes n}\rangle\right|^2 \propto \left|\int f_{\text{obj}}^* f_{\text{int}} dx\right|^2$$

- Relative error in the computation of the energy

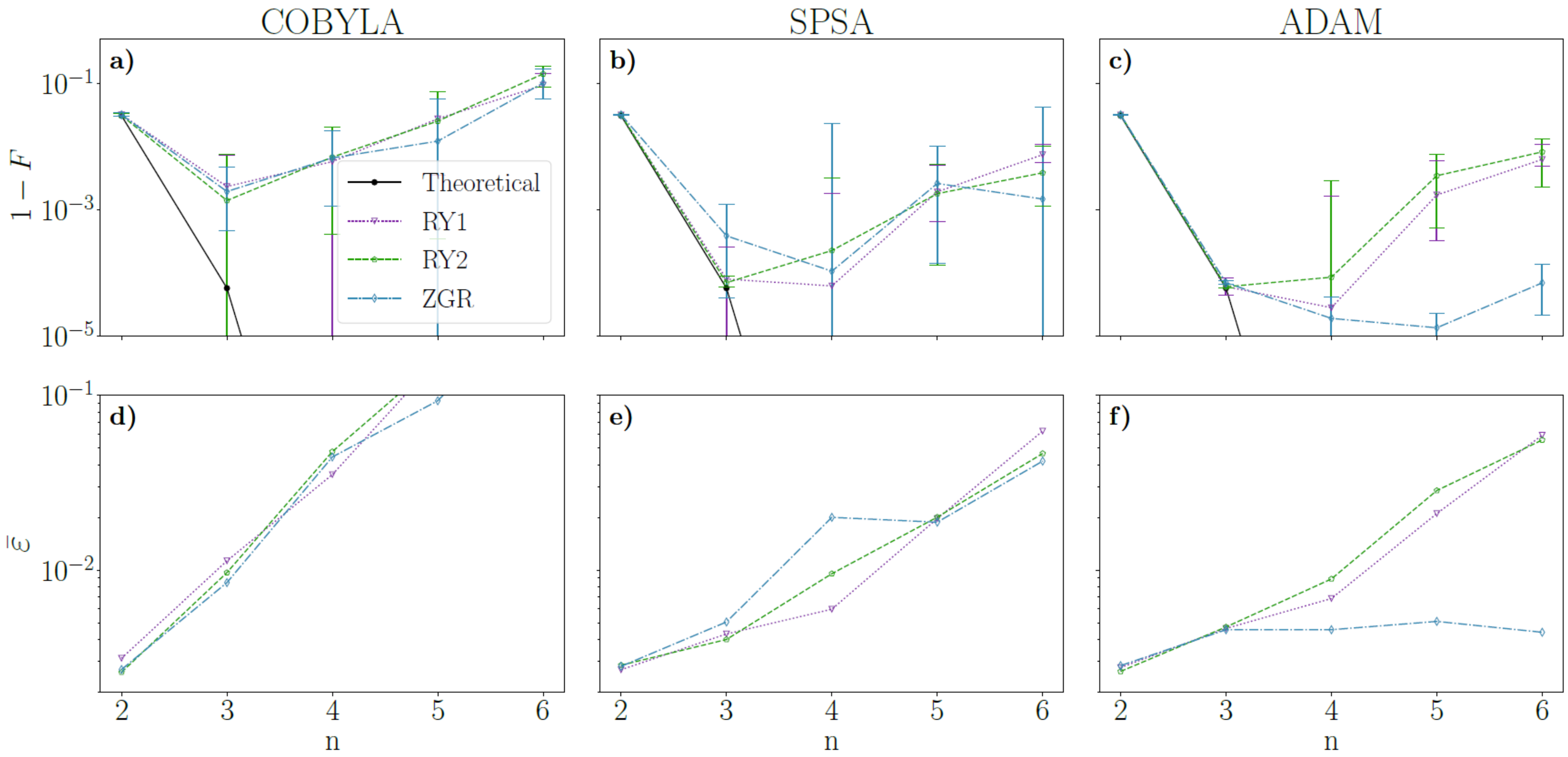
$$\varepsilon = \left|\frac{E_{t_n} - E_{\text{opt}}}{E_1 - E_0}\right|$$

Parameters for the simulations

- 8192 evaluations.
- 100 repetitions.
- $n + m = 12$.

Optimum classical optimizer and ansatz

H. Abraham, AduOffei, R. Agarwal, I. Y. Akhalwaya, and G. Aleksandrowicz et al. Qiskit: An open-source framework for quantum computing (2019).

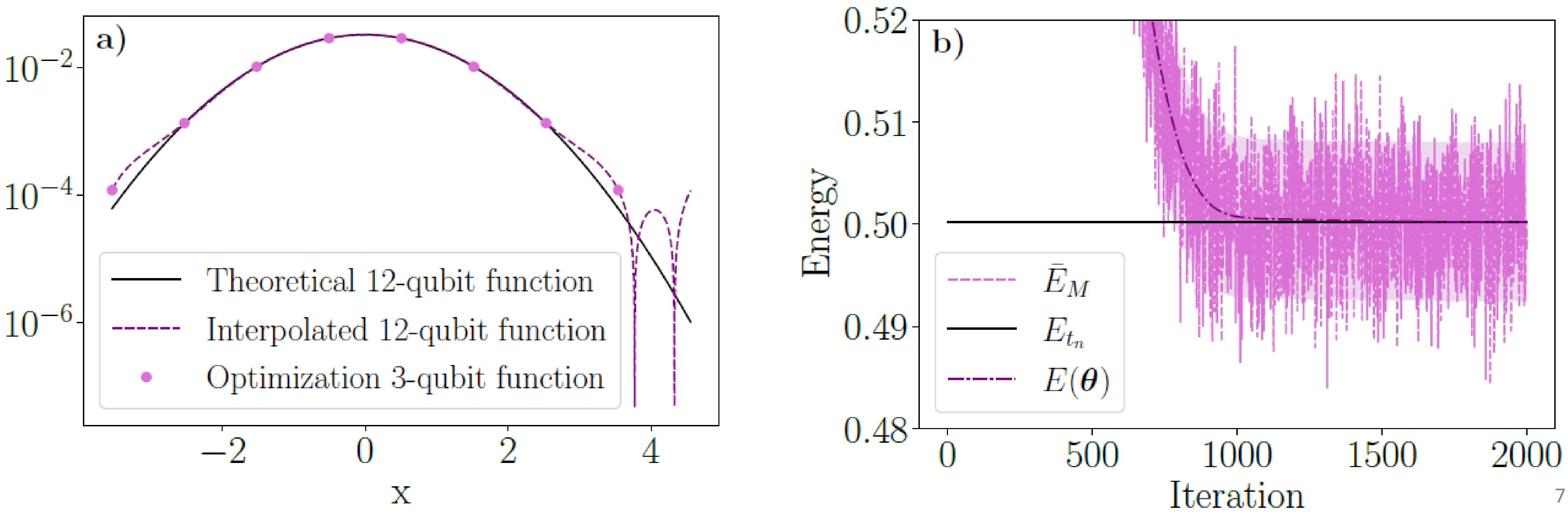


- ADAM best optimizer followed by SPSA. K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii. Phys. Rev. A 98(3) (2018). M. Schuld, V. Bergholm, C. Gogolin, J. Izaac, and N. Killoran. Phys. Rev. A 99(3) (2019).
- ZGR is the best variational ansatz as the state is smoothly constructed, contrary to the chaotic nature of R_Y (trapped in local minima for $n > 3$). J. R. McClean, S. Boixo, V. N. Smelyanskiy, R. Babbush, and H. Neven. Nature Communications, 9(1) (2018).
- Low infidelities of order $10^{-5} - 10^{-3}$ despite the statistical uncertainty in the evaluation of the cost function.

Wavefunction and optimization trajectory

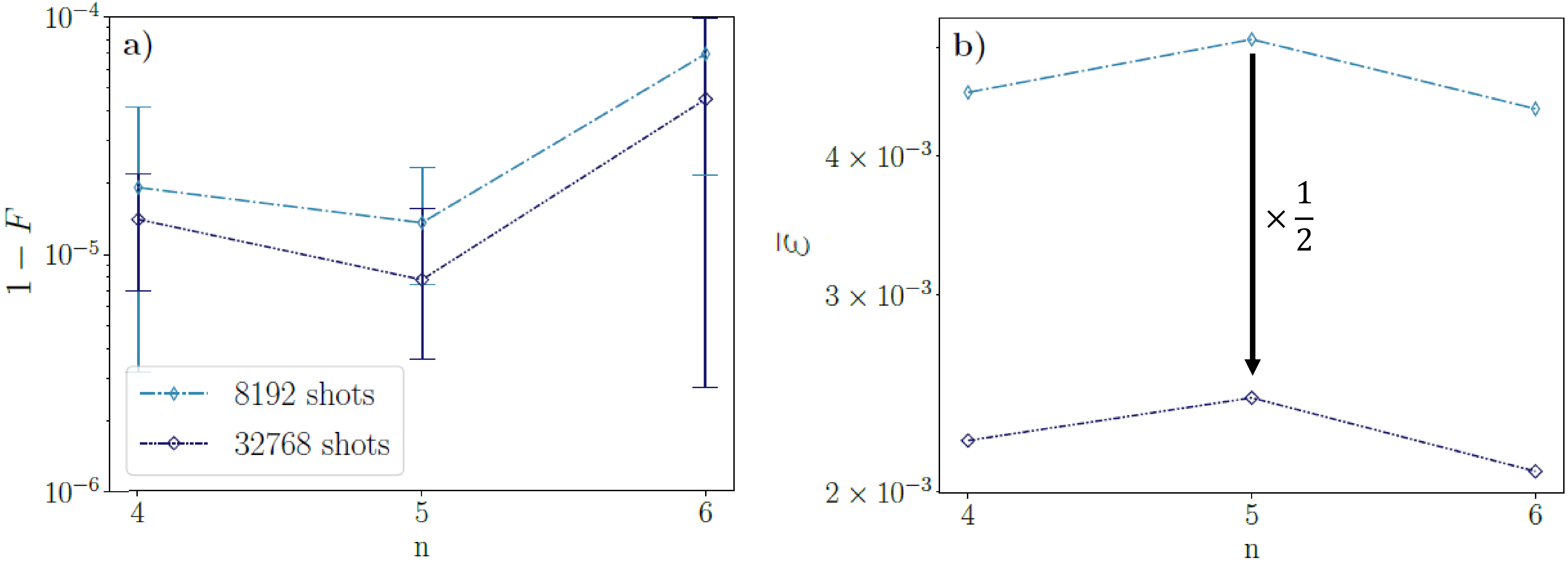
- Relative error below the statistical uncertainty.
- We recover the wavefunction with high fidelity using Fourier interpolation.

3 qubits
ZGR ansatz
ADAM optimizer



Increase in the number of evaluations

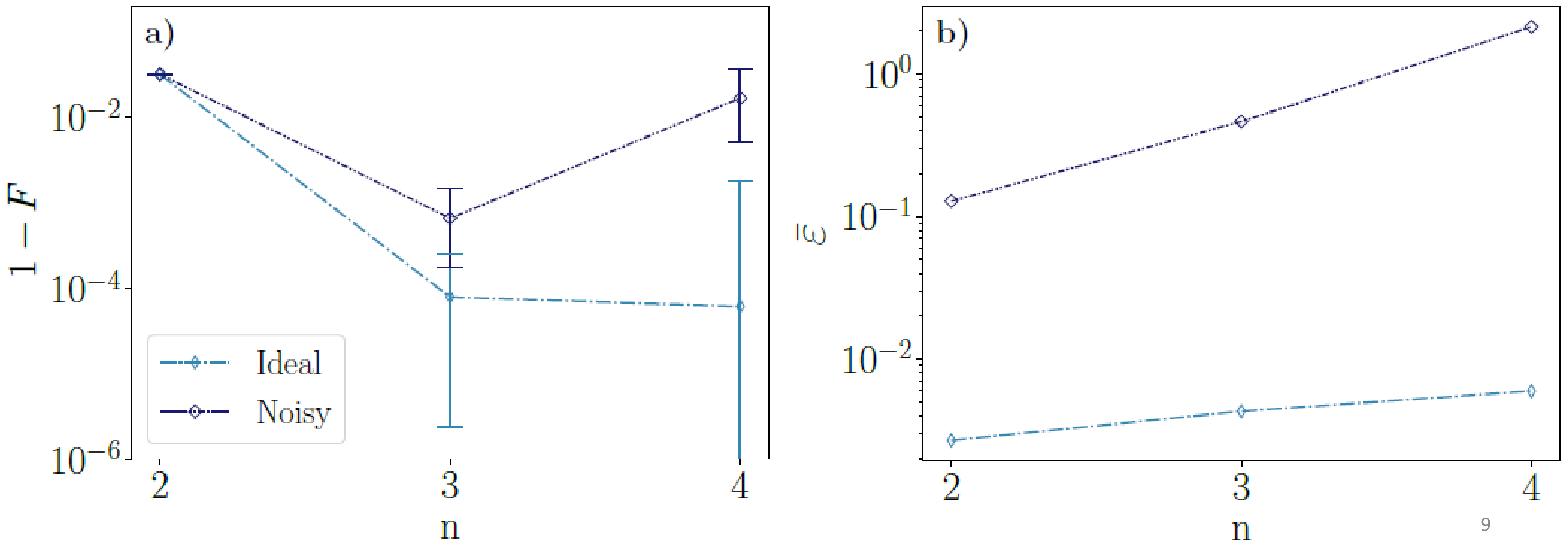
The precision of the algorithm is limited by the number of evaluations in the quantum computer, as the more evaluations the better the estimate of the expectation value.



Noisy simulation

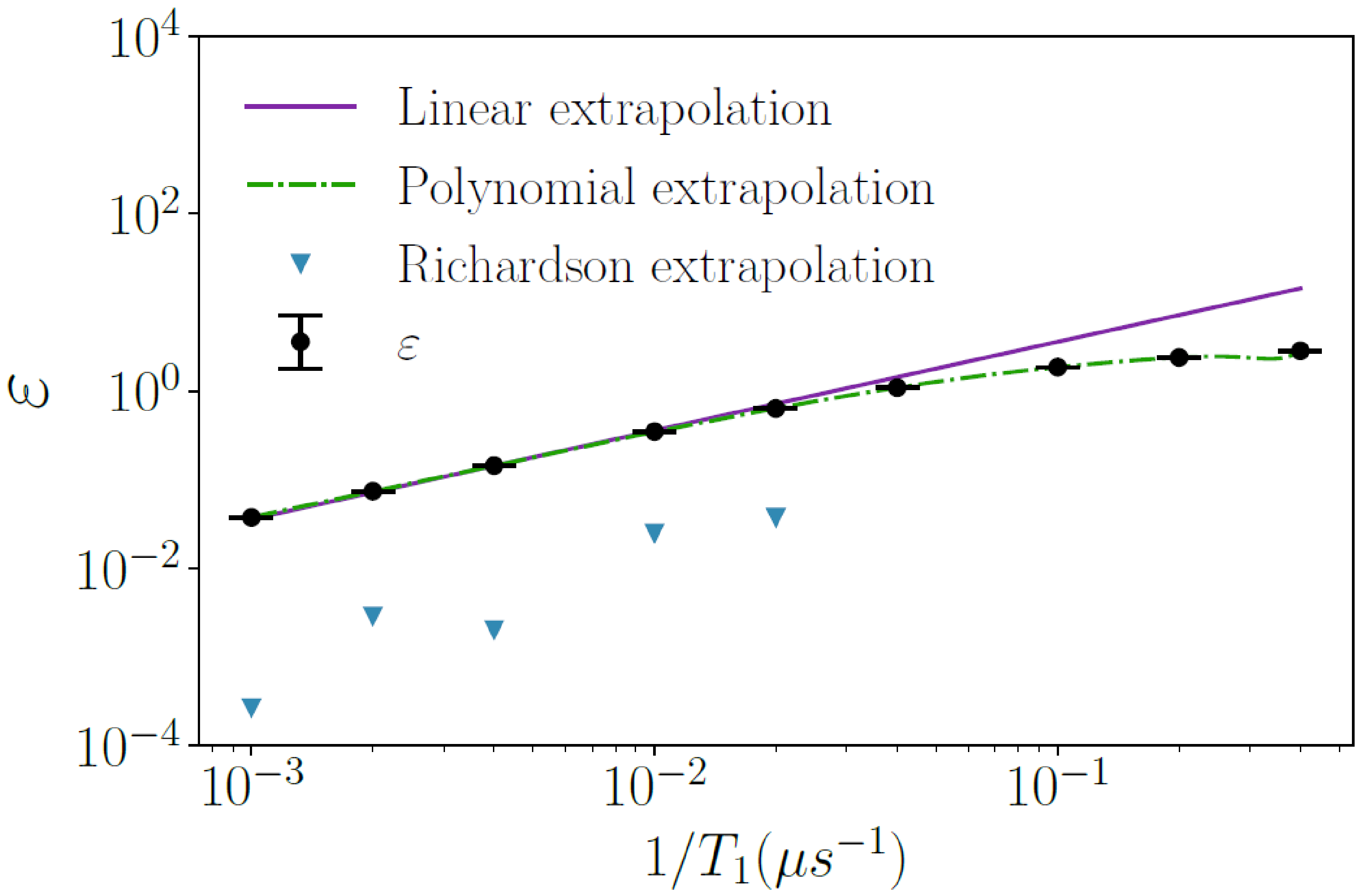
(R_y depth 1 + SPSA optimizer for the harmonic oscillator using the ibmq_santiago simulator)

- Noise resilient for a small (3) number of qubits, with infidelity of order 10^{-4}.
- Very significant error in the energy.



Error mitigation (zero-noise extrapolation)

A. Kandala, K. Temme, A. D. Córcoles, A. Mezzacapo, J. M. Chow, and J. M. Gambetta, Nature 567(7749):491–495 (2019).



- Thermal relaxation (ibmq_santiago simulator).
- R_y ansatz with depth 1 and 3 qubits for the harmonic oscillator optimum solution.
- It admits 5-th order Taylor expansion.

$$E(T_1) = E_0 + \sum_n \epsilon_n \frac{1}{T_1^n}$$

- Richardson extrapolation with energy error $\varepsilon \sim 10^{-2}$ for state of the art thermal relaxation times.

Conclusions

- We have developed a variational quantum algorithm to solve Hamiltonian PDE's based on Fourier interpolation to represent continuous functions in quantum registers, and new variational ansätze suited to describe continuous functions, or which include symmetries.

- We have obtained high fidelity results under ideal and noisy circumstances.

Future work

- Reduce the cost using new ansätze and less demanding gradient techniques.

  R. Sweke, F. Wilde, J. Meyer, M. Schuld, P. K. Faehrmann, B. Meynard-Piganeau, and J. Eisert, Quantum 4:314 (2020).

- Consideration of quantum-inspired methods (tensor networks). J. J. García-Ripoll, Quantum 5 431 (2021).

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Solving partial differential equations in quantum computers

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