NEURAL INFORMATION PROCESSING SYSTEMS

Physics-Informed Bayesian Optimization of Variational Quantum Circuits

Work in collaboration with: L. **Funcke**, T. **Hartung**, K. **Jansen**, S. **Kühn**, K. R. **Müller**, P. **Stornati**, P. **Kessel**, and S. **Nakajima**.

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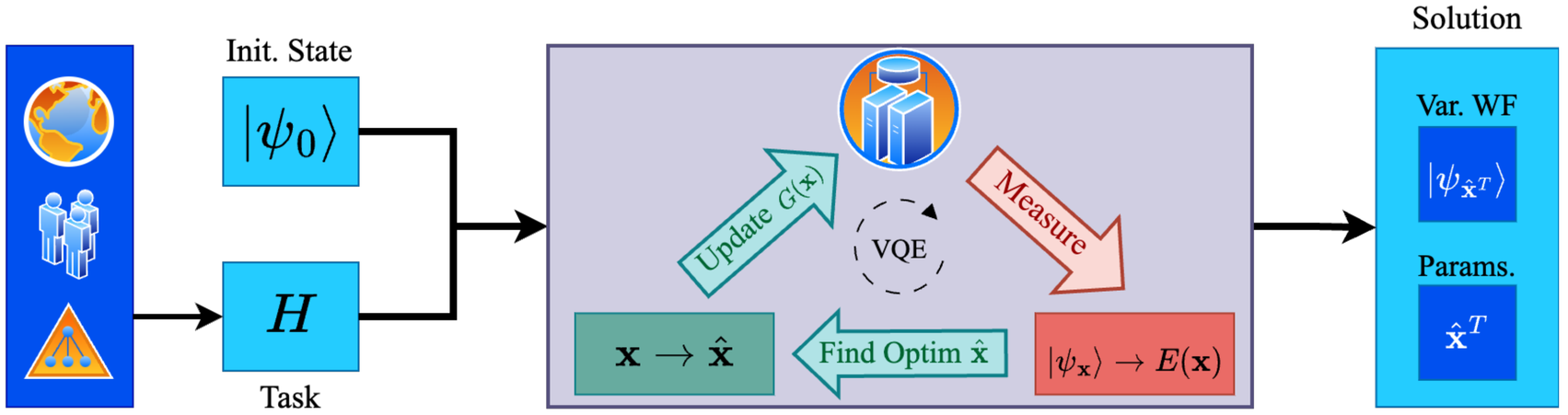
Talk by K. A. **Nicoli** and C. J. **Anders**

Variational Optimization of Quantum Circuits

⭐ **Goal**: Find optimal parameters of a quantum circuit to minimize the energy of a given Hamiltonian H.

a.k.a.

⭐ **Goal**: Find optimal parametric ansatz to minimize a suitable cost function.



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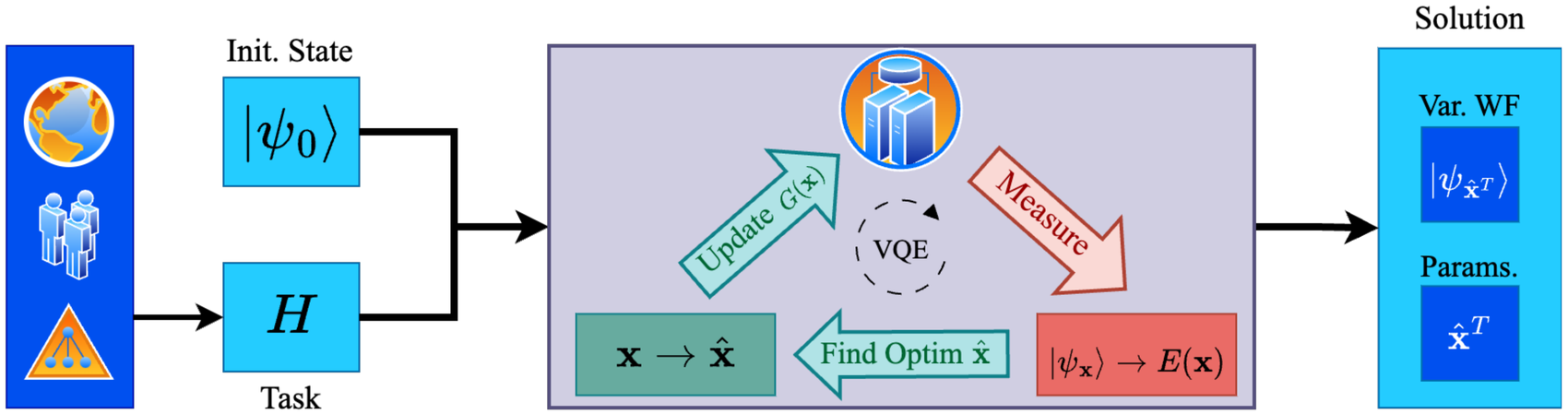

Cost function (Energy): expectation value of a given Hamiltonian H

$$H = -\sum_{i=\{X\,Y\,Z\}}\sum_{j=1}^{Q}(J_i\sigma_j^i\sigma_{j+1}^i + h_i\sigma_j^i)$$

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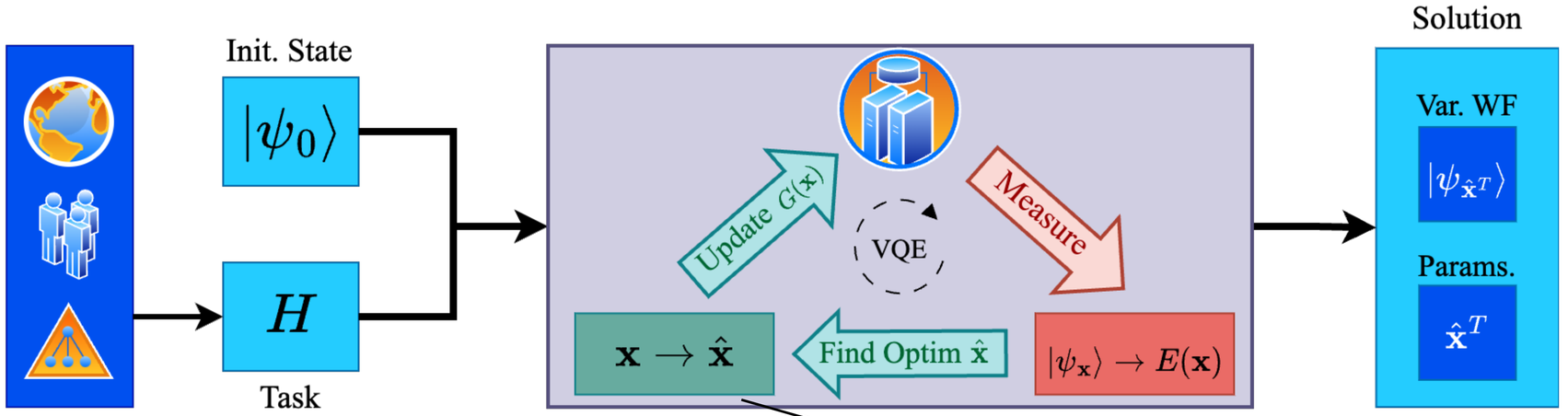

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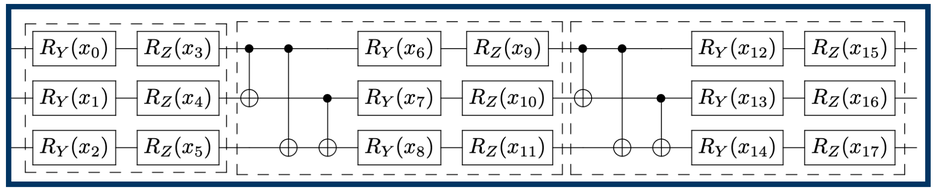
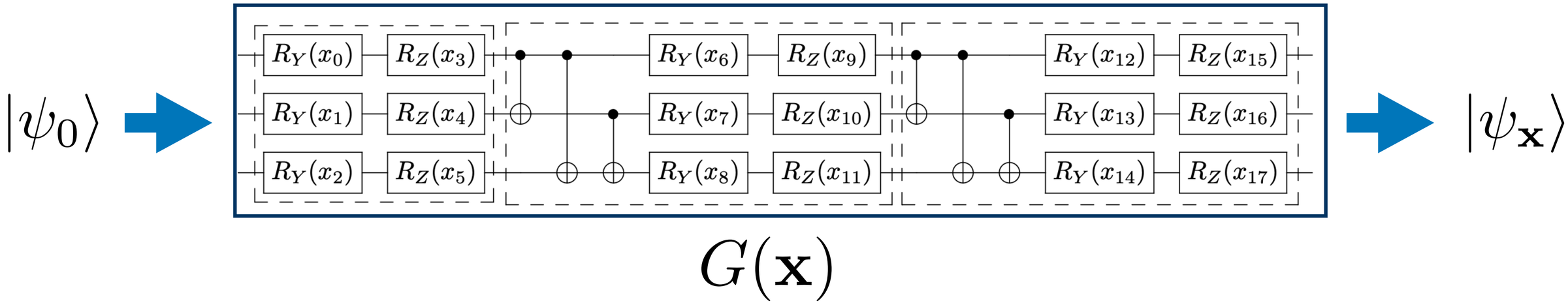
x parametrizes the **gates** $R_{Z,Y}$ of a parametric quantum circuit $G(\mathbf{x})$



Variational Quantum Eigensolvers (VQEs)



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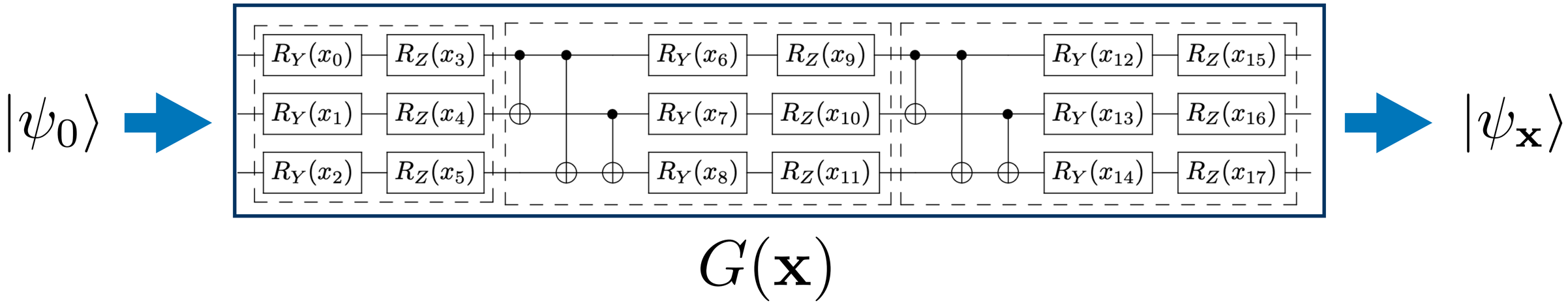

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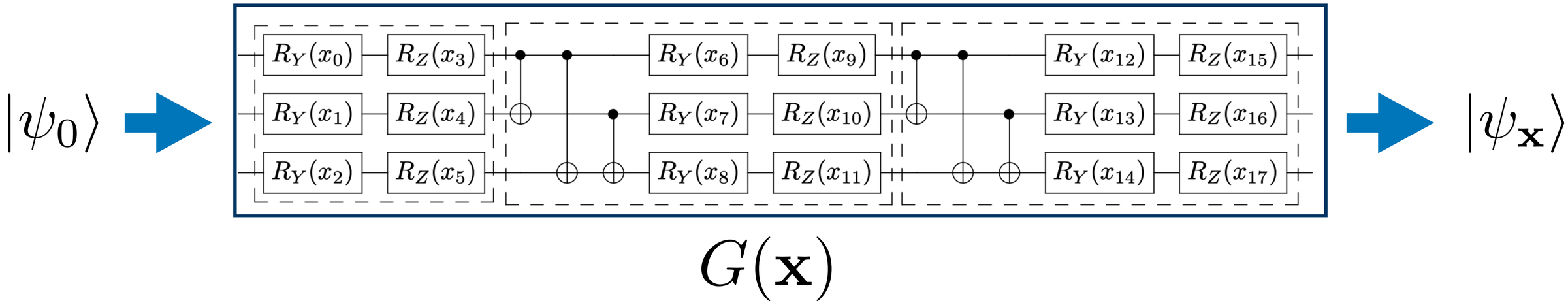

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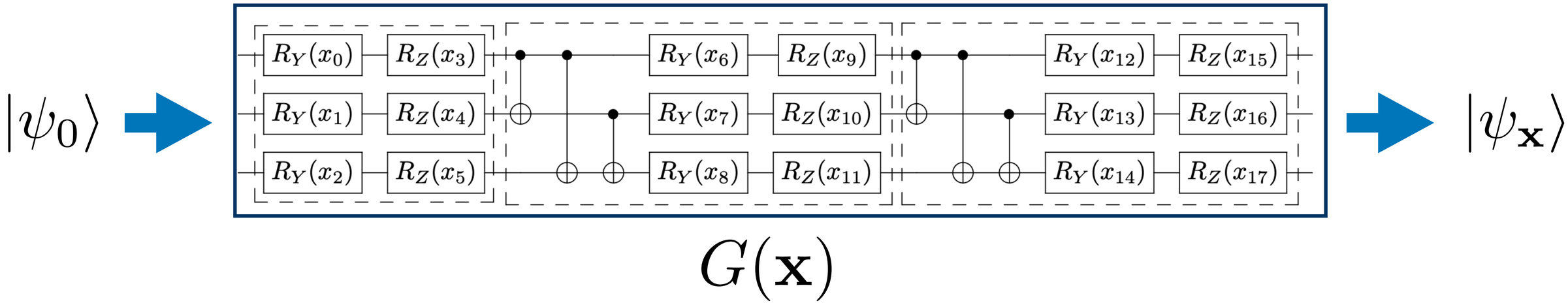

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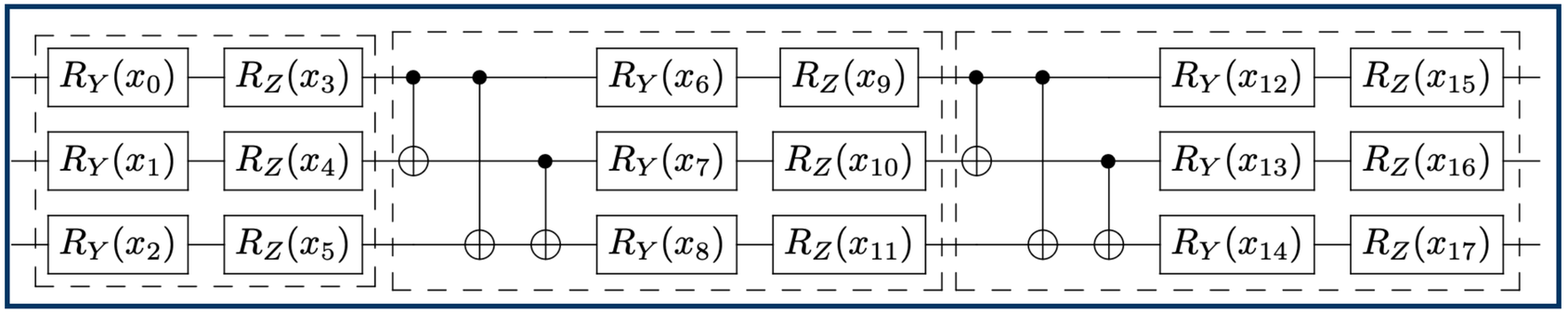
$|\psi_0\rangle$ 

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Variational Minimization Problem

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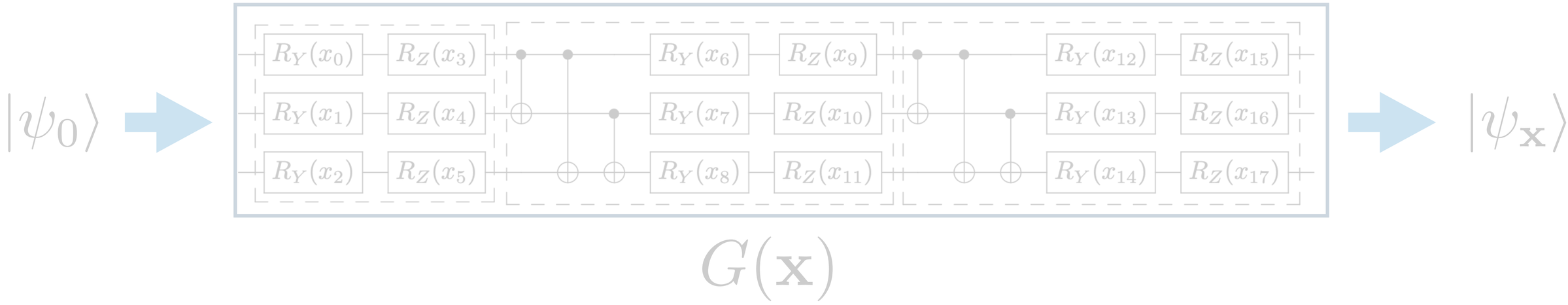

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Quantum operation: measurement on QC

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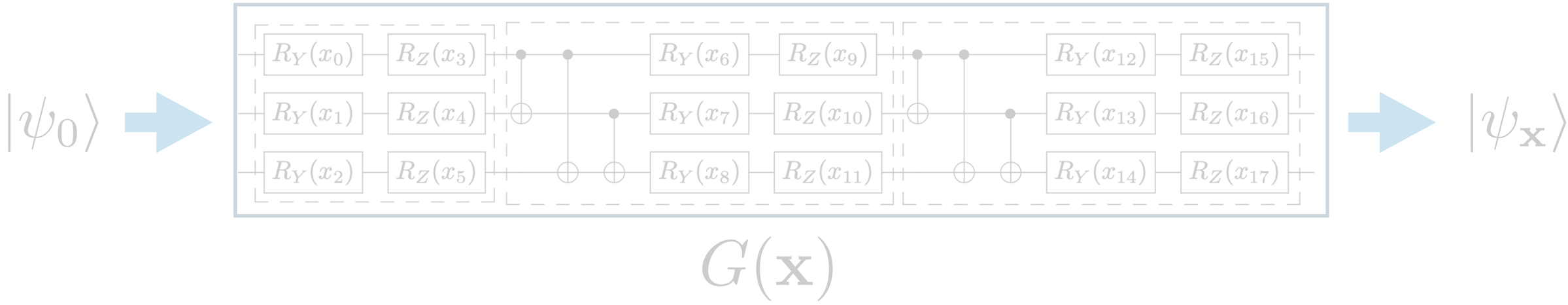

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Classical operation: runs on classical computer

Variational Minimization Problem

Bayesian Optimization for VQEs

We tackle the **classical optimization problem** from a **Bayesian Optimization** standpoint.

Approximate the true energy $E^*(\cdot) : \mathcal{X} \mapsto \mathbb{R}$

Using noisy observations from the QC $y = E^*(\mathbf{x}) + \varepsilon$ $\varepsilon \sim$ QC Hardware noise

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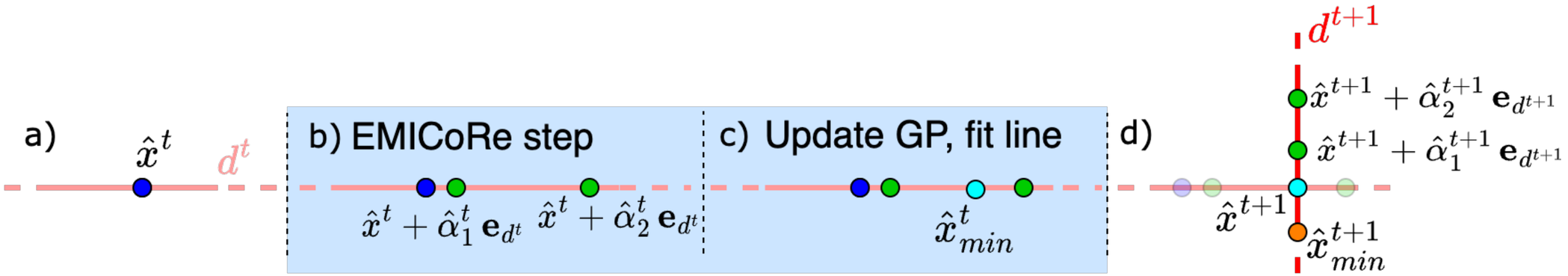
One question remains to be answered:

*At which point in parameter space we should perform the **next measurement**, on the quantum computer, to **maximize the information gain** and **minimize the quantum computer calls** needed to minimize the objective?*

Expected Maximum Improvement over Confident Regions



i. Take the best params $\hat{\mathbf{x}}^t$, which give the minimum value for the cost function at step $t-1$.

ii. Identify one direction $d^t \in D$ to optimize at step t.

iii. Use EMICoRe* to perform a grid search and find the best pair of shifts $\{\hat{\alpha}_1^t, \hat{\alpha}_2^t\}_{d^t}$ to add to the previous $\hat{\mathbf{x}}^t$.

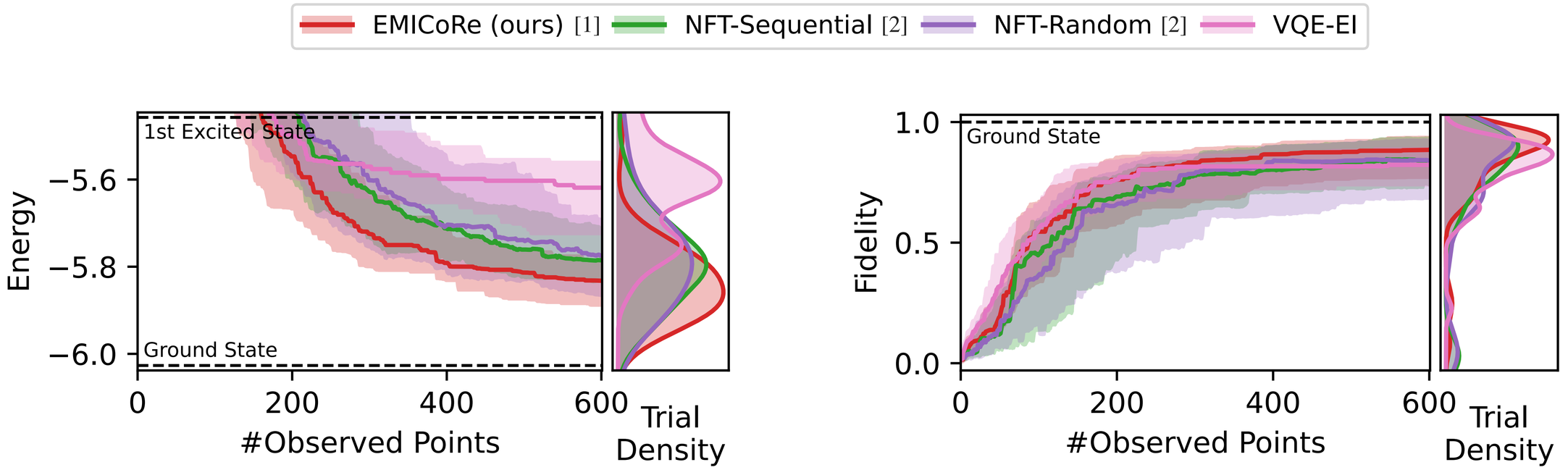
iv. Perform new observations at $y_1^t = \hat{\mathbf{x}}^t + \hat{\alpha}_1^t$ and $y_2^t = \hat{\mathbf{x}}^t + \hat{\alpha}_2^t$ and add these to the GP.

v. Perform least square minimization to find the new minimum $\hat{\mathbf{x}}^t_{min}$ which is the starting point for step $t+1$.

EMICoRe efficiently identifies the points in step iii. , using the *Core:* $\mathcal{Z}_{\widetilde{\mathbf{X}}} = \{\mathbf{x} \in \mathbf{X}^{\mathrm{Grid}}; s_{\widetilde{\mathbf{X}}}(\mathbf{x}, \mathbf{x}) \leq \kappa^2\}$

*EMICoRe uses a physics informed VQE-kernel introduced in this work. More details in the paper.

Results



Our experiments demonstrate:

- EMICoRe outperforms the baselines
- Faster convergence
- Stable optimization
- Smaller energy (median)

Applications:

- Lattice quantum field theory
- Material Science
- Quantum chemistry
- Optimization Tasks (flight gate assign.)

[1] Nicoli K. A. et al., NeurIPS (2023) - This work

[2] Nakanishi, K, Fujii K., and Todo S., Phys. Rev. Res. (2020)

Want to know more?

Poster #1308

Thursday 14th Dec, 5-7 p.m.
Great Hall & Hall B1+B2

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Go to the Paper

Go to GitHub