Theory and Phenomenology of Fundamental Interactions
UNIVERSITY AND INFN · BOLOGNA

INFN Istituto Nazionale di Fisica Nucleare
Sezione di Bologna

QUANTUM COMPUTING: a hybrid point of view

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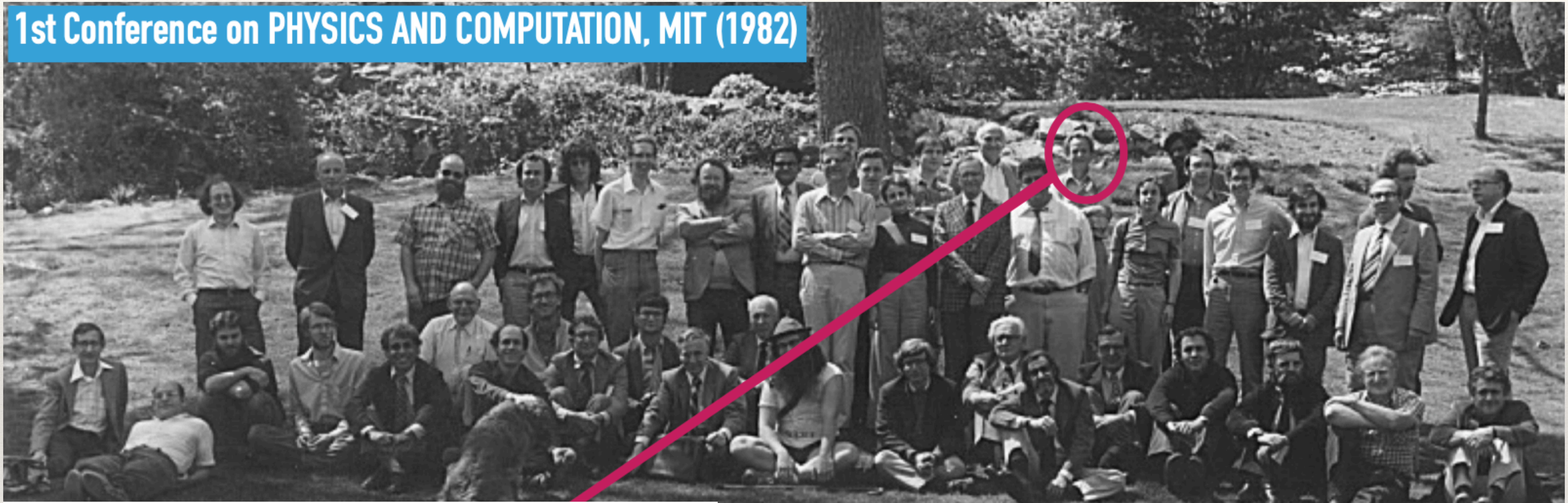
A Quantum Day in Bologna
Caligola Workshop
June 9, 2023

Quantum Simulations



Simulating Physics with Computers

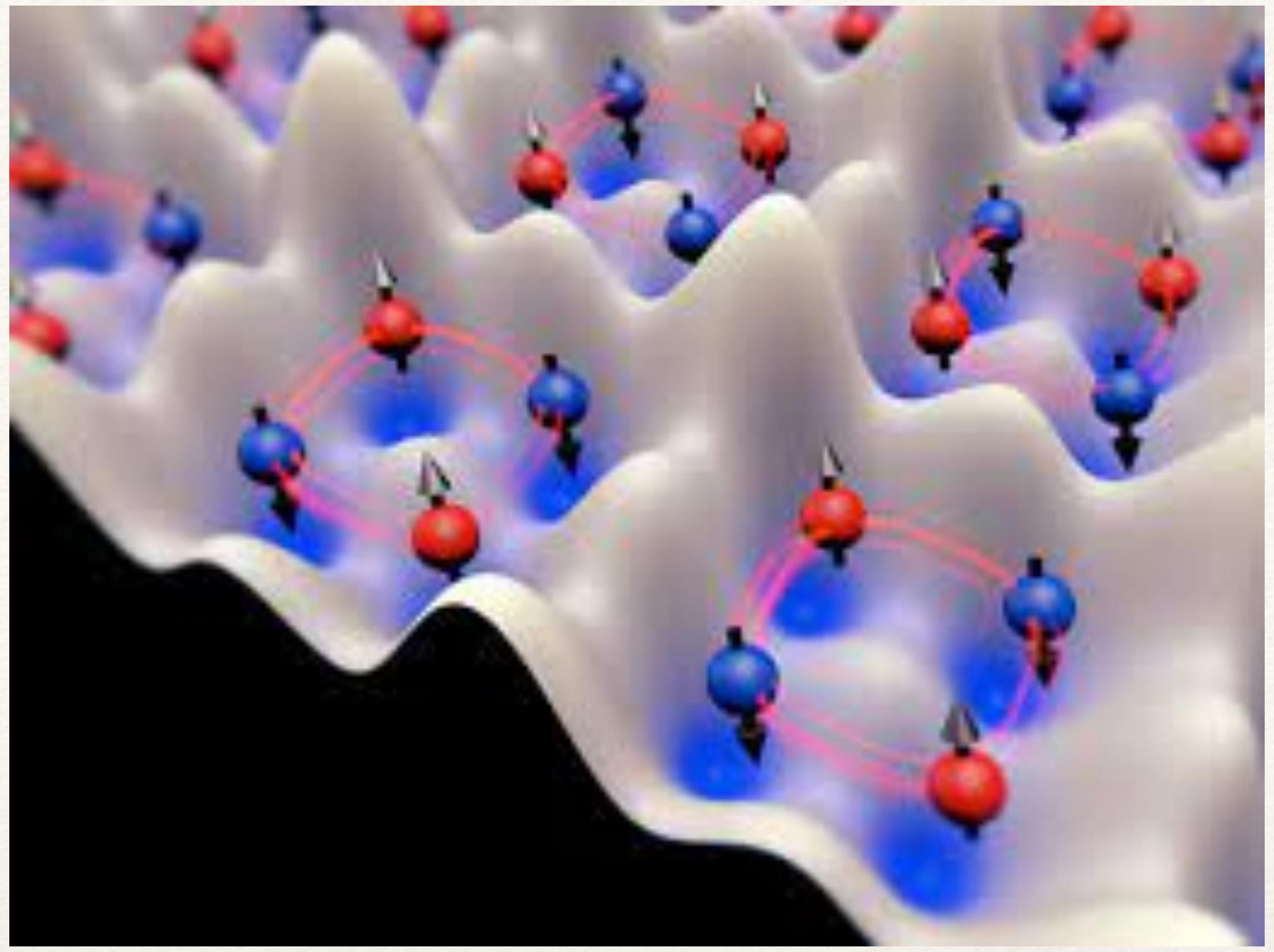
Richard P. Feynman

Now, what kind of physics are we going to imitate? First, I am going to describe the possibility of simulating physics in the classical approximation, a thing which is usually described by local differential equations. But the physical world is quantum mechanical, and therefore the proper problem is the simulation of quantum physics—which is what I really want to talk about, but I'll come to that later. So what kind of simulation do I mean?

I want to talk about the possibility that there is to be an *exact* simulation, that the computer will do *exactly* the same as nature.

International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

TRAPPED IONS/ATOMS

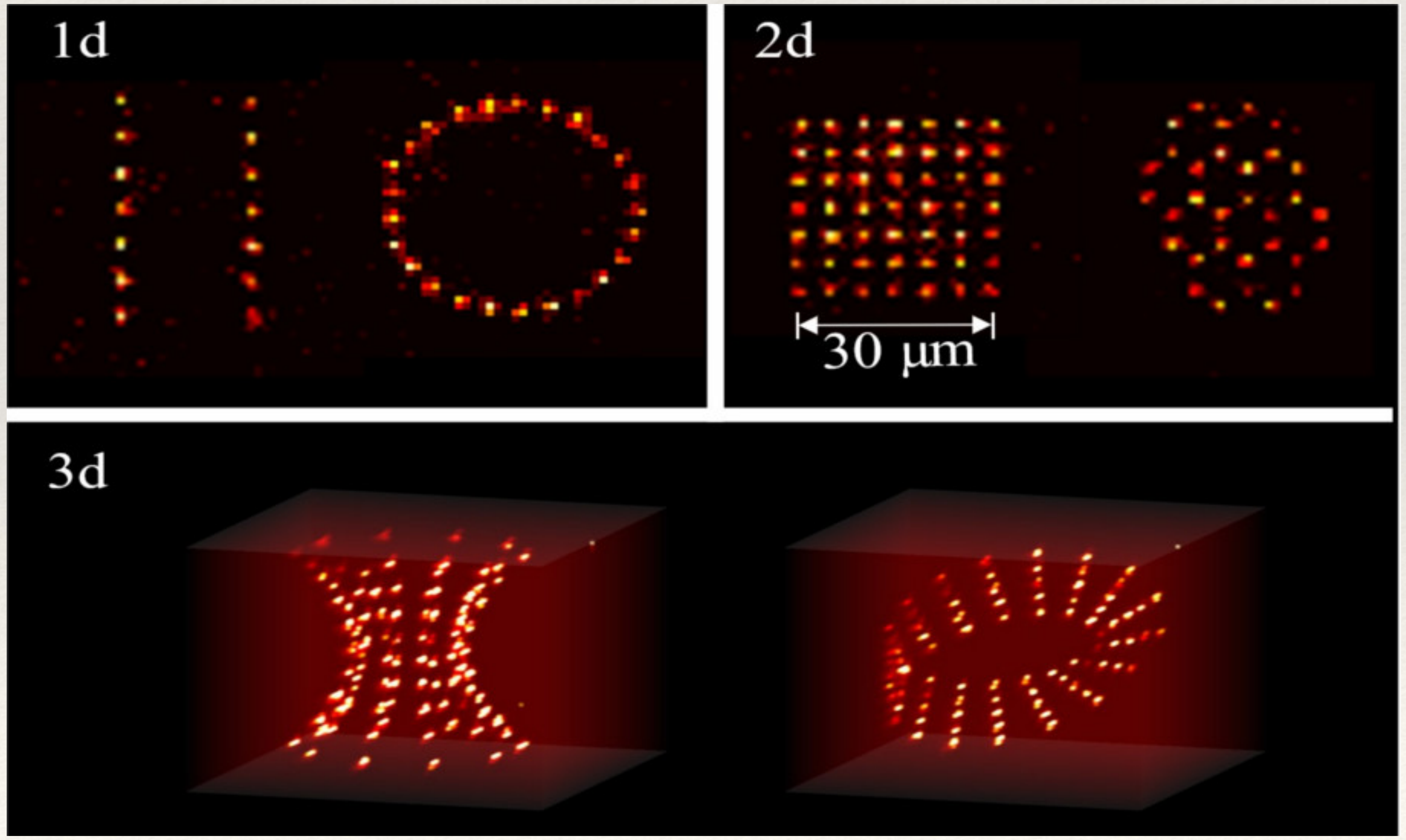


ANALOGUE SIMULATIONS

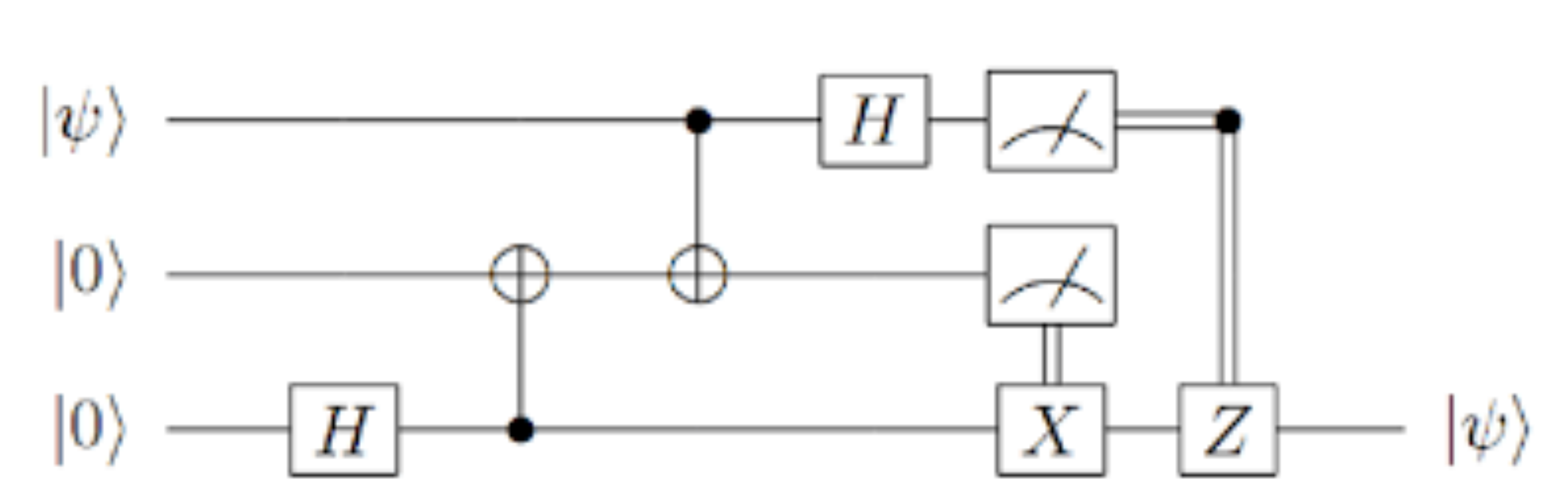
Single atoms/ions trapped in optical lattices

very versatile systems:

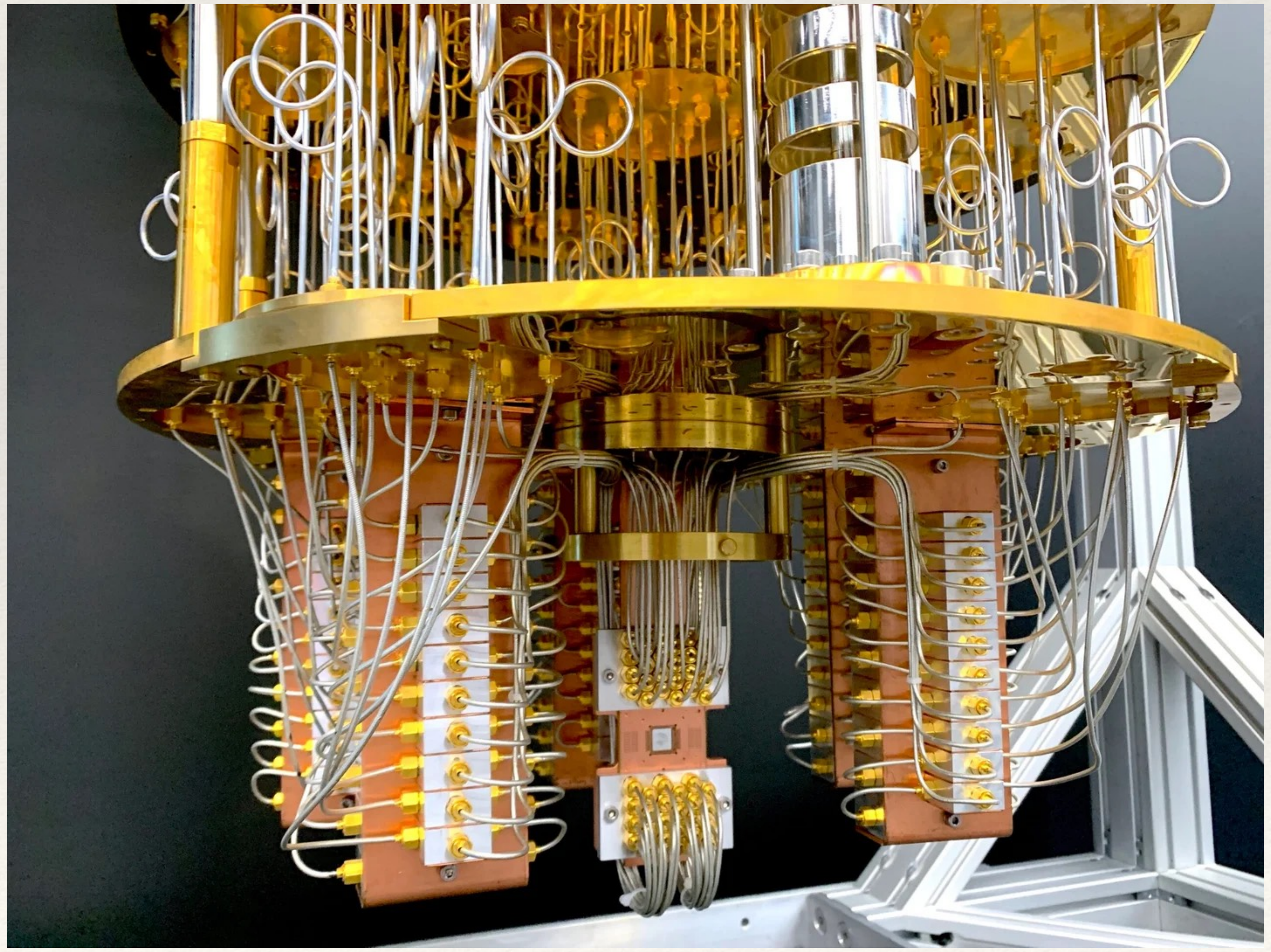
- different geometries
- tunable hopping velocities
- controllabile on-site & interaction potentials
- different statistics (bosons, fermions, anyons?, …)
- internal degrees of freedom



QUANTUM COMPUTING



DIGITAL SIMULATIONS



Mainly based on superconducting qubits

more developed from commercial side:

- low-T devices
- asy to interface
- scalability
- universality

OTHER IMPLEMENTATIONS

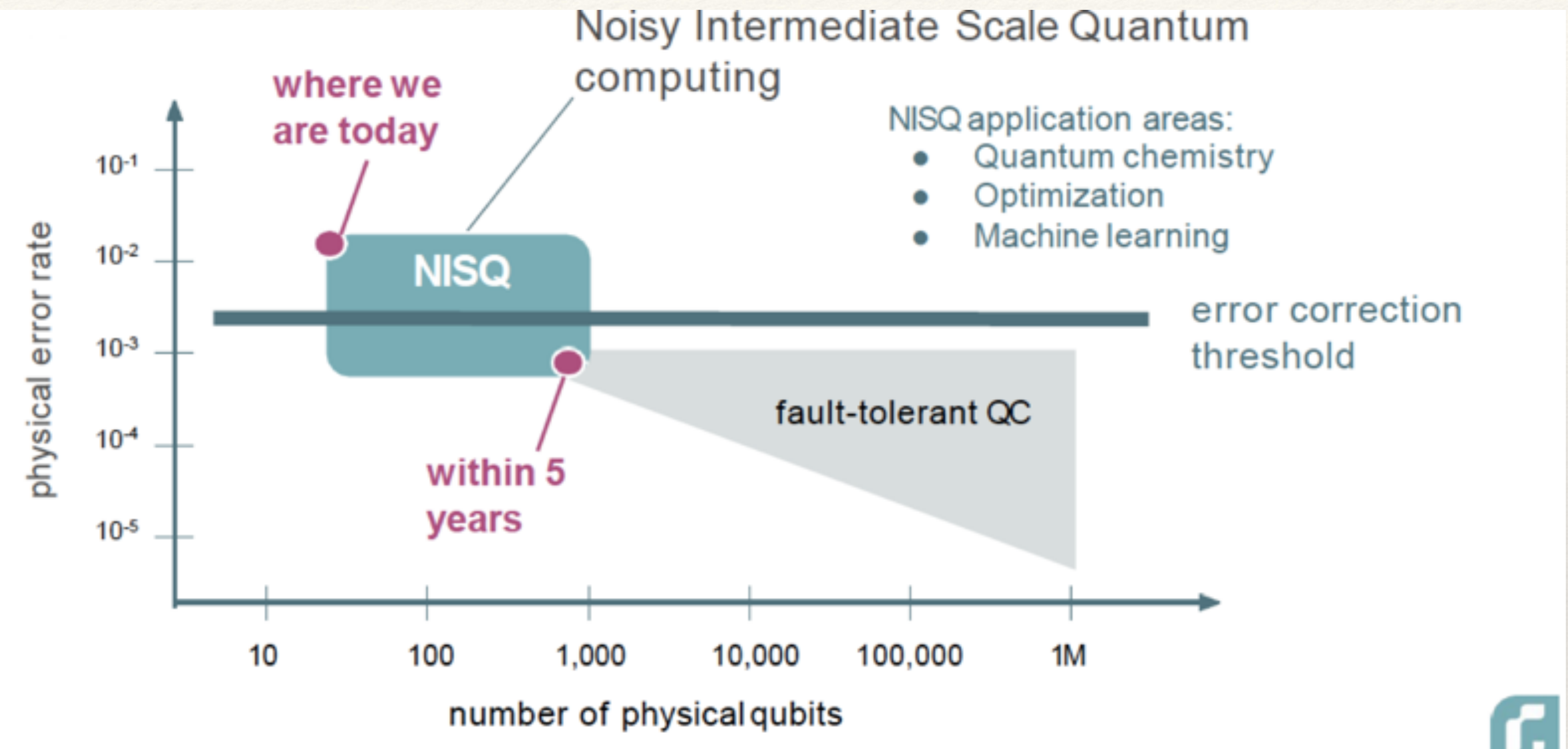
Ising machines
quantum annealing based

photonic
topological materials
cavity QED
quantum dots in silicon
vacancies in diamond
molecular magnets
…

BUT

DECOHERENCE!

NISQ DEVICES



"Quantum computing in the NISQ era and beyond" Preskill, 2018 https://arxiv.org/abs/1801.00862

HYBRID SOLUTIONS: both experiments and protocols

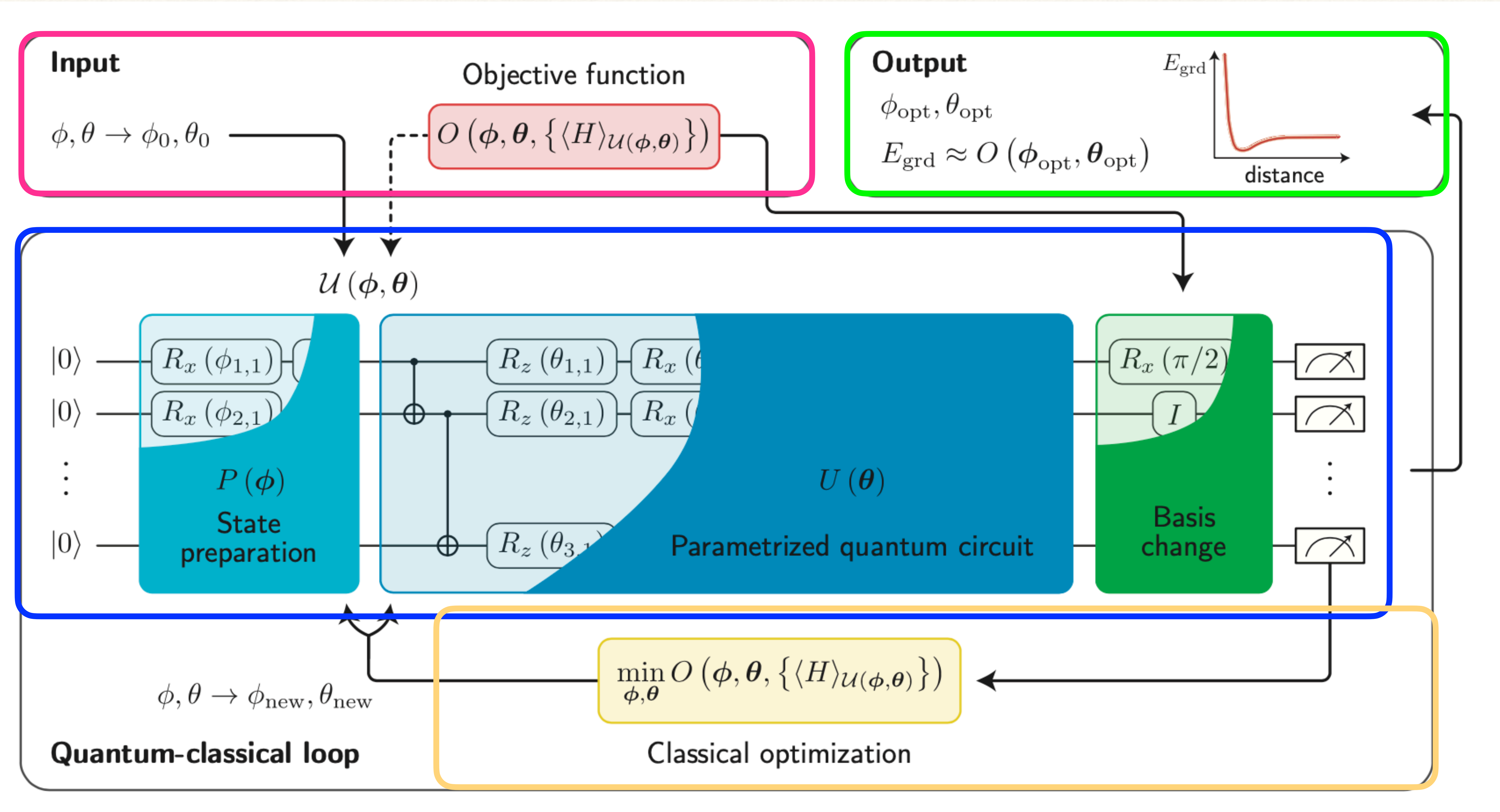
Applications in:

- classical hard (combinatorial) problems
- chemical compounds
- condensed matter models
- statistical mechanics models and critical phenomena
- fundamental interactions: particle physics and gravity

BEHIND: mathematical structure of quantum mechanics

- Hilbert space & operator algebra theory
- Probability (q.) & estimation theory
- Geometry of Hilbert space
- diff equations: Schroedinger or Lindblad

Quantum Approximation Optimization Algorithm (QAOA)



K. Barthi et al.; arXiv:2101.08448

QUANTUM RESOURCES

for preparation of a parametrised variational state

- embed dof in register of qubits & define (cost) Hamiltonian whose $\langle H_C \rangle$ has to be minimized
- use a quantum circuit built out of a set of parametrised unitary operators to span the the space of possible ground states $|\theta, \phi\rangle$
- make measurements to determine the objective function $\langle \theta, \phi | H_C | \theta, \phi \rangle$

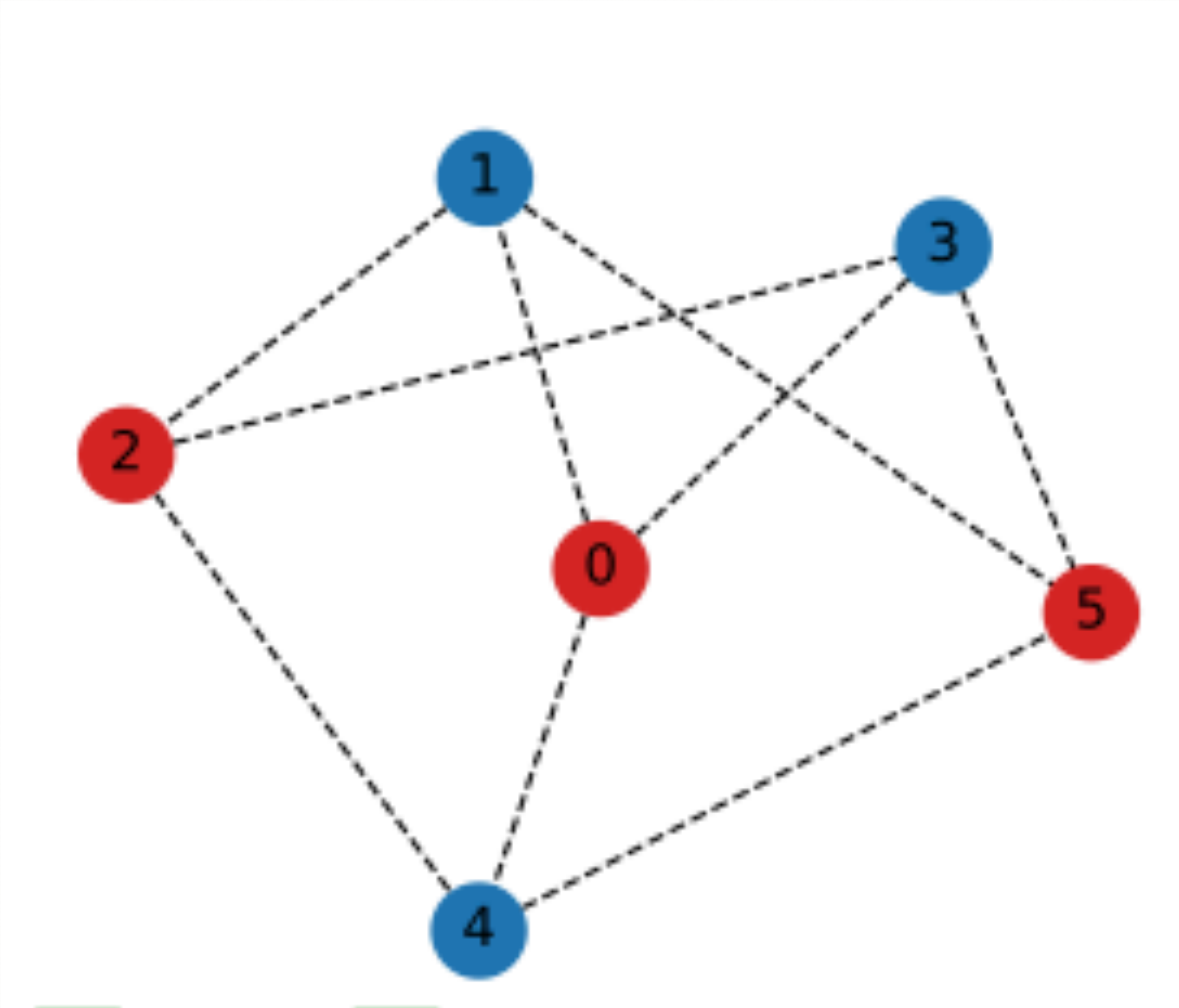
hybrid protocol: that exploits quantum resources to span the space of states and classical techniques for optimization

CLASSICAL RESOURCES

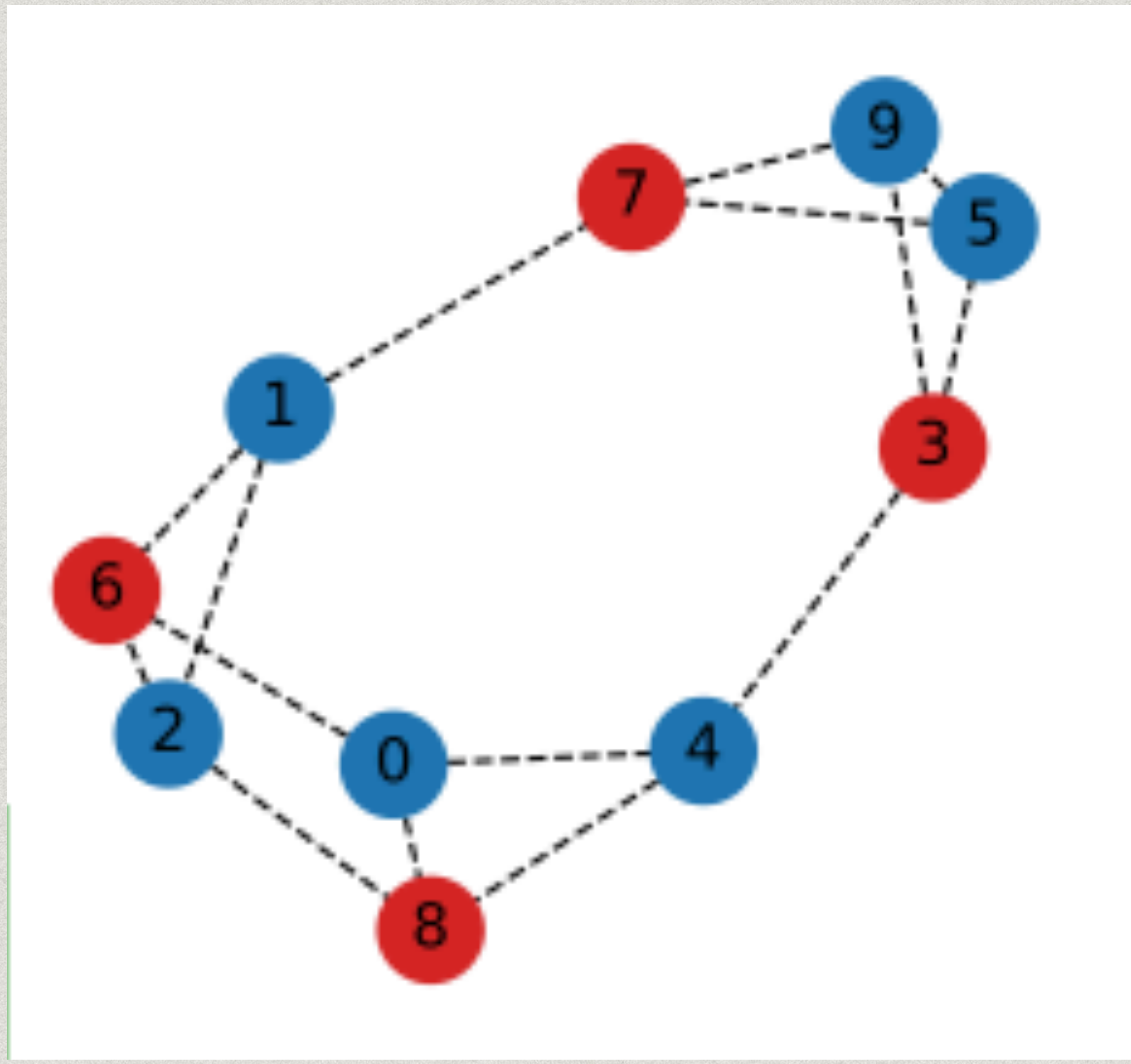
and techniques (local gradient, global, machine learning, …) to find the optimal values of the parameters and the corresponding ground state $|\theta_{opt}, \phi_{opt}\rangle$

- **Solution of Combinatorial problems on Graphs** (NP-hard)

MIS problem: find the largest set of nodes not adjacent



Max-Cut problem: partition the graph in two sets of nodes interconnected by the largest number of links



• Ground State Preparation for Nontrivial Quantum Hamiltonians

$\mathbb{Z}_2$ Lattice Gauge Theory

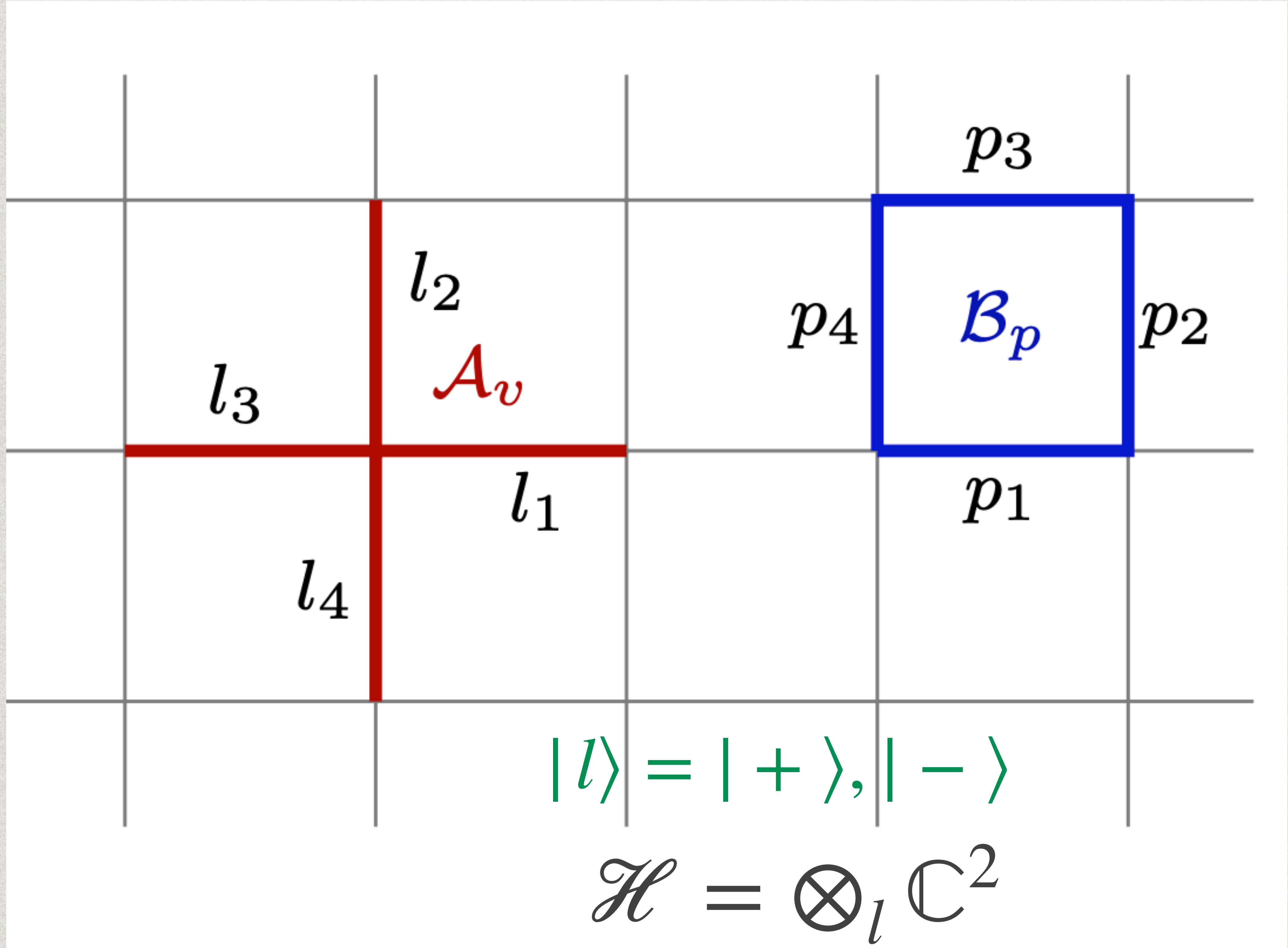
$$H(h) = H_E + h\, H_B$$

electric contribution

$$H_E = \sum_l (1 - \sigma_l^x)$$

magnetic contribution

$$H_B = -\sum_p \mathscr{B}_p = -\sum_p \sigma_{p_1}^z \sigma_{p_2}^z \sigma_{p_3}^z \sigma_{p_4}^z$$



$$\mathscr{A}_v |\psi\rangle_{phys} = |\psi\rangle_{phys} \qquad \mathscr{A}_v = \prod_{l \in v} \sigma_l^x$$

$$E_P(\gamma, \beta) = \langle \psi_P(\gamma, \beta) \,|\, H(h) \,|\, \psi_P(\gamma, \beta) \rangle$$

Initialisation of the state

❖ Combinatorial Problem

$$|\Omega_0\rangle = \bigotimes_x |+\rangle_x$$

simple product state, prepared by Hadamard gate

EMBEDDING of data might be crucial for efficiency

$$(0,0,1,0,1,\cdots,1,1,1,0) \mapsto |\psi\rangle \in \mathscr{H}$$

❖ Quantum Hamiltonian

$$|\Omega_B\rangle = \mathscr{N} \sum_\Gamma \mathscr{W}_\Gamma |\Omega_E\rangle$$

such states might have entanglement ->
complicated circuit that cannot be done in parallel on plaquettes

(consistent with results that O(L) circuit depth to
prepare states with topological entanglement)

Parametrised quantum evolution

❖ Combinatorial Problem

$$|\psi_P(\gamma,\beta)\rangle = \left(\prod_{m=1}^{P} e^{-i\beta_m H_M} e^{-i\gamma_m H_B}\right)|\psi_0\rangle$$

$$H_C^{(MIS)} = \sum_x Z_x + \omega \sum_{xy} Z_x Z_y$$

$$H_M^{(MIS)} = \sum_x X_x$$

$$[H_M, H_C] \neq 0$$

❖ Quantum Hamiltonian (similar to a Suzuki-Trotter decomposition)

$$|\psi_P(\gamma,\beta)\rangle = \left(\prod_{m=1}^{P} e^{-i\beta_m H_E} e^{-i\gamma_m H_B}\right)|\psi_0\rangle$$

$$[H_E, H_B] \neq 0$$

gauge invariant

Quantum circuit for each step ($m = 1, \cdots, P$) of the QAOA to implement the evolutions through H_1 , H_1

Classical optimisation

$$E_P\left(\gamma,\beta\right) = \langle \psi_P(\gamma,\beta) \,|\, H_C \,|\, \psi_P(\gamma,\beta) \rangle$$

Energy landscape -> rugged; barren plateaus

1) Standard gradient-descent methods (Vanilla, Stochastic, ..)

2) Global optimisation (basin-hopping, differential evolution…)

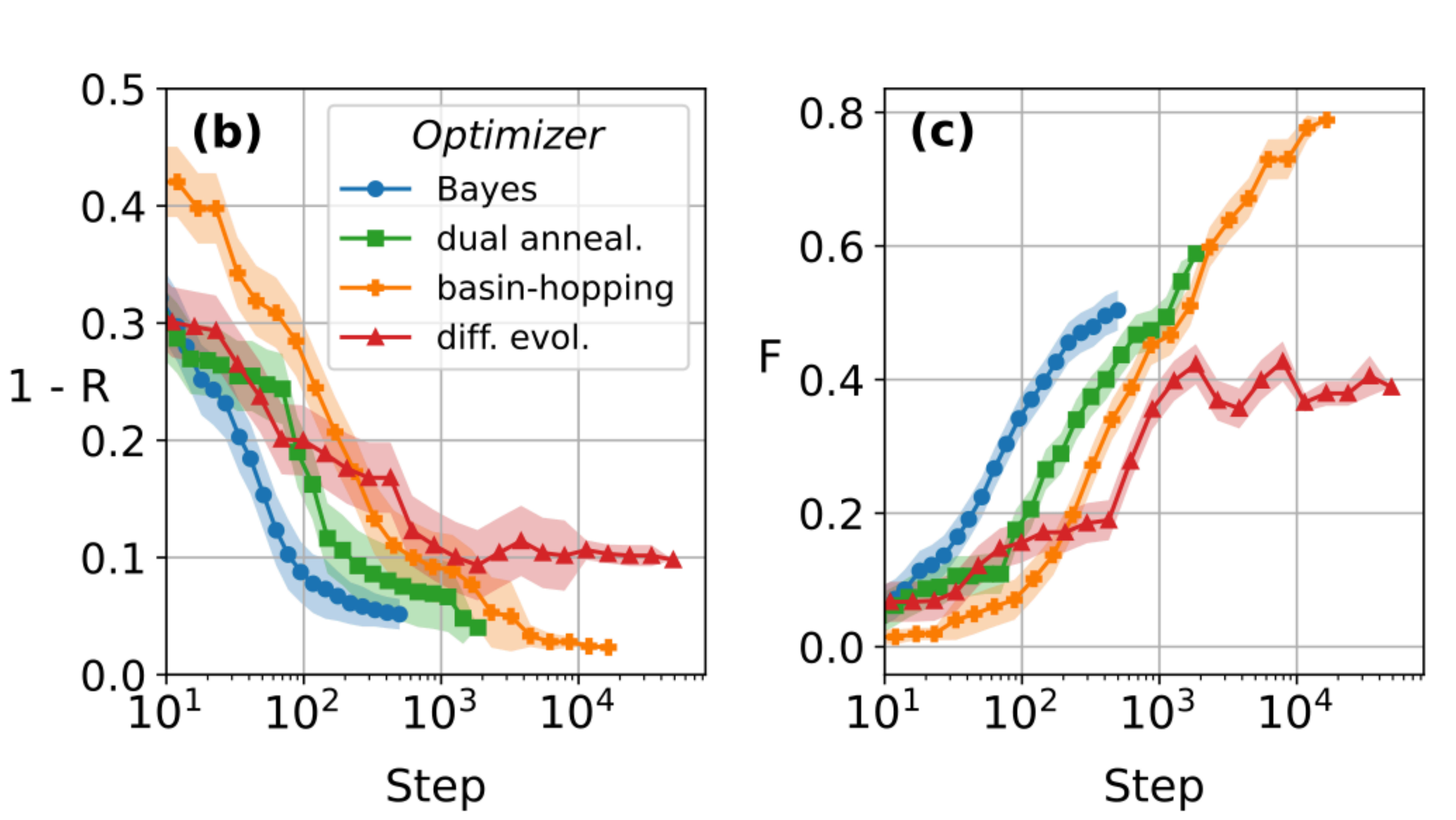
3) Quantum annealing

4) Bayesian approach based on tstaistical inference

5) Natural and Quantum Natural Gradient

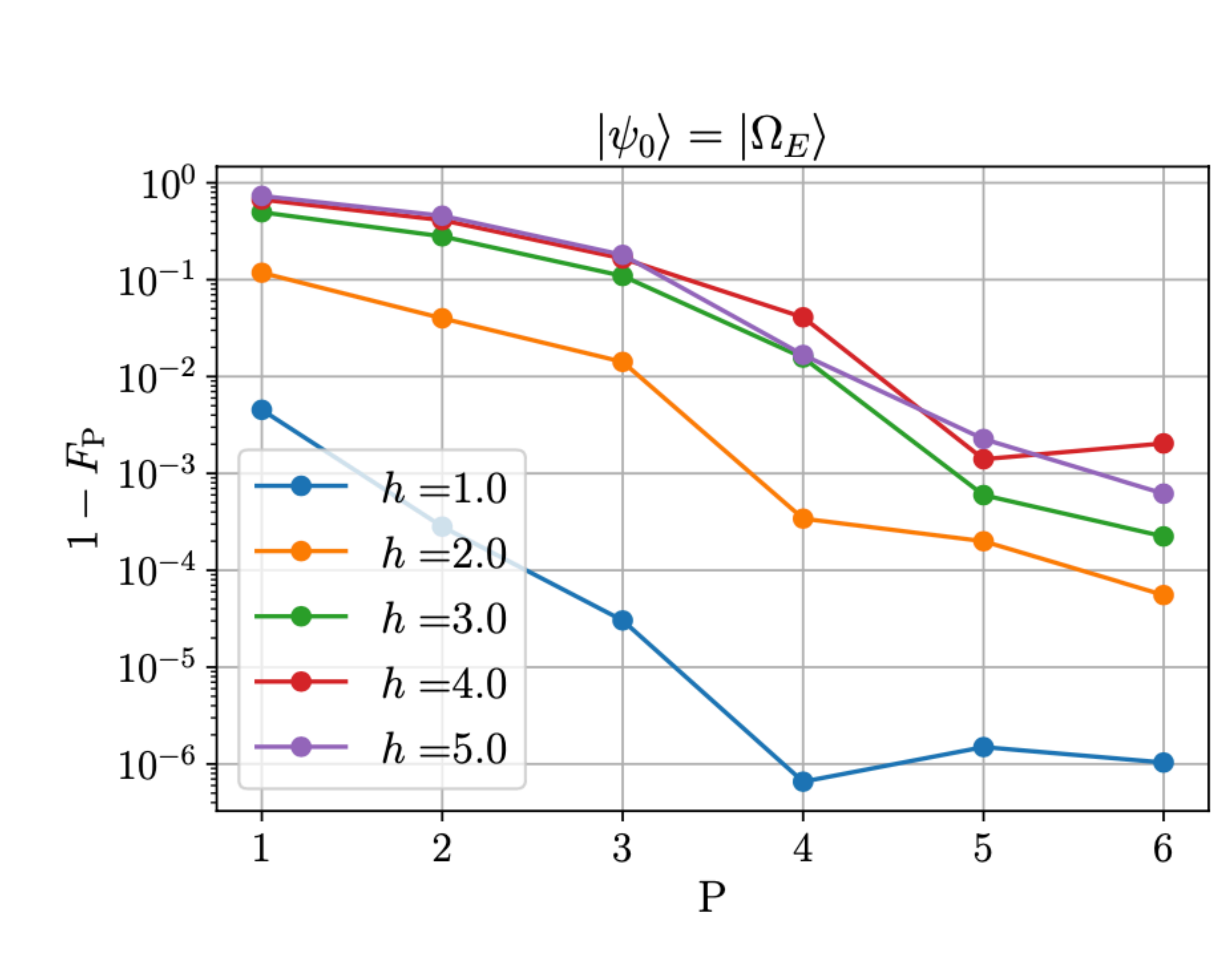
Some results:

❖ Combinatorial Problem



$$R = E(\boldsymbol{\theta})/E_{GS}$$

❖ Quantum Hamiltonian



$$F = |\langle \boldsymbol{\theta} | z^{\star} \rangle|^2$$

QAOA EVOLUTION + CLASS. OPT.

=

PATH IN HILBERT SPACE

→ "OPTIMAL" PATHS?

- ADIABATIC THEOREM PREVENTS EFFICIENT EVOLUTION IF THE HAMILTONIAN GAP BECOMES ZERO:

  SHORTCUT TO ADIABATICITY?

- CAN WE EXPLOIT THE GEOMETRY OF HILBERT SPACE?

  GEODESICS?

$$
\begin{array}{ccc}
\mathbb{R}_+ \hookrightarrow & \mathcal{H}_0 = \mathbb{C}^d \setminus \{\mathbf{0}\} & \\
& \downarrow & \\
\mathsf{U}(1) \hookrightarrow & \mathbb{S}^{2d-1} & , \\
& \downarrow & \\
& P\mathcal{H} \sim \mathbb{CP}^{d-1} &
\end{array}
$$

Optimizers

- Pick the initial values for $\boldsymbol{\theta}$.
- Calculate the gradient of the cost function: $\nabla E(\boldsymbol{\theta})$.

Vanilla Gradient Descent

- Update the parameters $\boldsymbol{\theta}$, such that:

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \nabla E(\boldsymbol{\theta}_t).$$

Natural Gradient Descent

- Compute the Fisher Information Matrix [3]:

$$F_{ij}(\boldsymbol{\theta}) = \sum_{x \in [N]} p(x, \boldsymbol{\theta}) \left(\frac{\partial \log p(x, \boldsymbol{\theta})}{\partial \theta_i} \right) \left(\frac{\partial \log p(x, \boldsymbol{\theta})}{\partial \theta_j} \right)$$

- Update the parameters $\boldsymbol{\theta}$, such that:

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta F^{-1}(\boldsymbol{\theta}_t) \nabla E(\boldsymbol{\theta}_t).$$

Quantum Natural Gradient Descent

- Compute the Fubini-Study metric [4] $g(\boldsymbol{\theta}) = Re[G(\boldsymbol{\theta})]$, where:

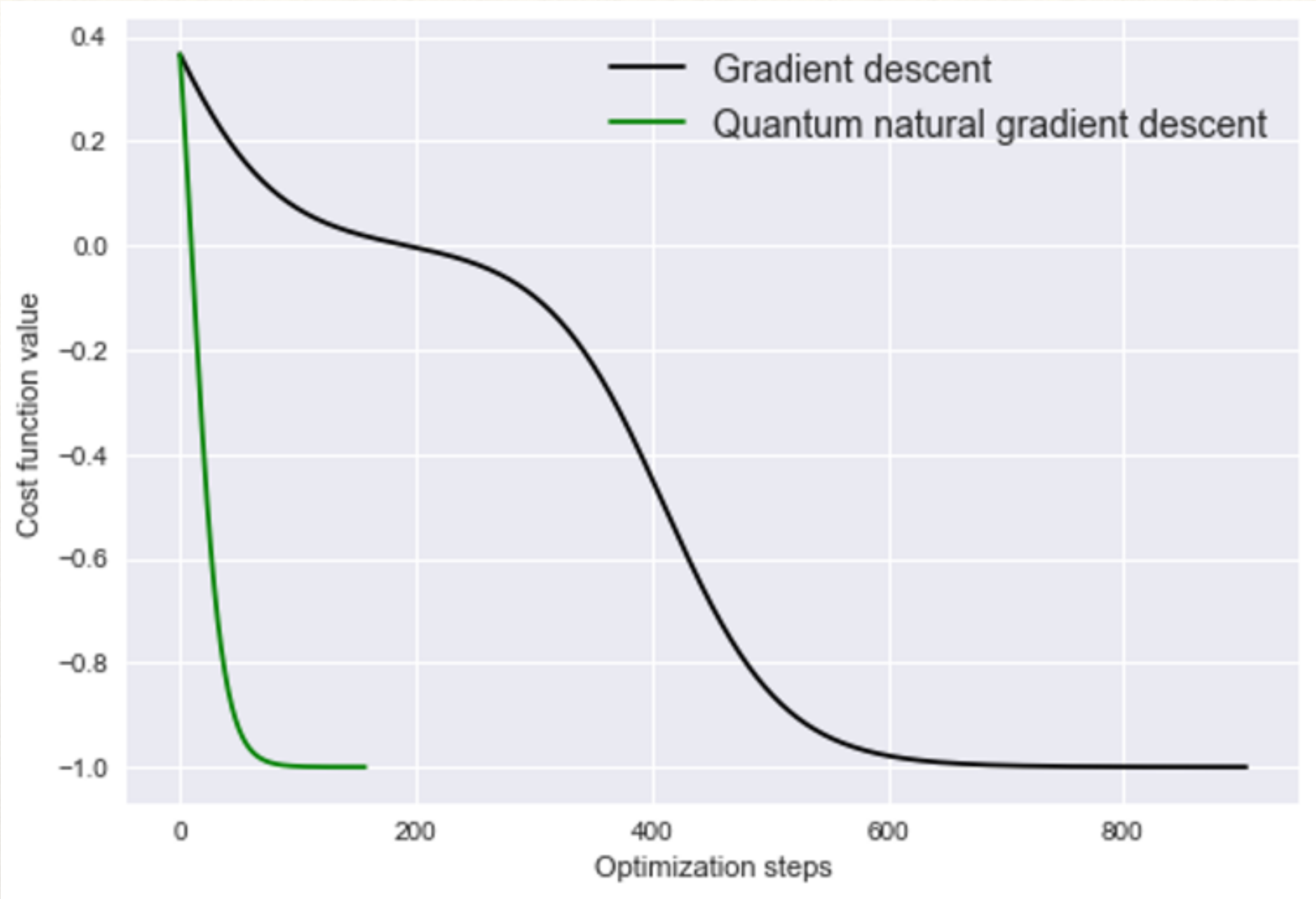
$$G_{ij}(\boldsymbol{\theta}) = \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \psi_\theta \right\rangle \left\langle \psi_\theta, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle$$

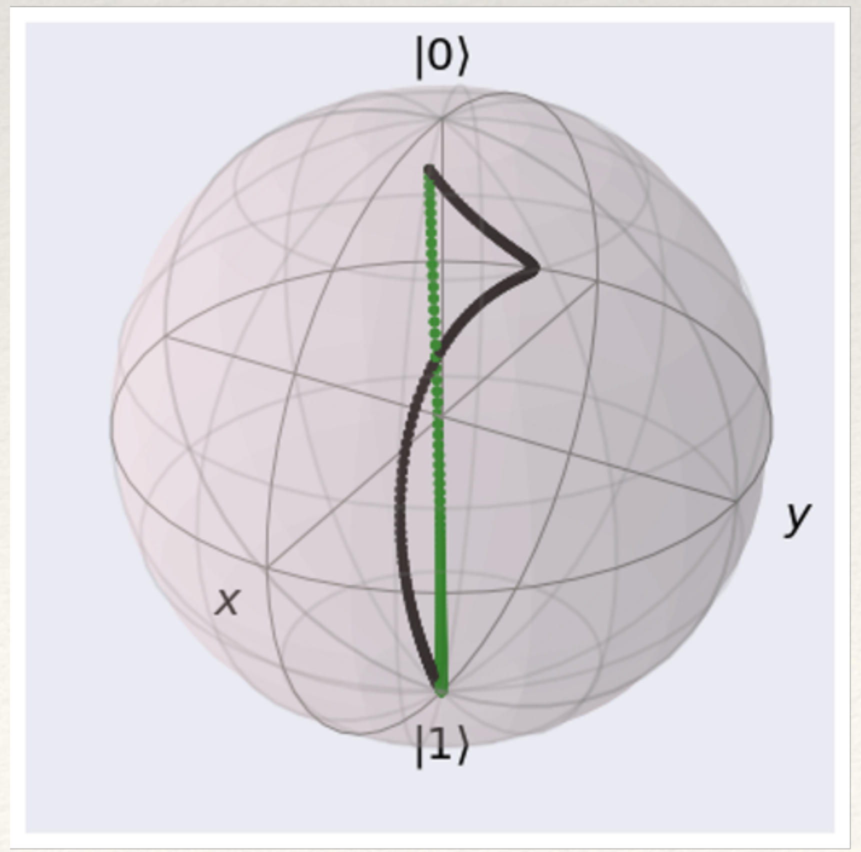
- Update the parameters $\boldsymbol{\theta}$, such that:

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta g^{-1}(\boldsymbol{\theta}_t) \nabla E(\boldsymbol{\theta}_t).$$

in the QAOA algorithm, the metric tensor can be computed via an additional quantum circuit single qubit

$$H_C = \sigma_z$$





Ising chain

$$H = \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - t \sum_{i=1}^{N} \sigma_i^x$$