KMI School 2024

Quantum Computing for Particle Physics and Astrophysics
Nagoya University, March 6, 2024

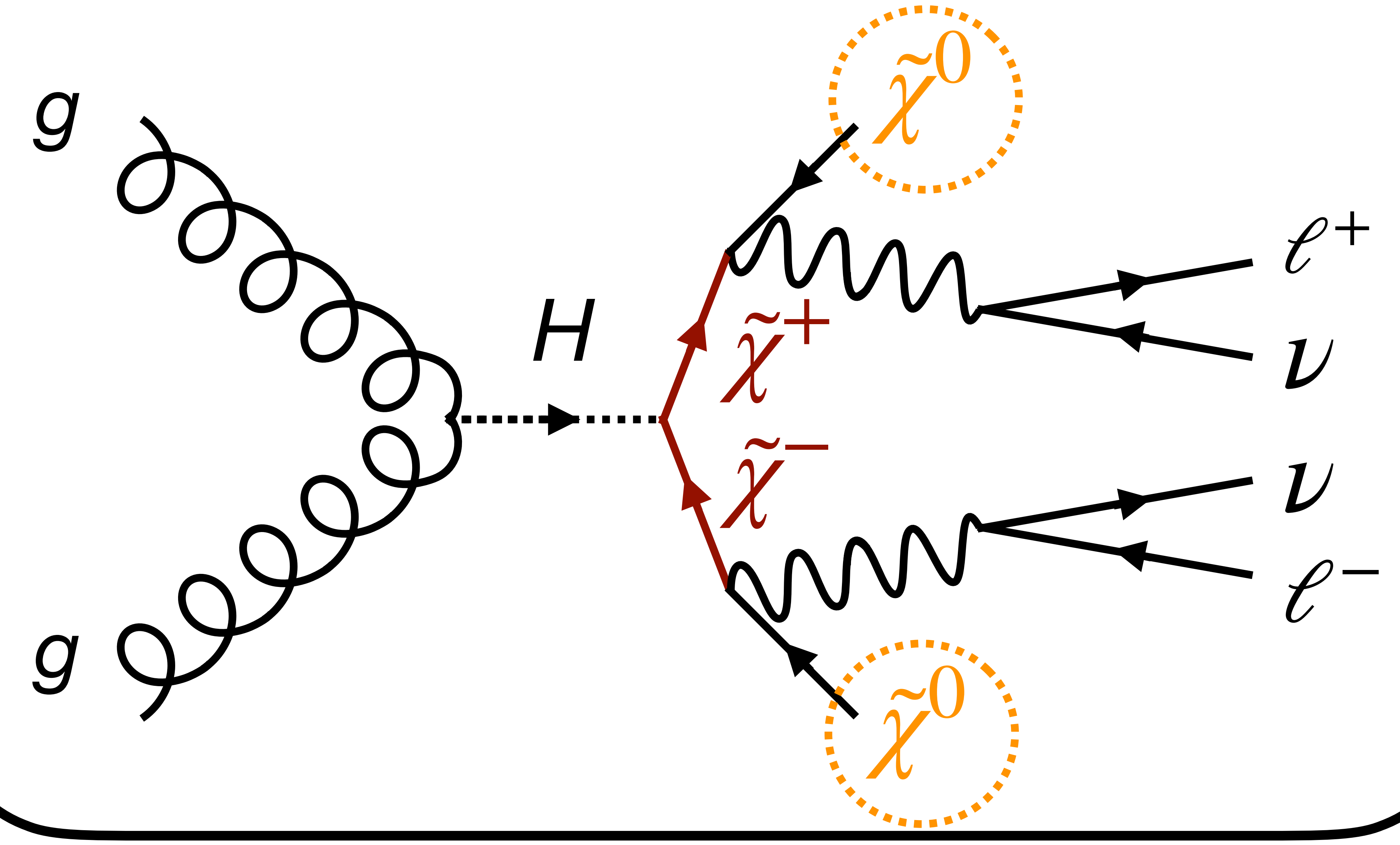
Quantum Computing Applications to HEP

ICEPP, The University of Tokyo
Koji Terashi

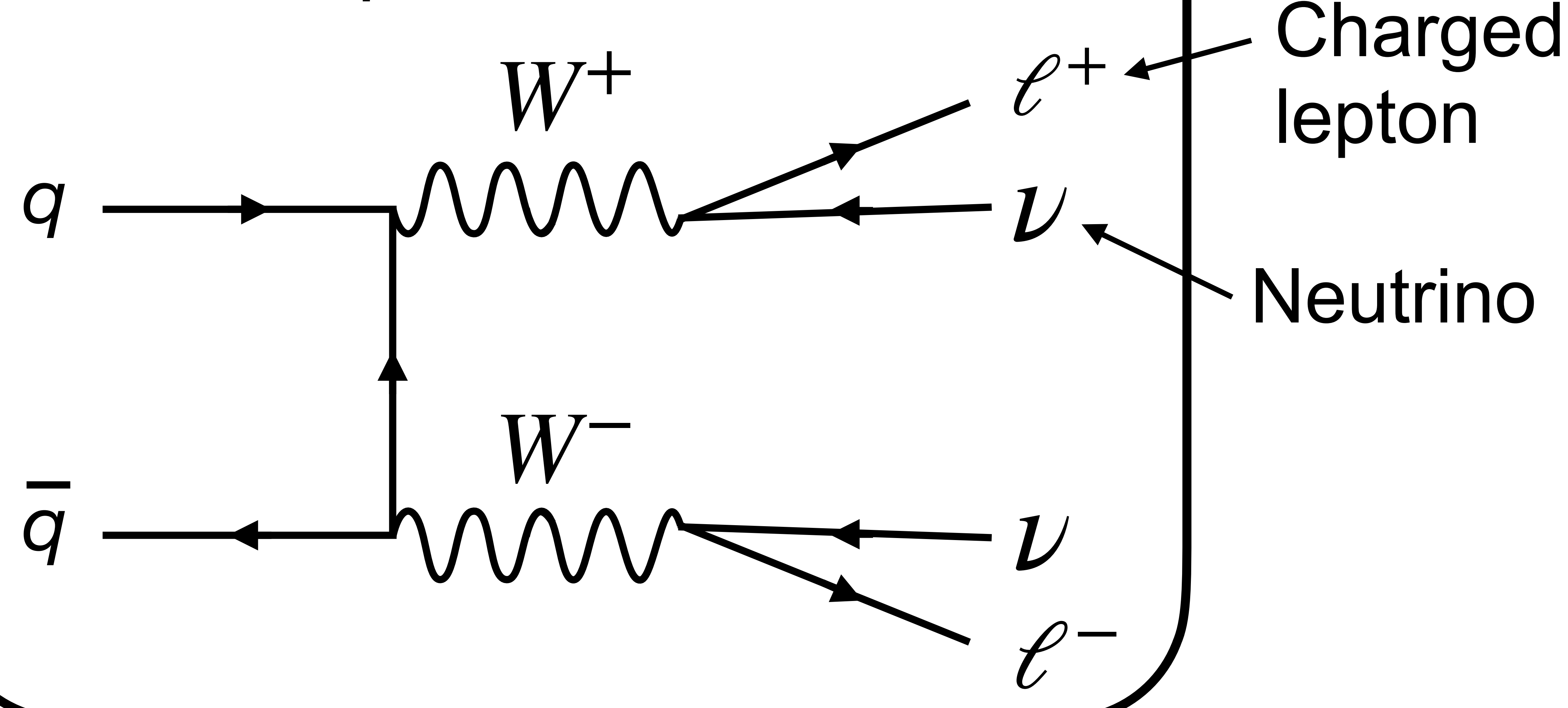
Reminder: QML Application to Event Classification

Classify events that contain new physics signal from background events

Signal event with unknown particles



Background event without unknown particles

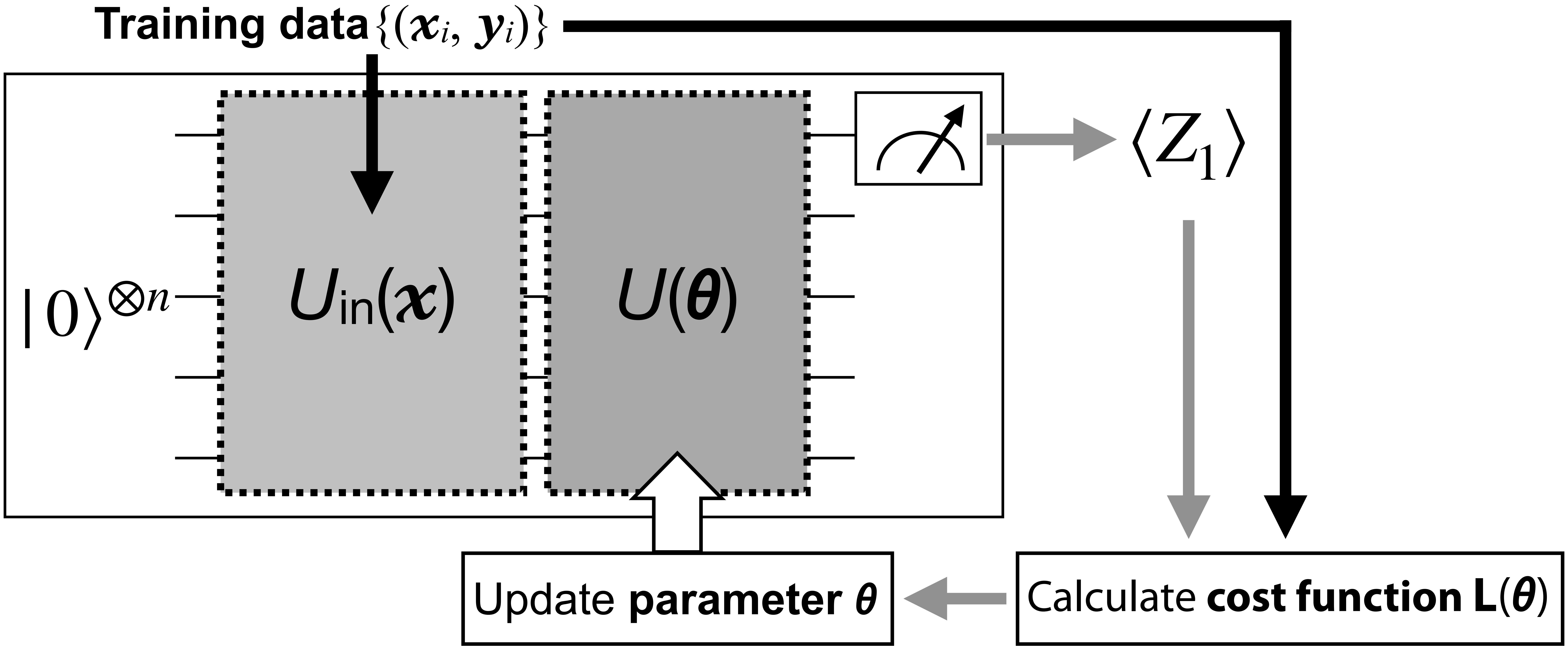


Neutralino ➡ Not observed by the detector, like SM neutrino

Use differences in kinematical properties due to the presence of *H* and $\tilde{\chi}^{\pm}/\tilde{\chi}^0$ to classify signal from background

Reminder: QML Application to Event Classification

Conventional **Quantum Neural Network (QNN)** model for supervised machine learning task



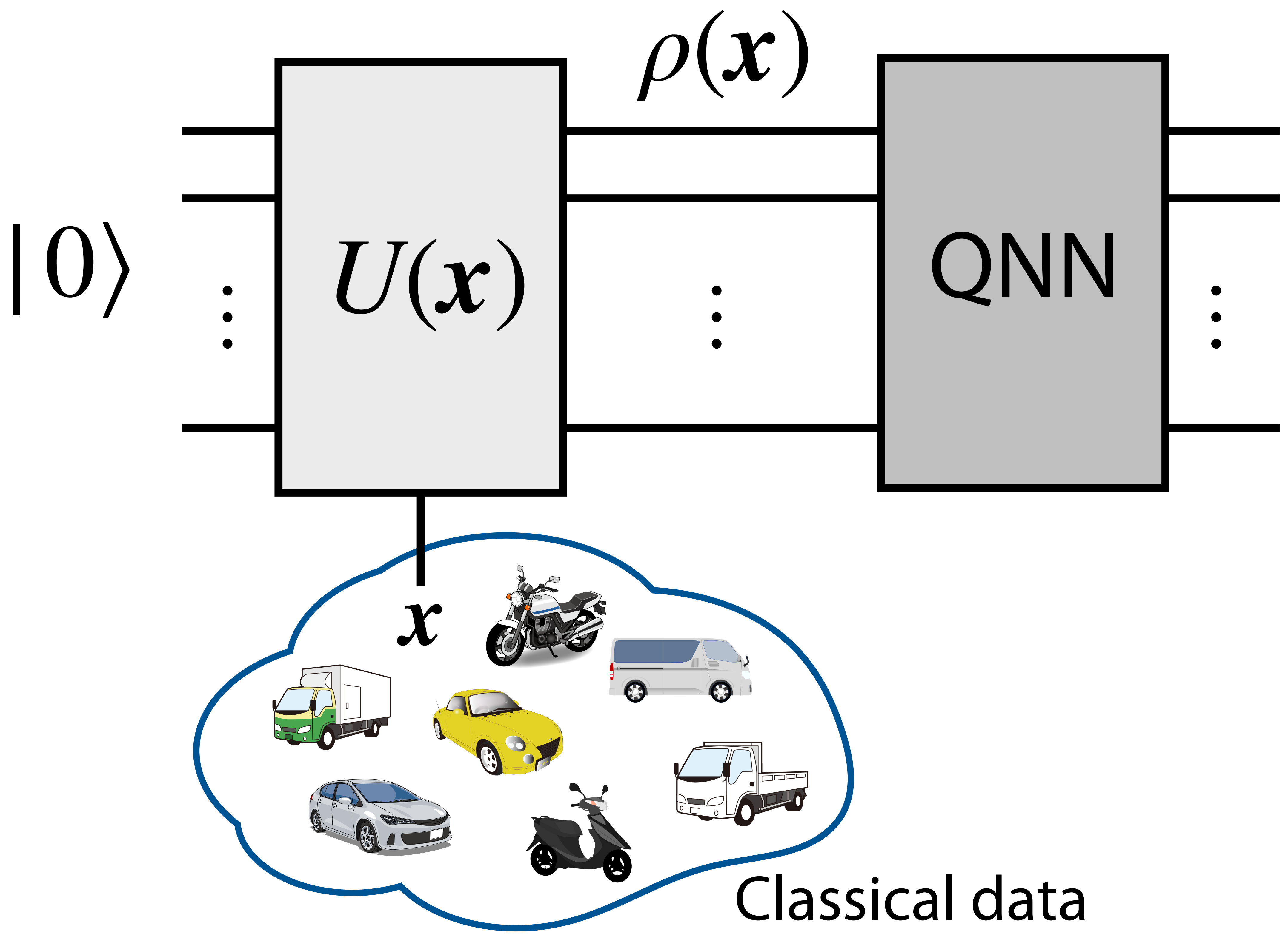
Learning on Quantum Data

Considered so far classification problem of classical data

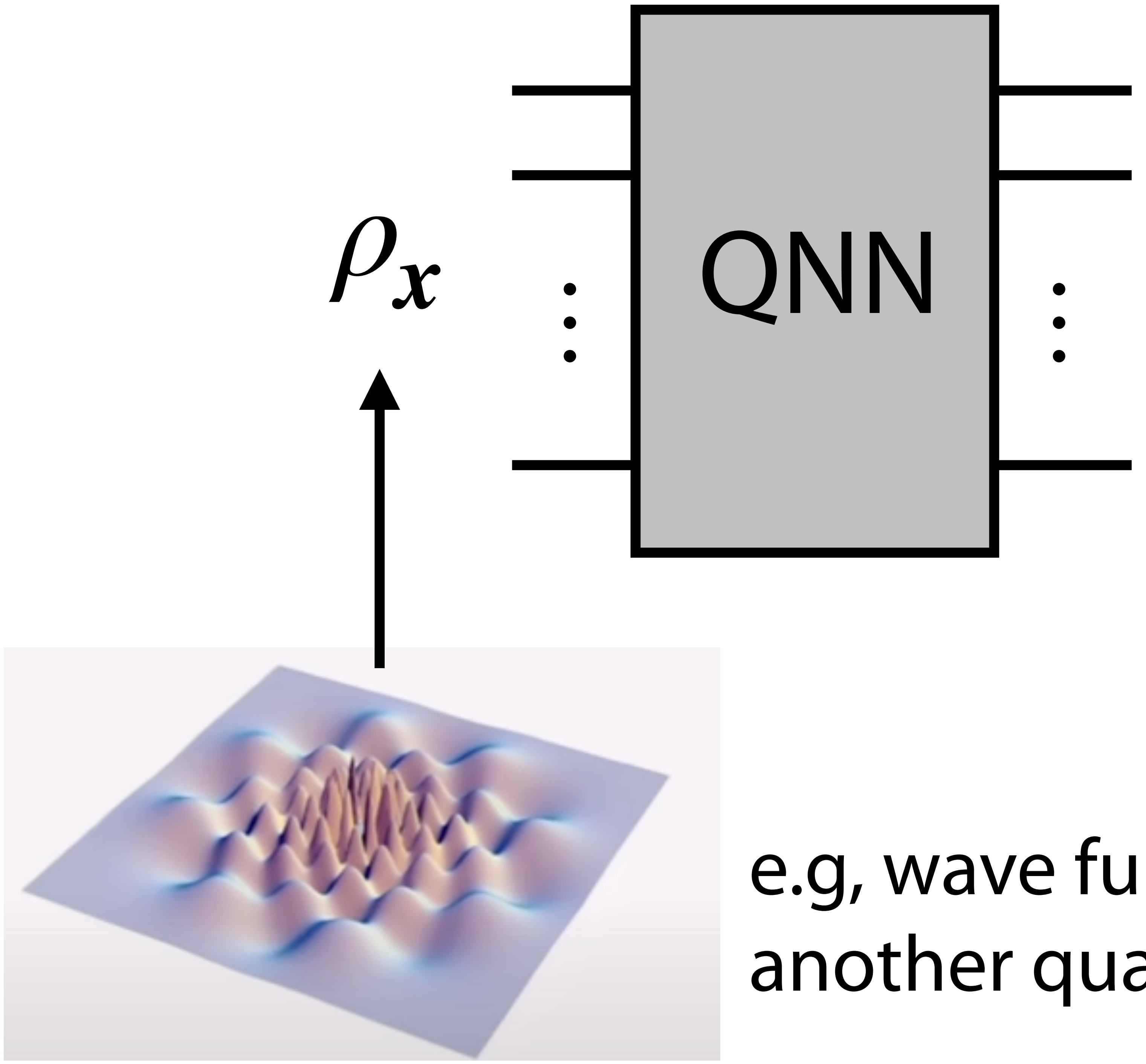
Caveat: classical analysis methods such as deep neural networks quite powerful…

Let us think more *quantum-friendly* problem suitable for quantum computer

Learning classical data $\boldsymbol{x}$



Learning quantum data $\rho_{\boldsymbol{x}}$



e.g, wave functions from another quantum system

QML Application to Quantum Data

Extract physical properties by learning various quantum states generated by quantum simulations

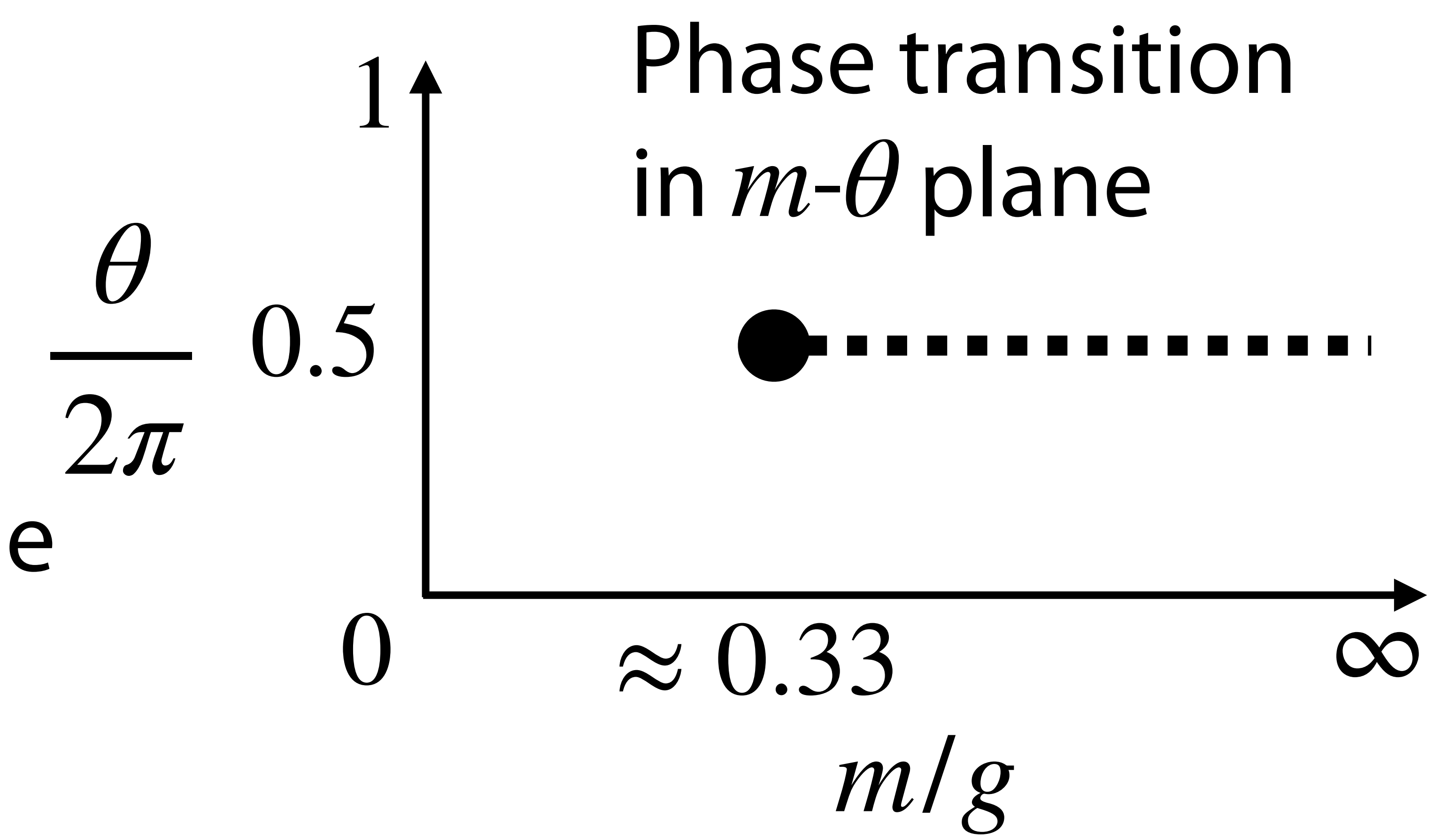
L. Nagano, A. Miessen, T. Onodera, I. Tavernelli, F. Tacchino, K. Terashi, arXiv:2306.17214

Possible to determination of classical parameters that control a physical system (e.g, Hamiltonian parameters)?

QML Application to Quantum Data (I)

$(1+1)d\ U(1)$ Gauge Theory (Schwinger Model)

$$H = J \sum_{j=0}^{N_s-2} \left(\sum_{k=0}^{j} \frac{Z_k + (-1)^k}{2} + \frac{\theta}{2\pi} \right)^2 + \frac{\omega}{2} \sum_{j=0}^{N_s-2} (X_j X_{j+1} + Y_j Y_{j+1}) + \frac{m}{2} \sum_{j=0}^{N_s-2} (-1)^j Z_j$$

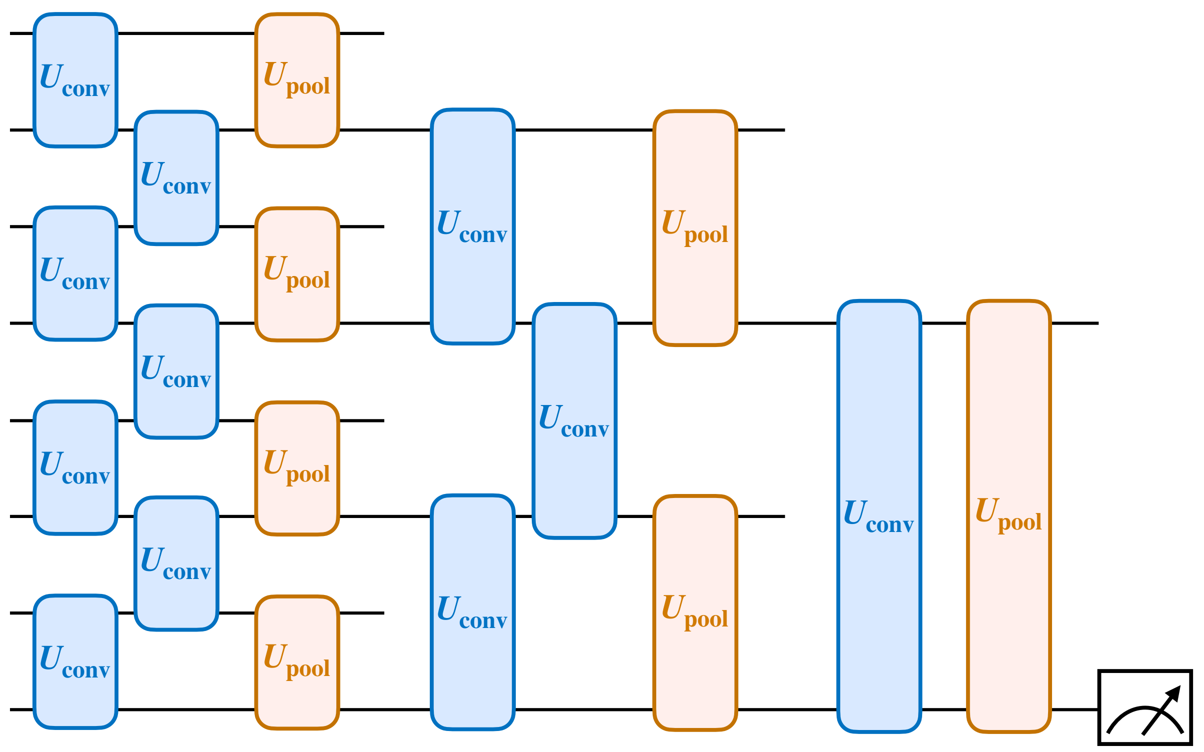


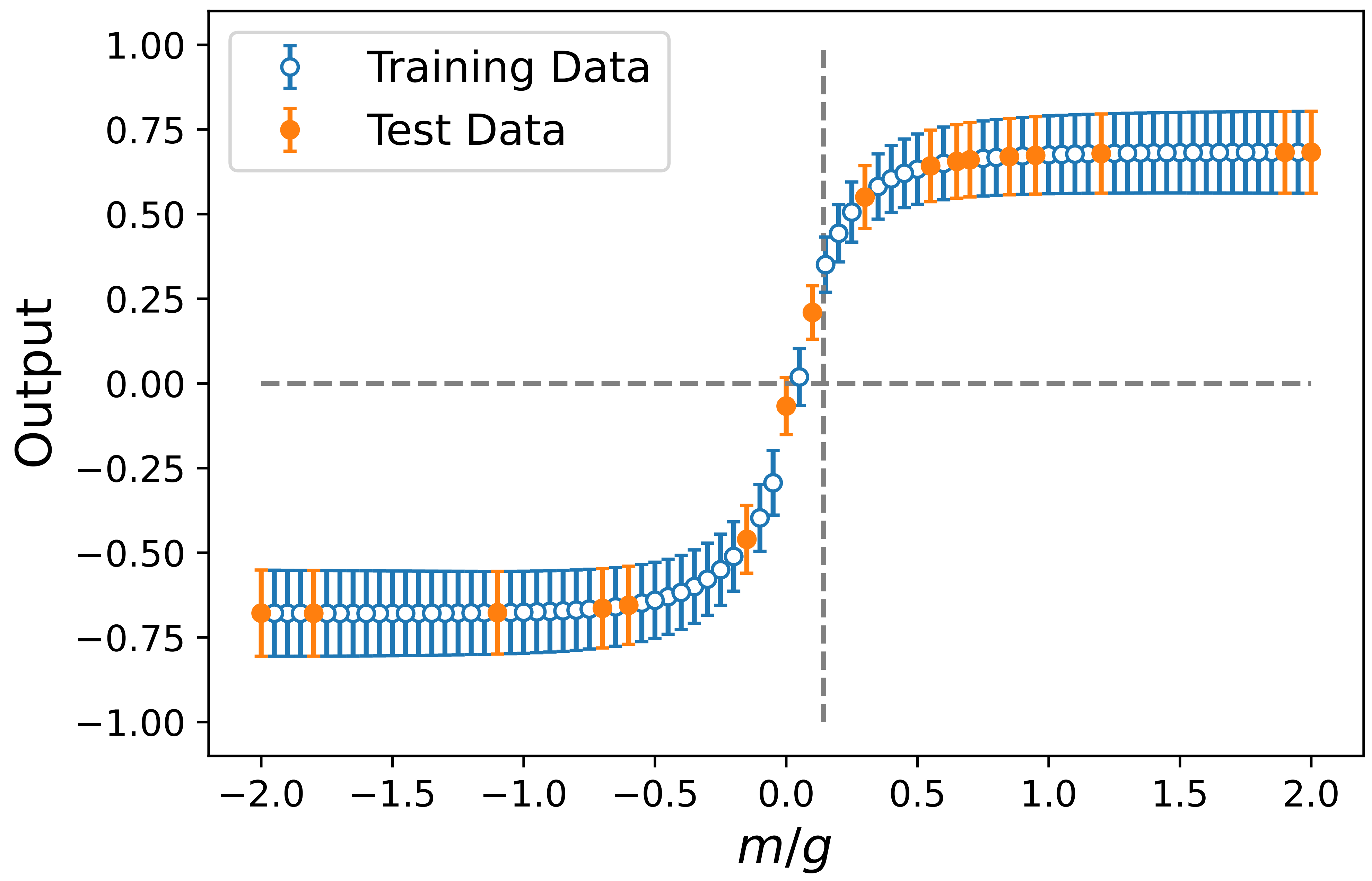
- Non-trivial properties such as chiral condensate, though the model is simple
- Phase transition at $\theta = \pi, m/g = m_c/g \approx 0.33$ due to topological term

Quantum data generation and classification

- Physical parameters: $N = N_s = 8, ag = 2, \theta = \pi$
- Generate ground states $|\psi_{\mathrm{GS}}(m)\rangle$ using VQE within parameter range of $m/g \in [-2,2]$
- Phase recognition as a classification with label:

$$y_m = \begin{cases} +1 & (m > m_c) \\ -1 & (m < m_c) \end{cases}$$





QML Application to Quantum Data (II)

$(1+1)d\ \mathbb{Z}_2$ Gauge Theory

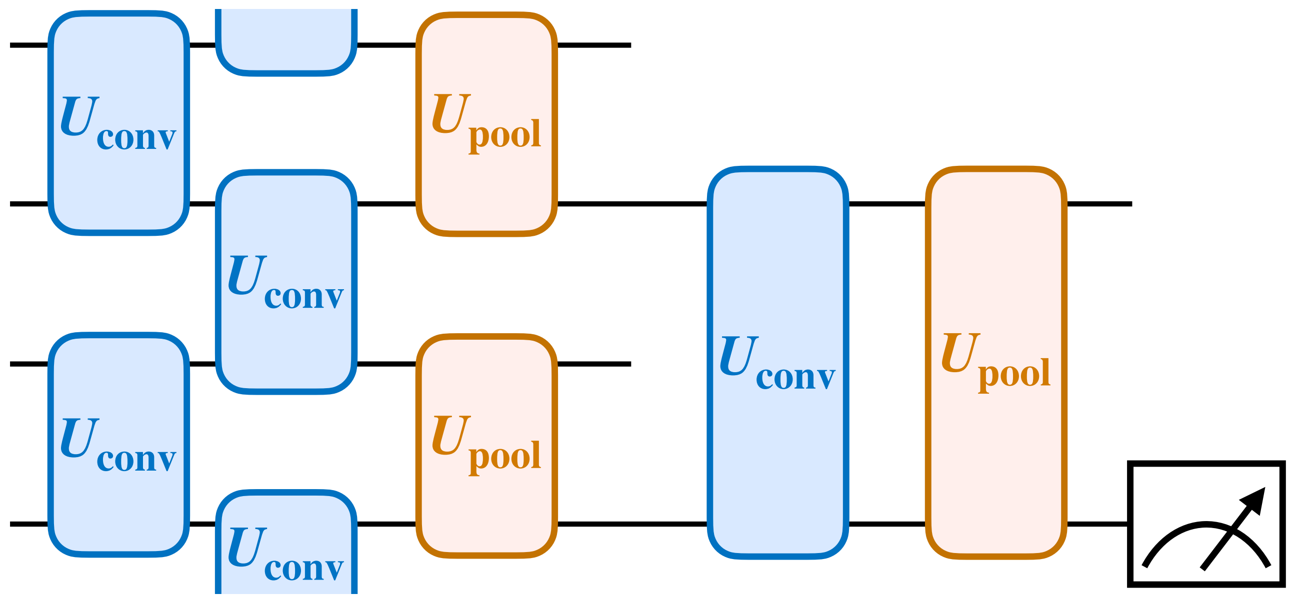
$$H = -\frac{J}{2}\sum_{j=0}^{N_s-1}(X_j Z_{j,j+1} X_{j+1} + Y_j Z_{j,j+1} Y_{j+1}) - f\sum_{j=0}^{N_s-2} X_{j,j+1} + \frac{m}{2}\sum_{j=0}^{N_s-1}(-1)^j Z_j$$

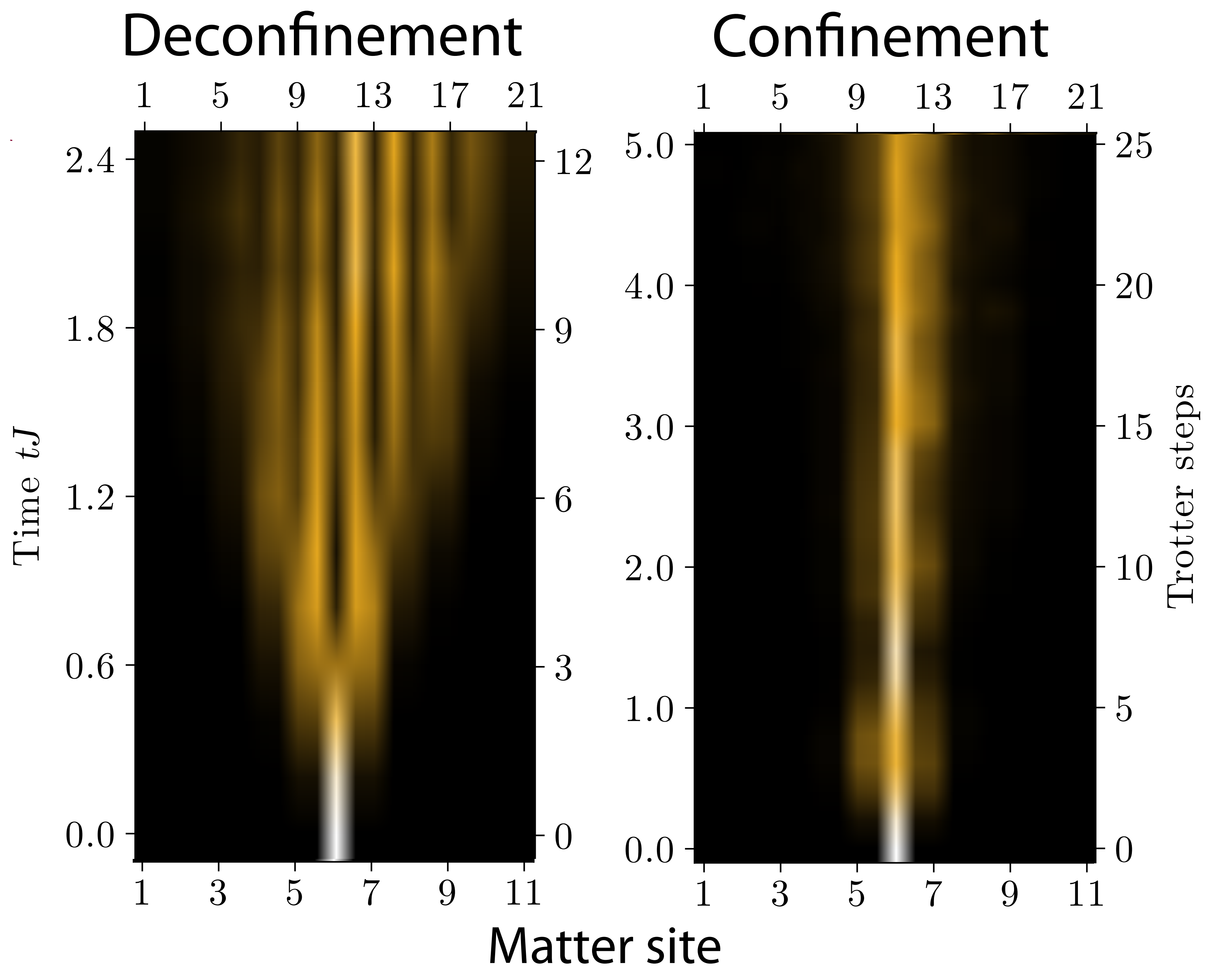
- Confinement ($f \neq 0$) and Deconfinement ($f = 0$) phases depending on the presence of background electric field

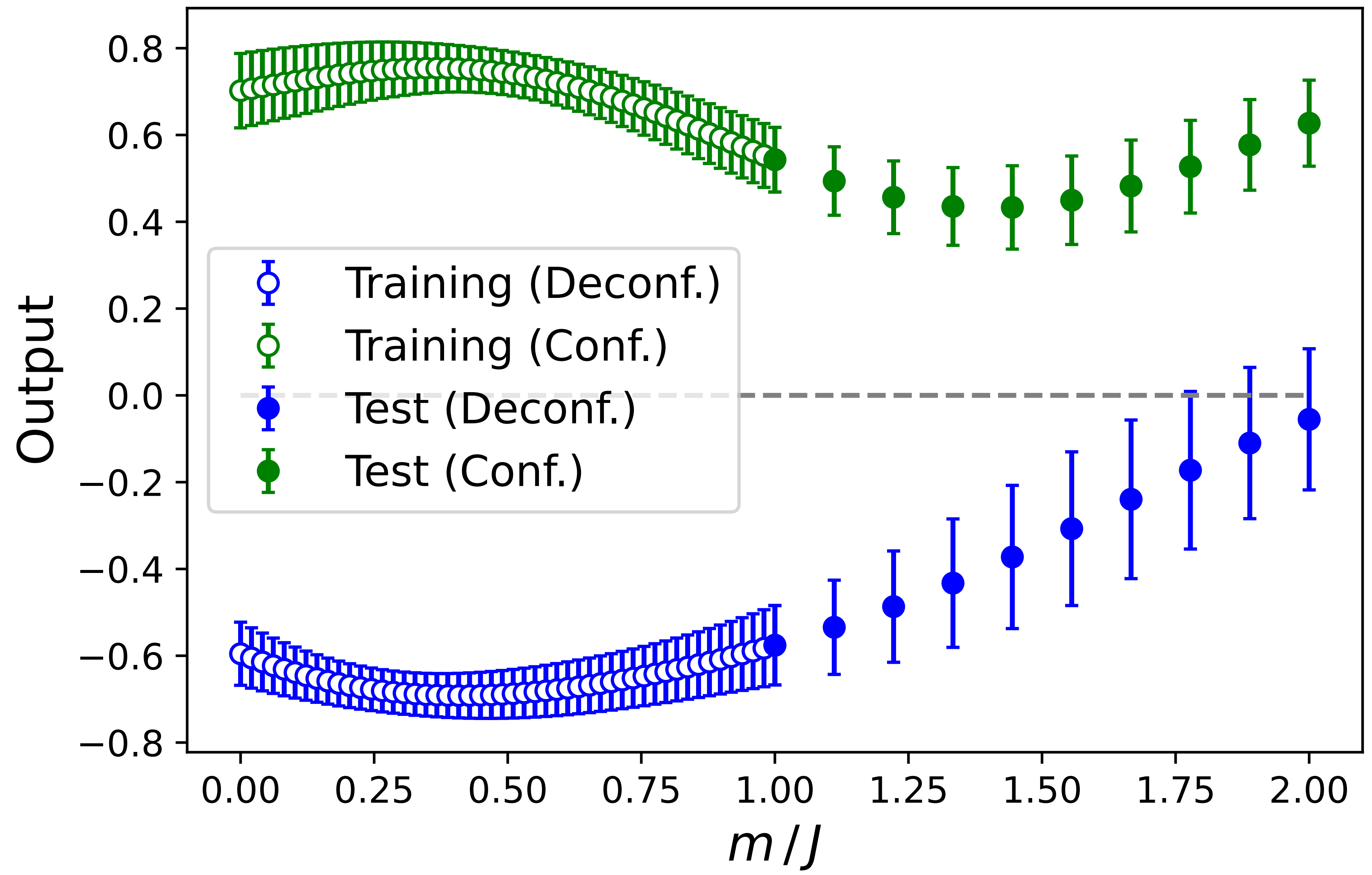
Quantum data generation and classification

- Physical parameters: $N = 2N_s = 4, J = 1, T = 2$
- Generate time-evolved states $|\psi(m,f)\rangle = e^{-iH(m,f)T}|\psi_0\rangle$ using Suzuki-Trotter decomposition within $m \in [0,2], f \in \{0,3\}$
- Phase recognition as a classification with label:

$$y_m = \begin{cases} +1 & (f \neq 0) \\ -1 & (f = 0) \end{cases}$$







QML Application to Quantum Data (III)

Parton Shower

$$L_{PS} = \bar{f}_1(i\partial\!\!\!/ + m_1)f_1 + \bar{f}_2(i\partial\!\!\!/ + m_2)f_2 + (\partial_\mu\phi)^2$$
$$+g_1\bar{f}_1f_1\phi + g_2\bar{f}_2f_2\phi + g_{12}[\bar{f}_1f_2 + \bar{f}_2f_1]\phi$$

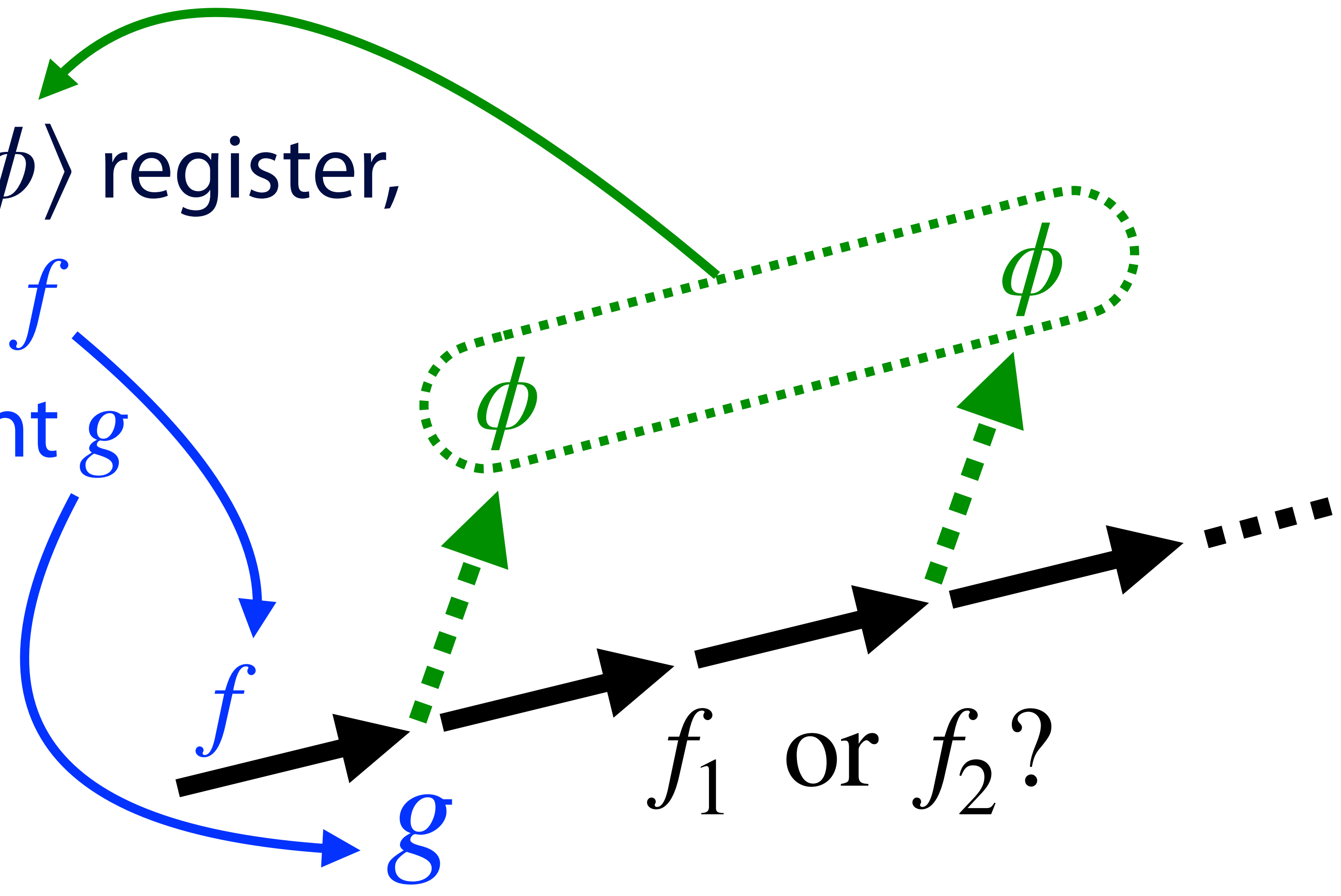
- Interference between unobserved intermediate states due to $g_{12}(\neq 0)$ term

B. Nachman et al., [Phys. Rev. Lett. 126, 062001 (2021)]

From the states in $|\phi\rangle$ register,

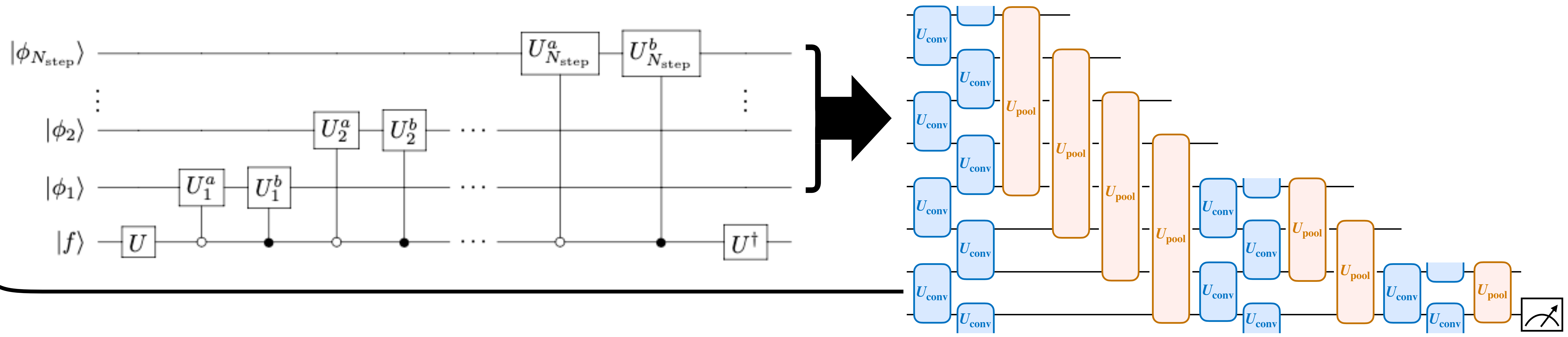
- Flavor of fermion f
- Coupling constant g between f and ϕ

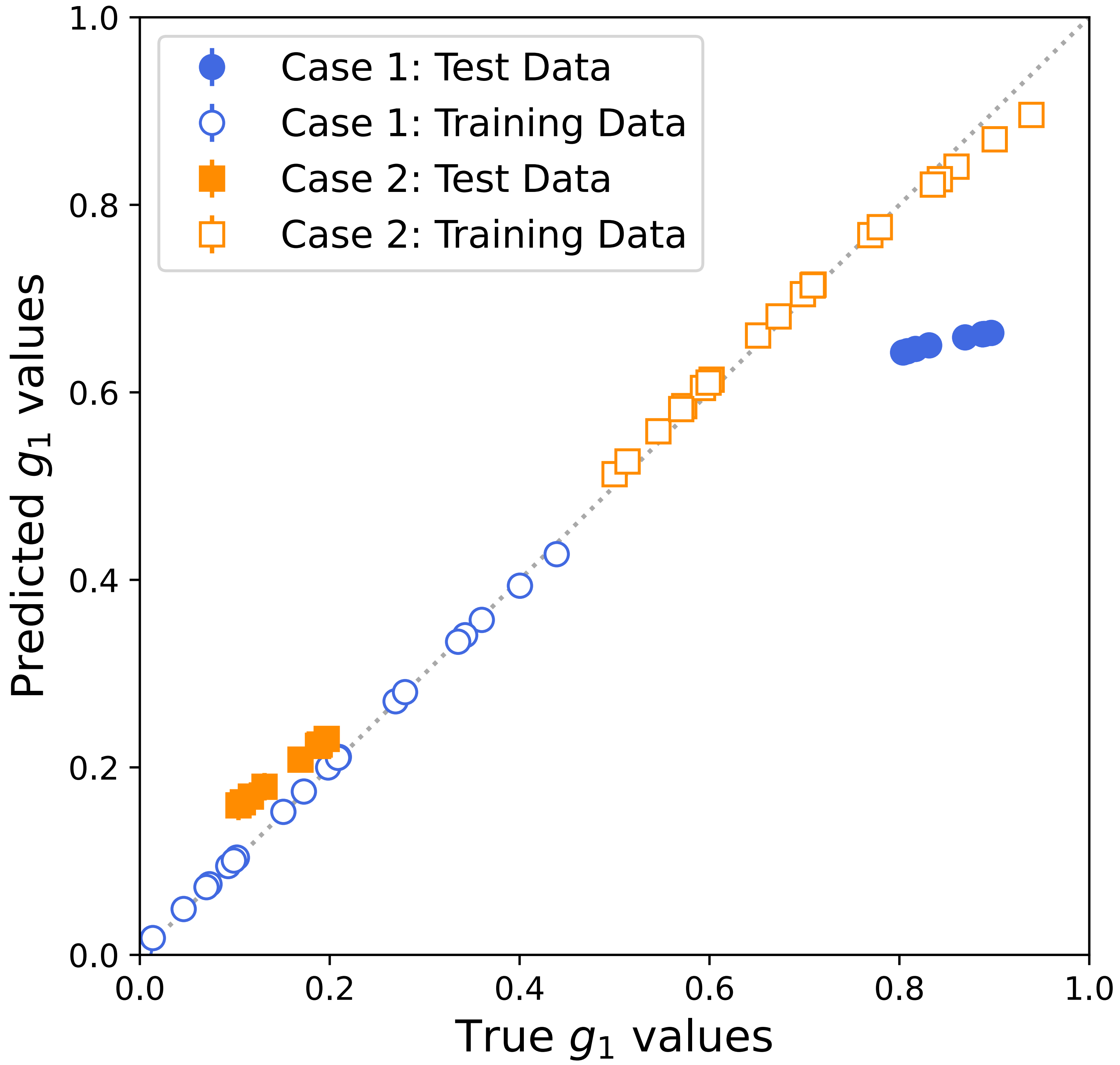
are extracted



Quantum data generation and classification

- Number of emission steps $N_{step} = 8$
- Generate various states with different flavors of input particle f or coupling constant g
- Flavor classification or regression of g values





Exercise of QML on Quantum Data

Consider a problem:

- Prepare a dataset of ground states for the transverse-field Ising model with different transverse-field strengths h
- Train a QNN model to learn the h values in the dataset

VQE

Prepare the ground states $|\psi(\mathrm{GS})\rangle = U(\boldsymbol{\theta})\,|0\rangle$ of Ising model with VQE ansatz:

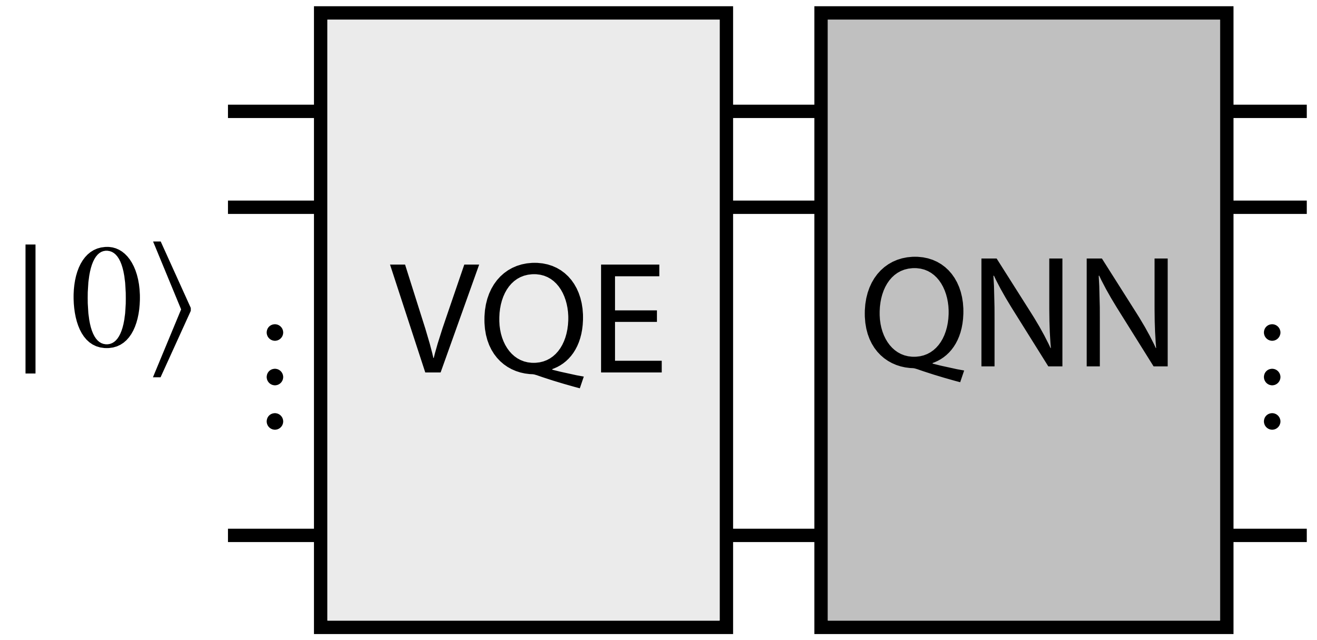
$$U(\{\theta_j^l\}) = \prod_{l=1}^{d}\left(\left(\prod_{j=1}^{n} R_j^Y(\theta_j^l)\right)\cdot U_{\mathrm{ent}}\right)\cdot \prod_{j=1}^{n} R_j^Y(\theta_j^0)$$

$$U_{\mathrm{ent}} = \prod_{j=1}^{n} C^{j}_{j\%n+1}[Z]$$

QNN

Learn the h value in the dataset

- VQE circuit fixed with optimized parameters
- QNN circuit similar to that used in VQE
- Mean squared error as a cost function
- SLSQP optimizer

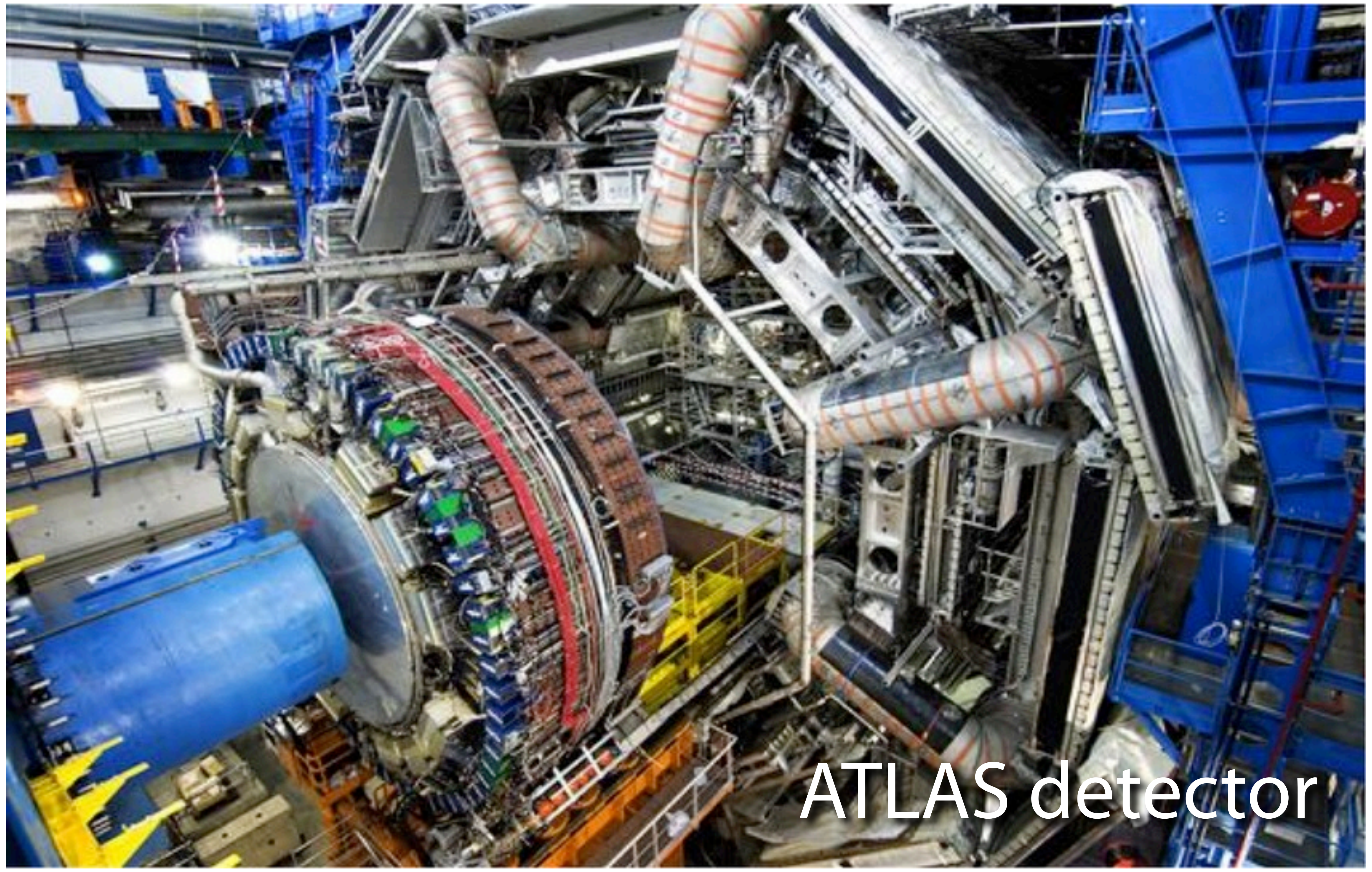


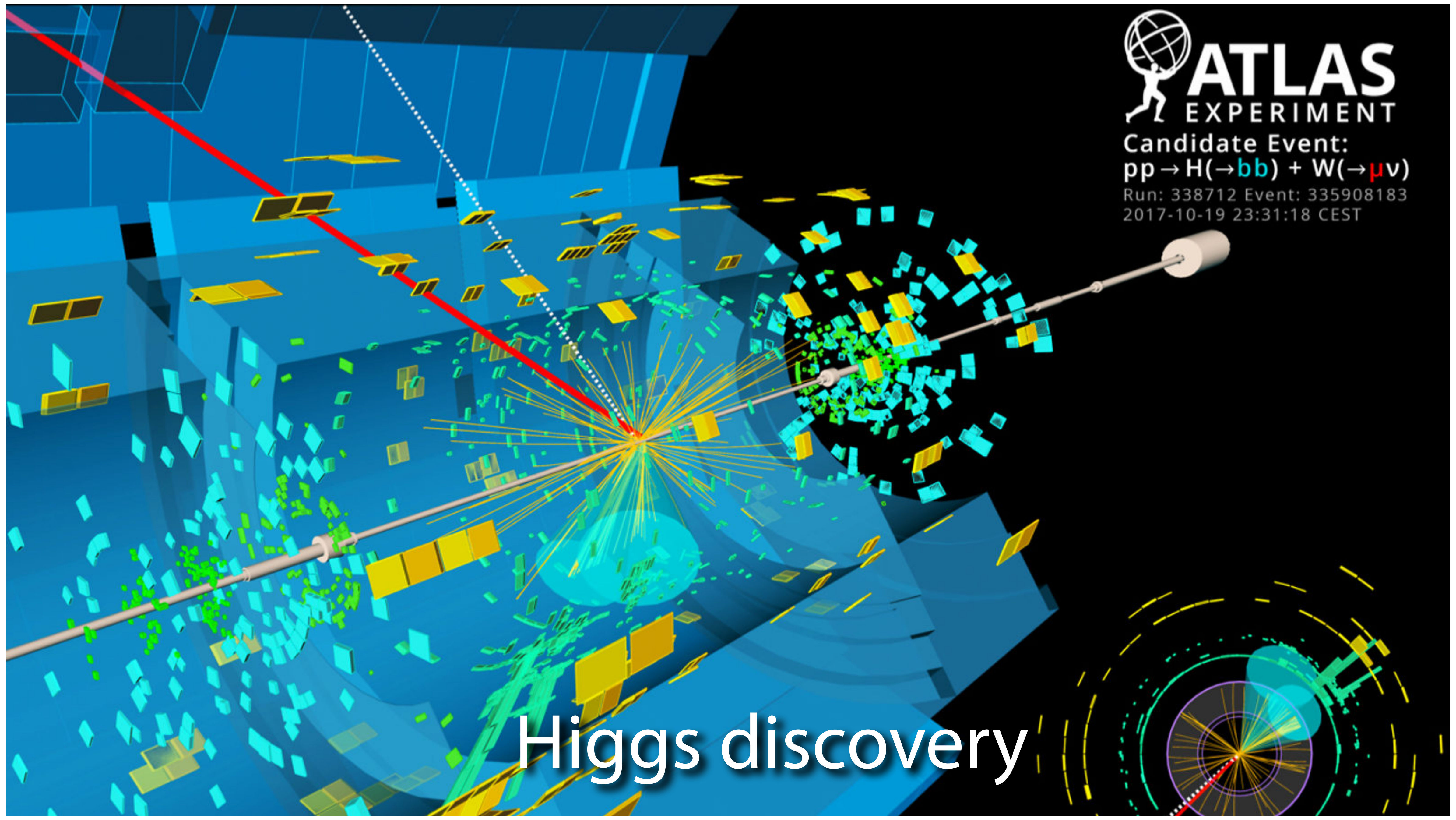
Hands-on Exercise (II)

- Quantum Machine Learning :
  - Determination of Hamiltonian parameter with quantum data

High-Energy Physics Experiment

- Particle collisions produced in high-energy accelerator
- Measure produced particles by precision detectors to study fundamental properties of particles and interaction mechanism
- Hadron colliders (e.g, LHC at CERN) primarily target new physics search beyond the Standard Model

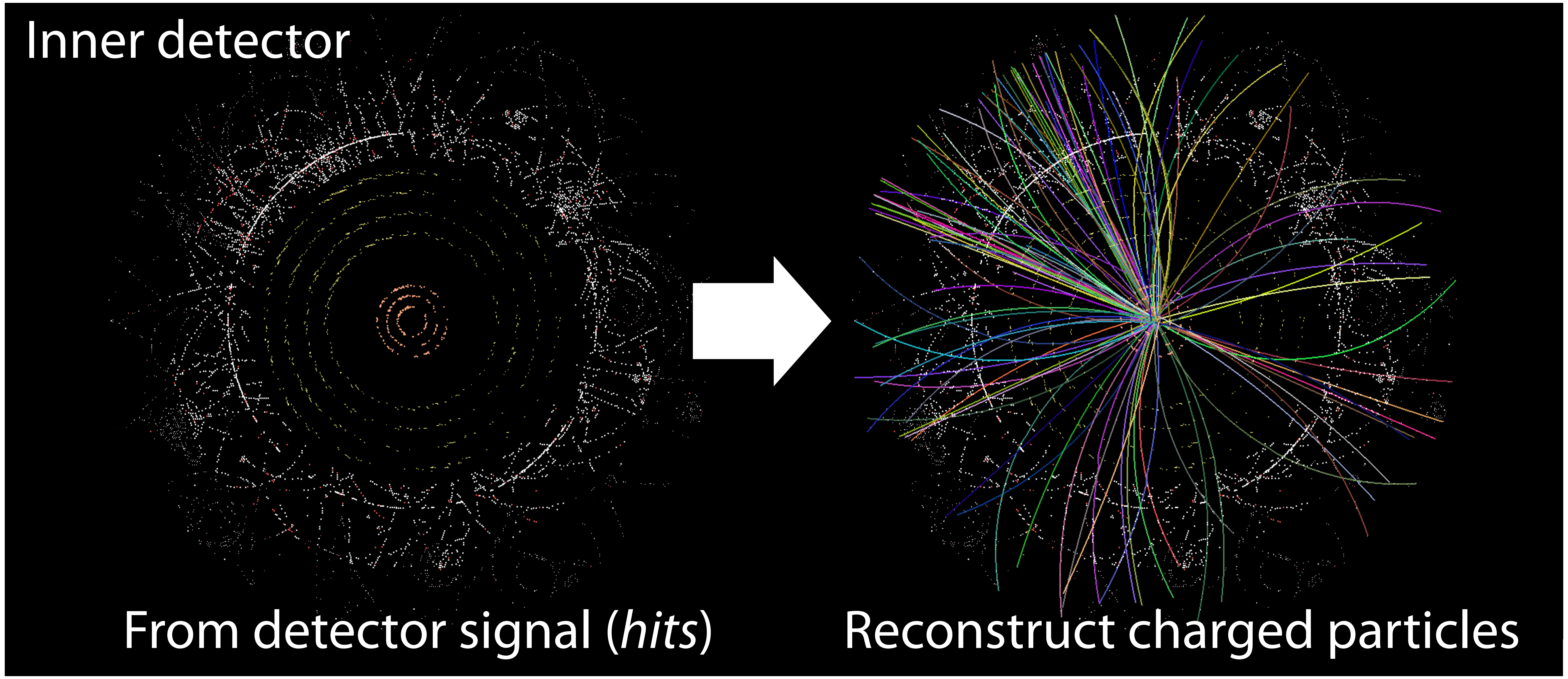

ATLAS detector

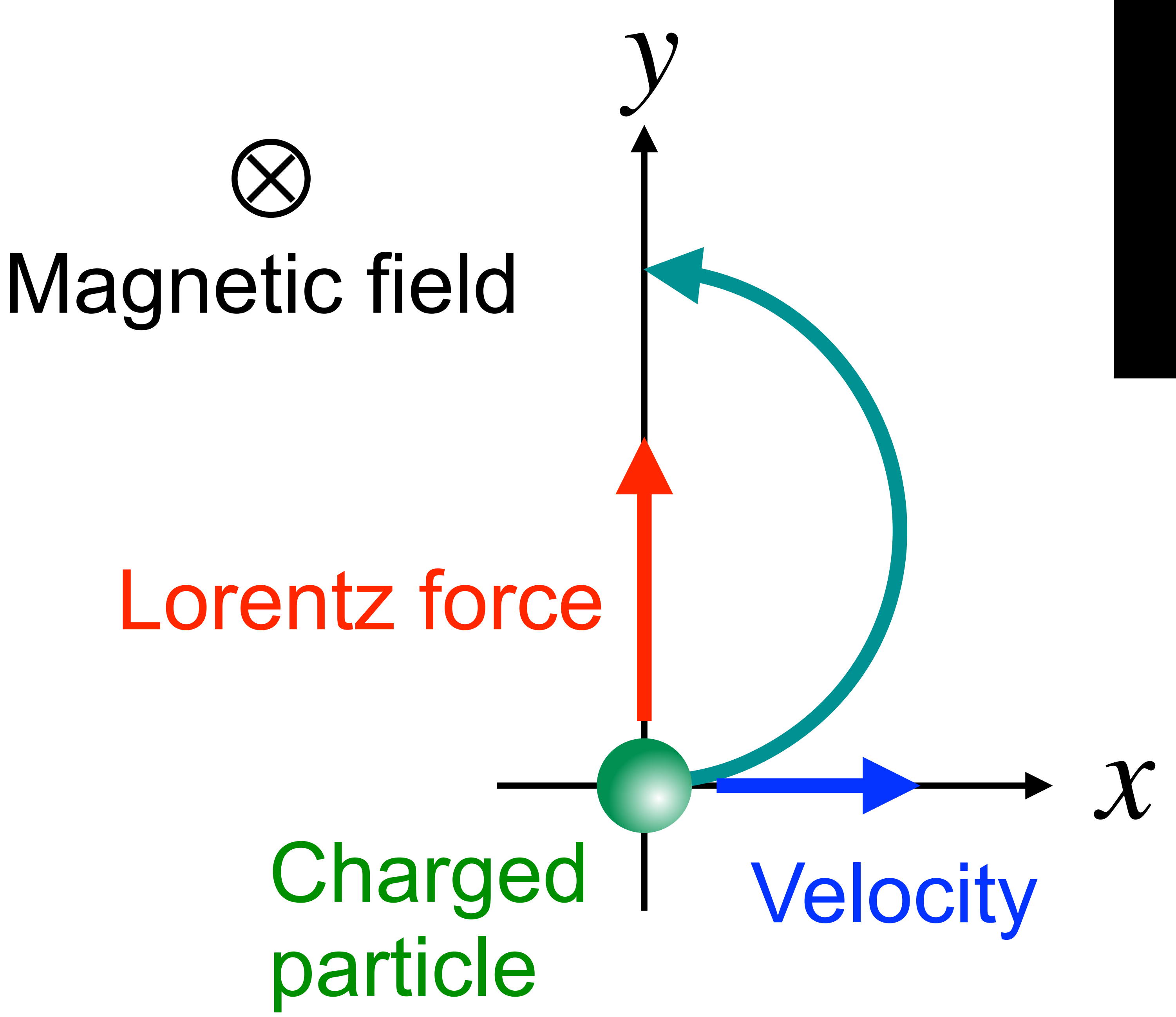


Higgs discovery

High-Energy Physics Experiment

Reconstruct produced particles from detector signal and measure their energy and momenta as a first step



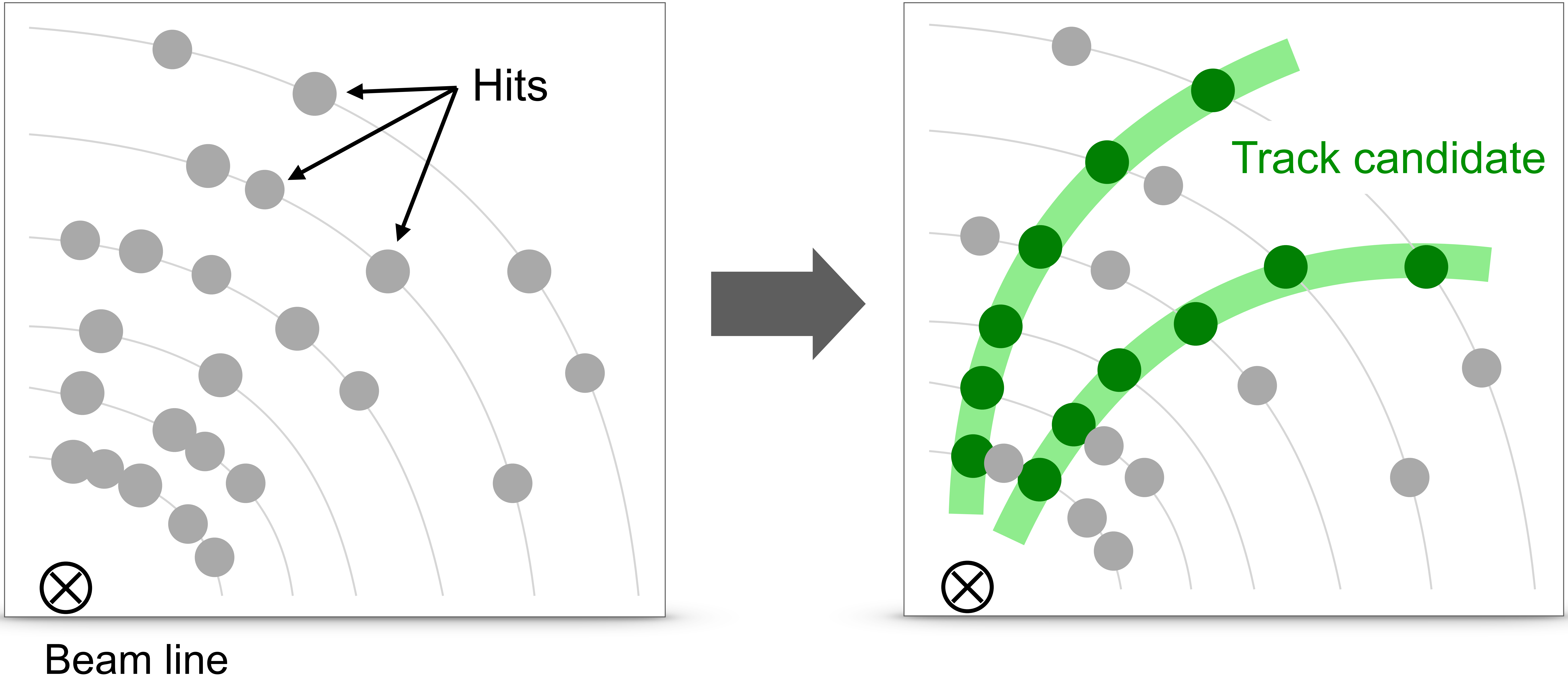


Find particle trajectory that matches the sequence of hits with a constant curvature

➡ **Tracking**

Charged Particle Tracking

Projected detector hits onto a plane perpendicular to the beam line



Check combinations of detector hits *in parallel* and choose correct ones based on expected pattern

➡ Possible to use quantum computing technique!

Exercise of Charged Particle Tracking

Consider a problem of selecting segments that constitute the same track

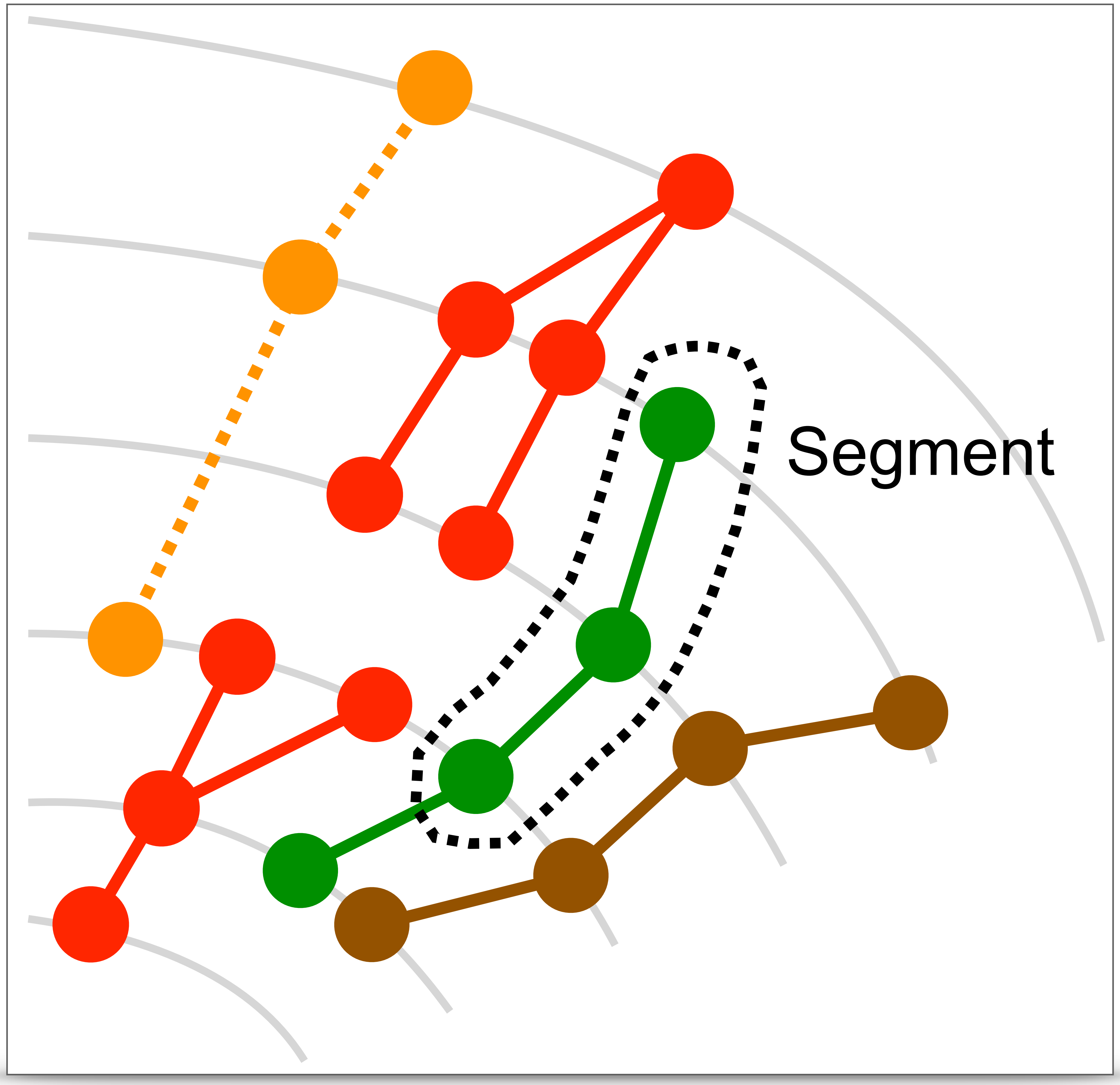
Preprocessing

- Form "***segments***" (= set of 3-consecutive layer hits) from detector hits using classical computer
- Calculate curvature in (x, y) plane, (r, z) angle, impact parameter, etc.
- Determine *weights* for each segment and each pairing of segments

Weight

- Largest positive weight (+1) for a segment pair with shared hits like red ones
- Large weight (> -1) for a zigzag pair or a pair with a hole in the middle
- Large negative weight (~ -1) for a segment pair with consistent curvatures and 2 shared hits like green

Segment = 3-consecutive layer hits



Exercise of Charged Particle Tracking

Solve as **Quadratic Unconstrained Binary Optimization (QUBO)** by minimizing

$$O(b,T) = \sum_{i=1}^{N} b_{ii} T_i + \sum_{i=1}^{N} \sum_{j=1\ (i<j)}^{N} b_{ij} T_i T_j$$

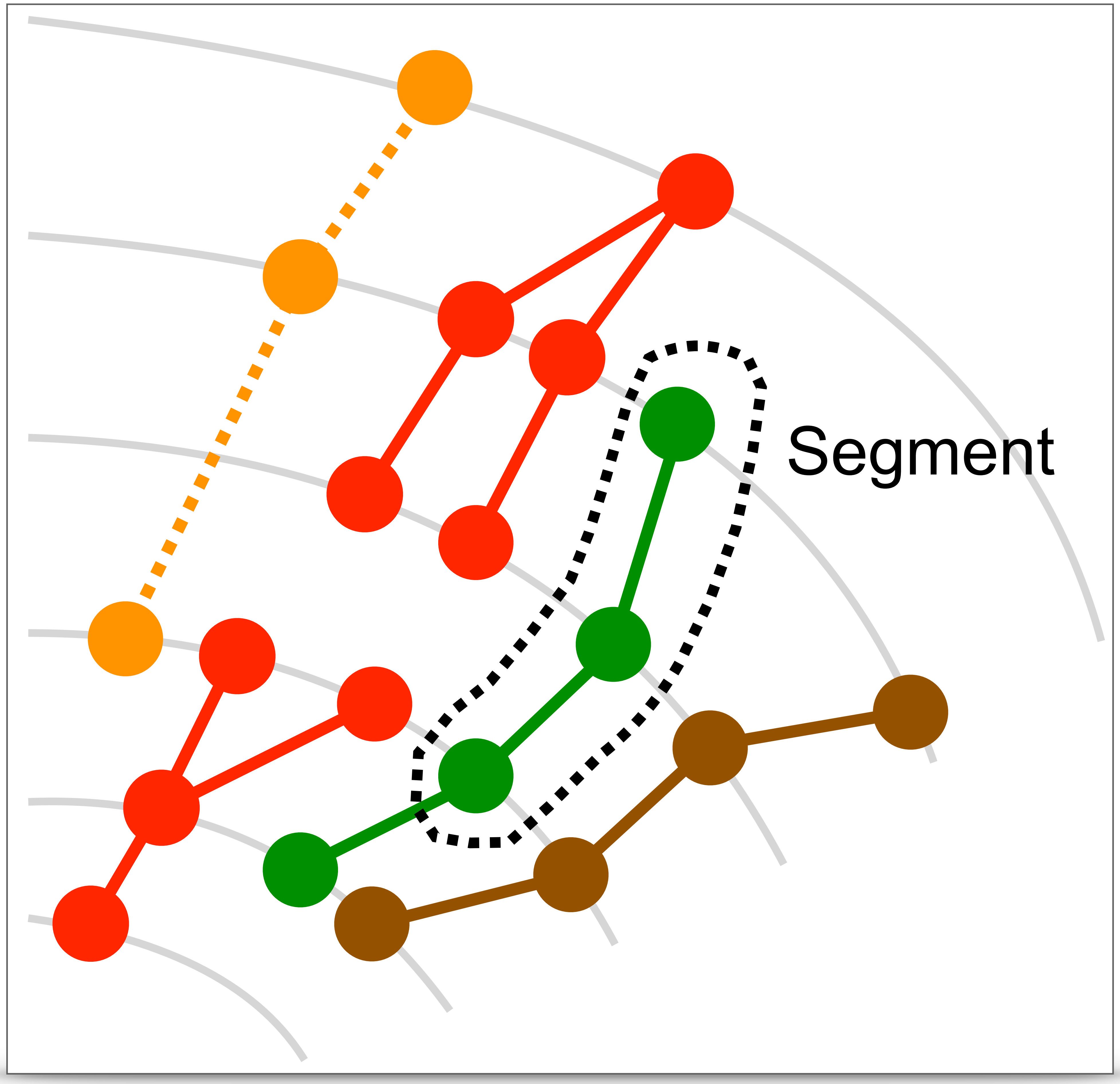
$$T \in \{0,1\}$$

Weight $b_{ij} = \begin{cases} -S(T_i, T_j) & \text{Green Brown Orange} \\ 1 & \text{Red} \\ 0 & \text{Others} \end{cases}$

$S(T_i, T_j)$ is set within $[0,1]$ based on relative angles between segments T_i and T_j

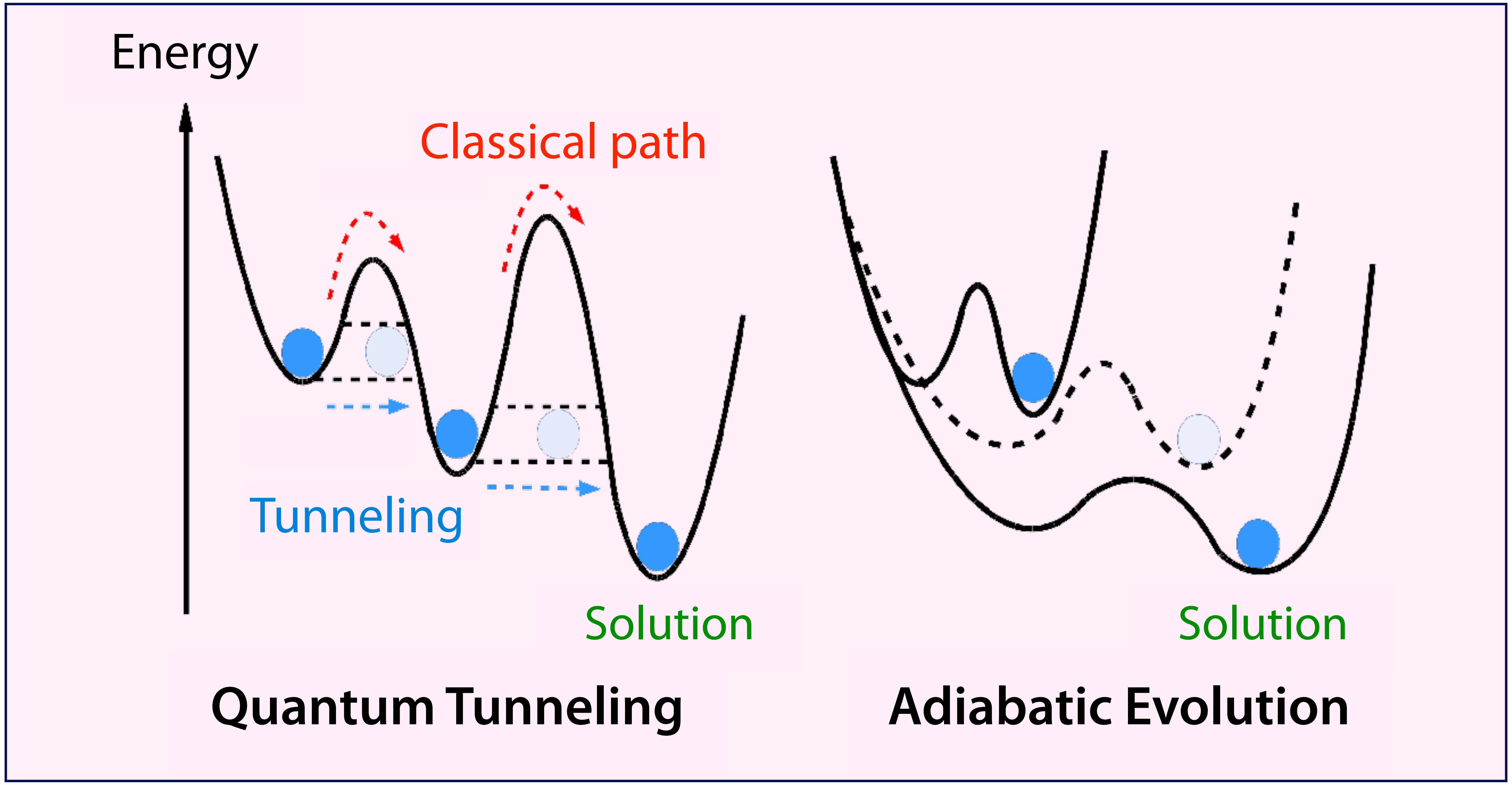
(closer to 1 as the curvatures get closer)

Segment = 3-consecutive layer hits

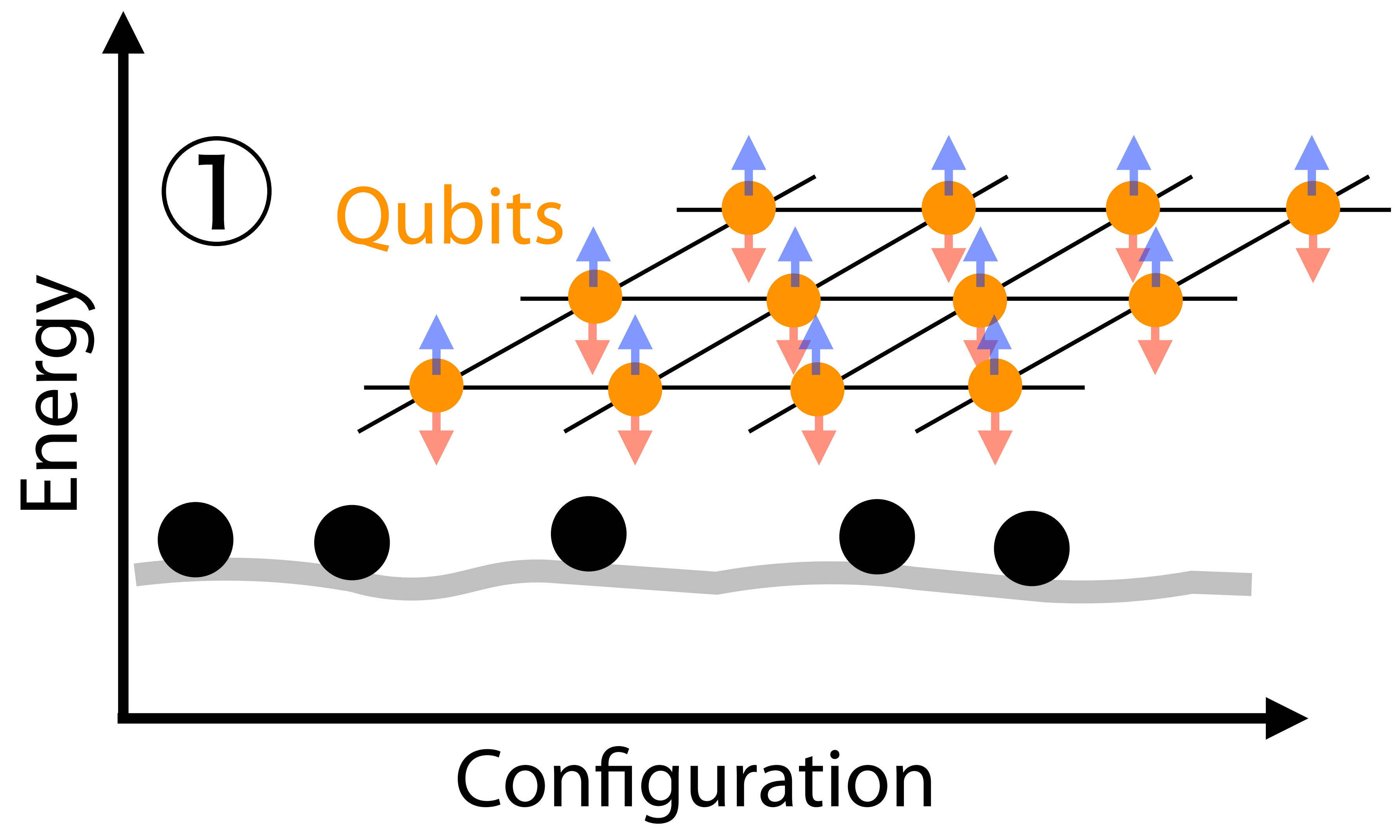


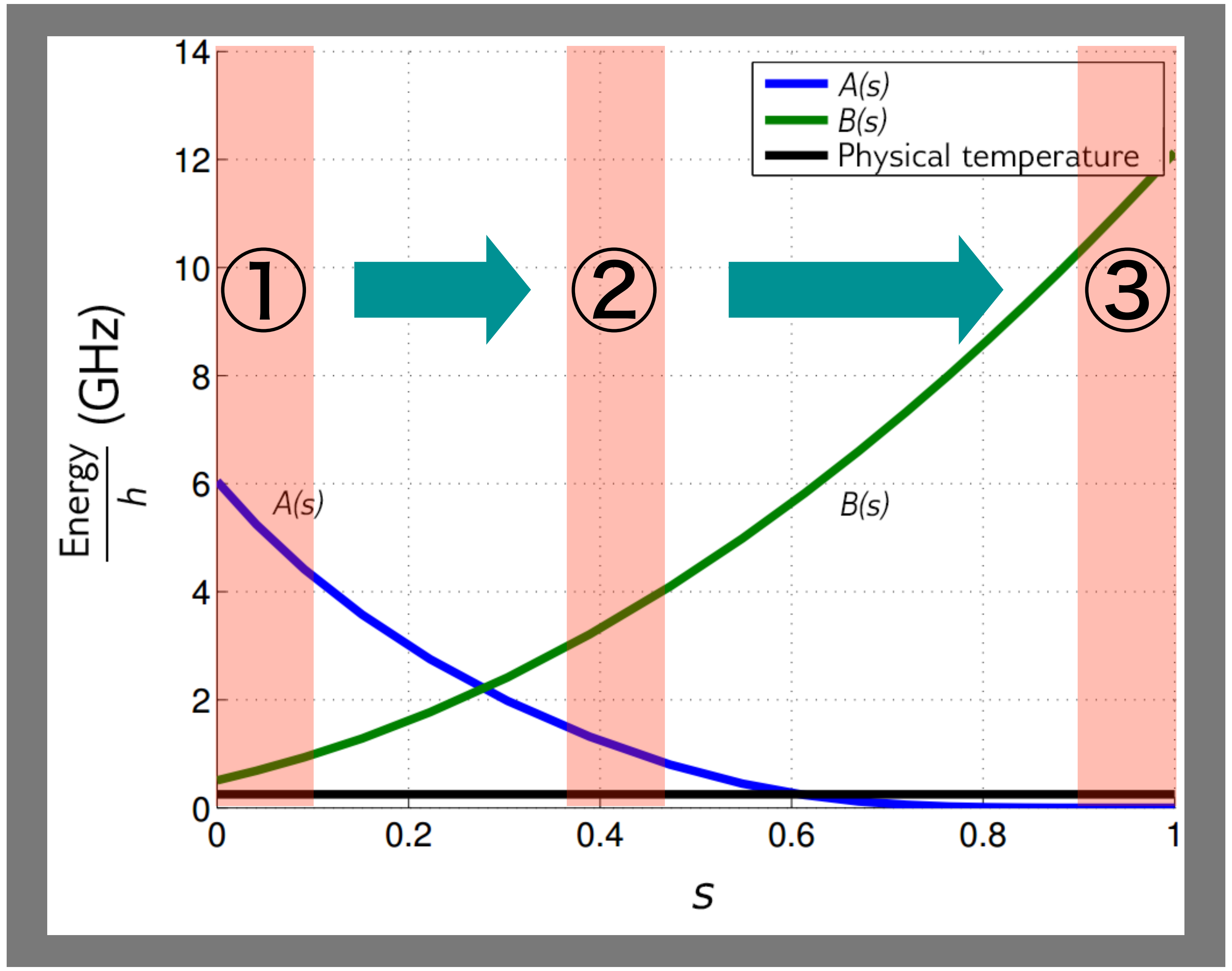
Quantum Annealing

- Formulate problem such that the solution corresponds to the lowest energy state
- Extract the solution by slowly (*adiabatically*) introducing problem hamiltonian
- Suitable for optimization problem



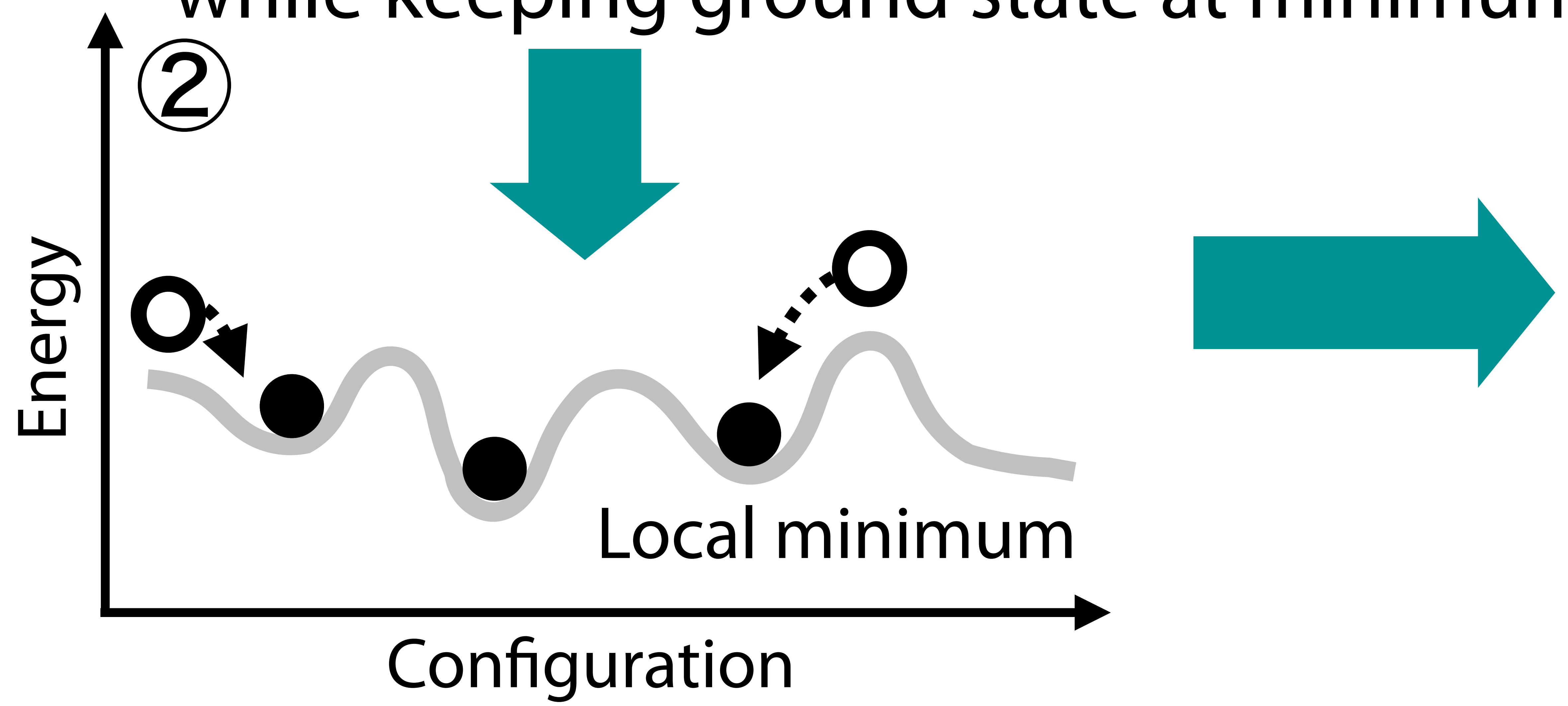
Quantum Annealing at Work

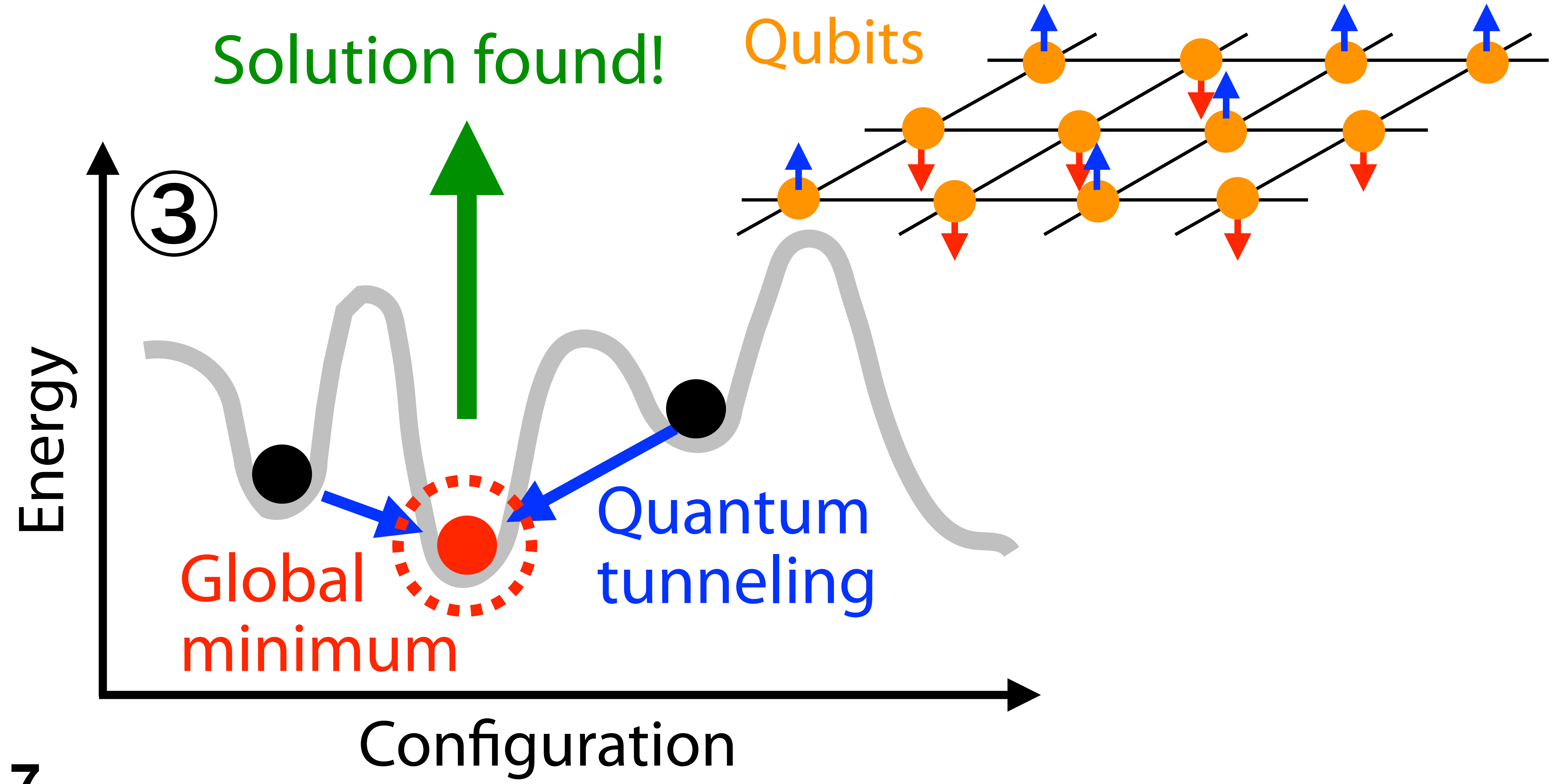




All configurations at ground state for **initial hamiltonian**

Slowly introduce **problem hamiltonian** while keeping ground state at minimum

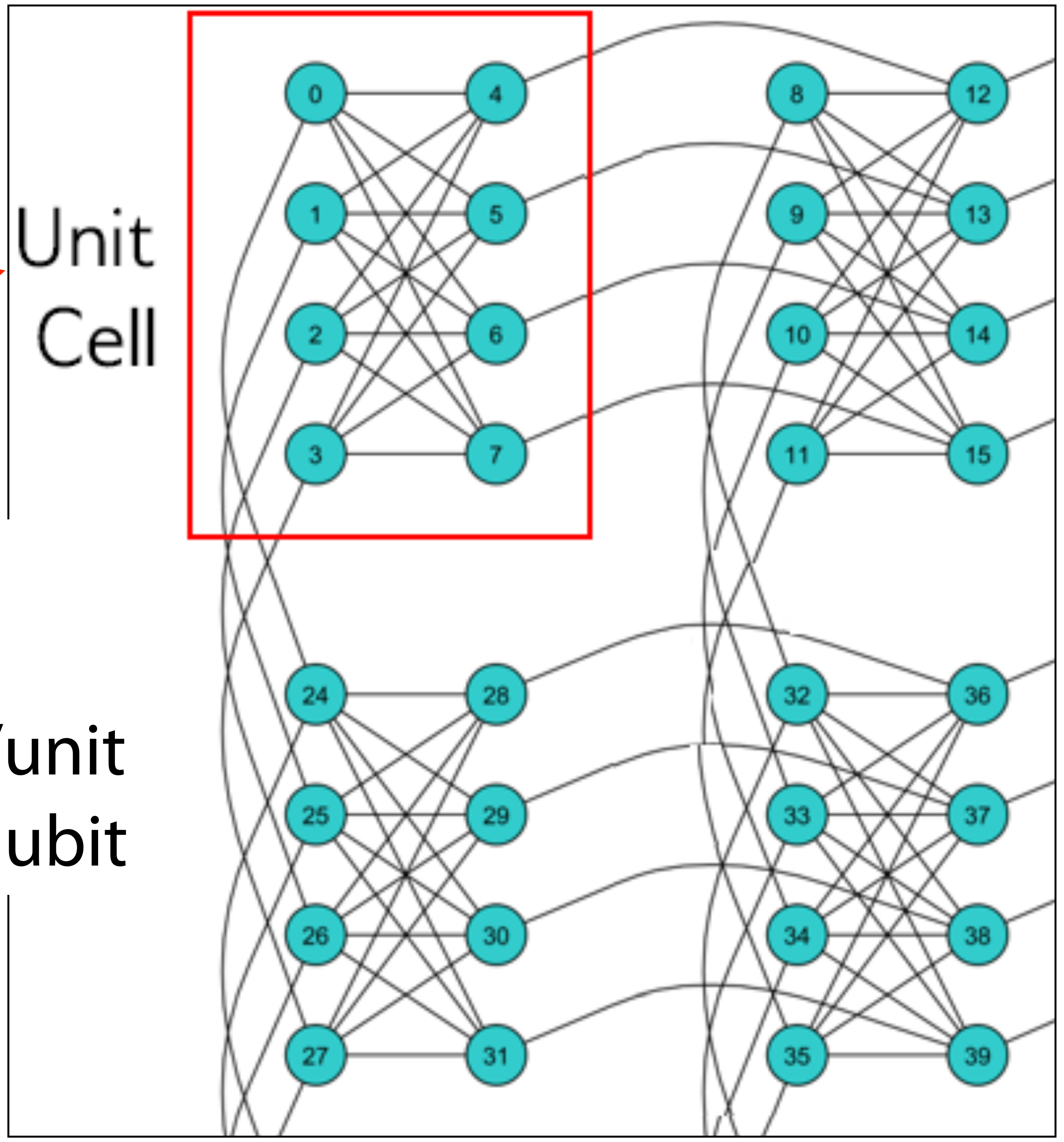




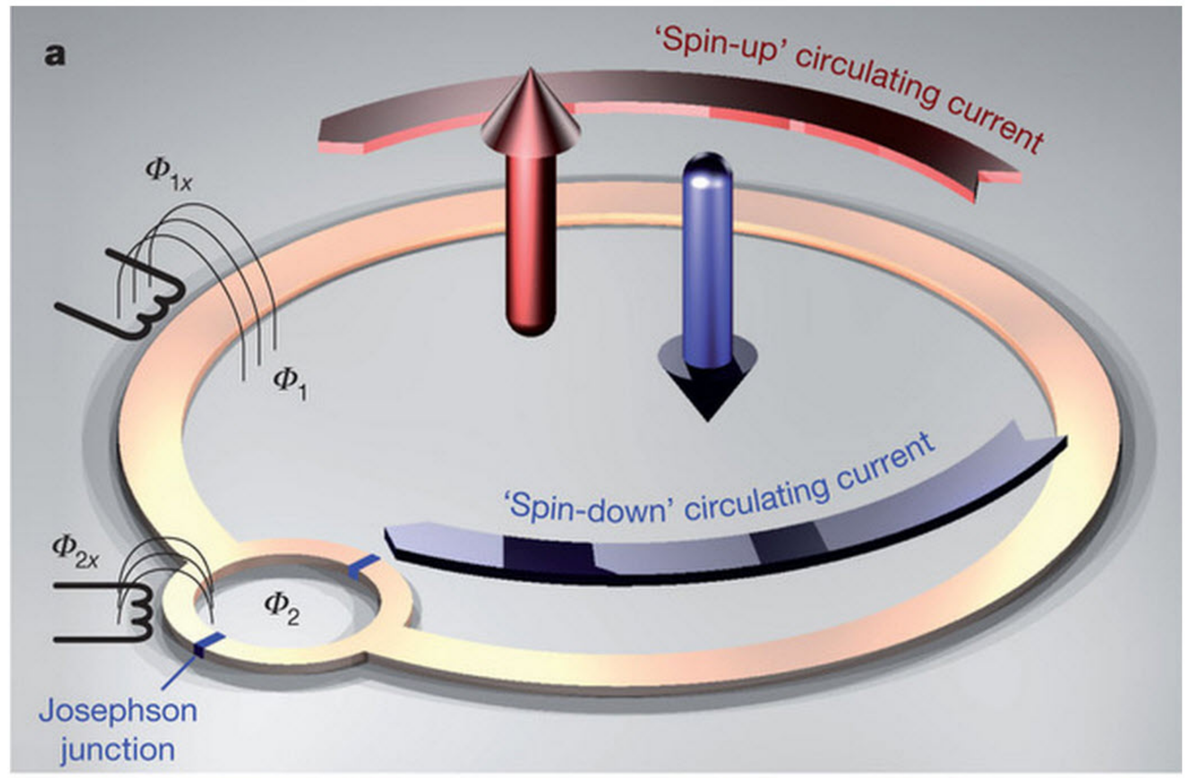
Quantum Annealing at Work

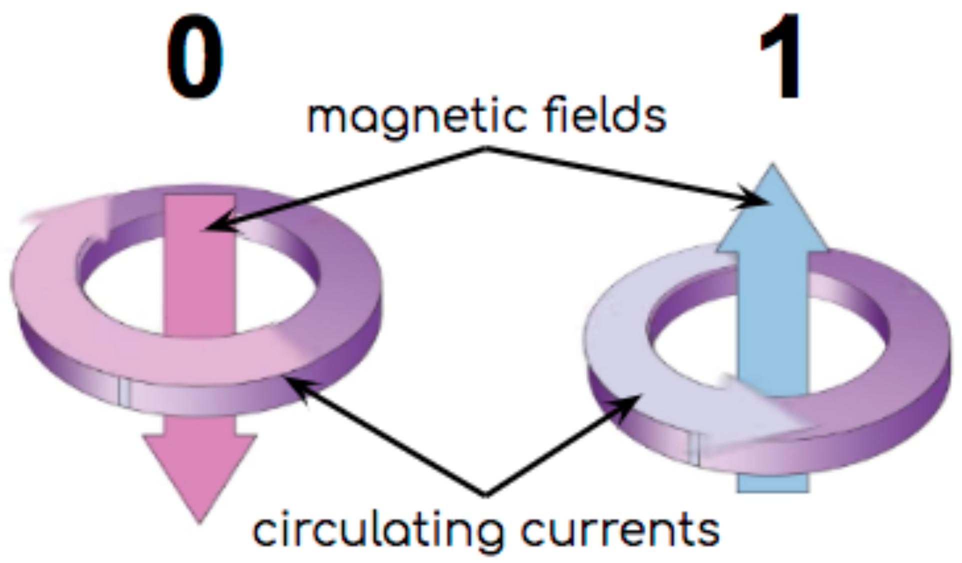
D-Wave Quantum Annealer

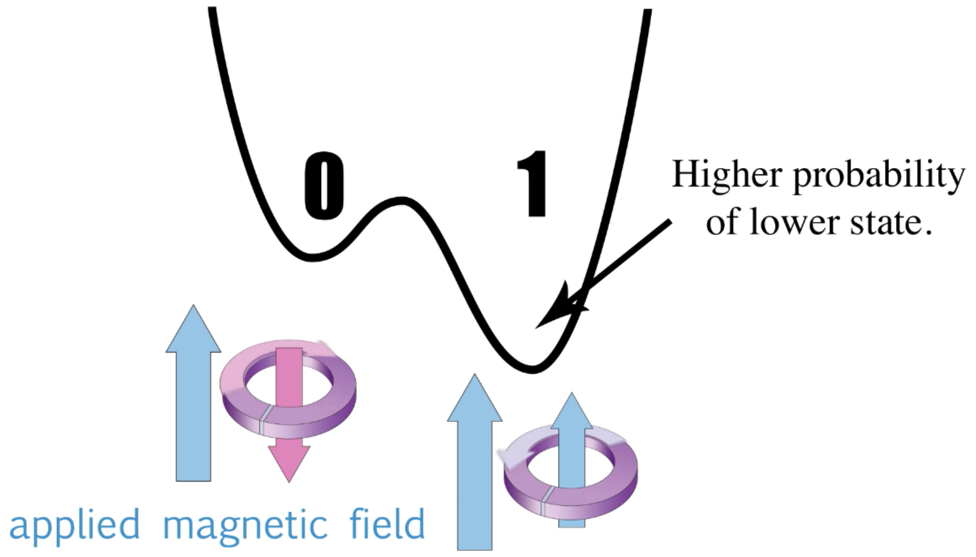
- Superconducting qubits (T~15 mK)
- >5000 qubits (D-Wave Advantage)
  2048 qubits (D-Wave 2000Q) used in studies
- Annealing time = 1~2000 μs, Coherence time ~ O(ns)

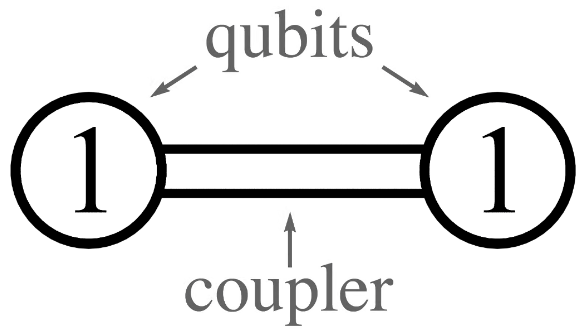


Connection via *Chimera* graph for 2000Q:
- 16×16 units, 8 qubits/unit
- 5-6 connections per qubit





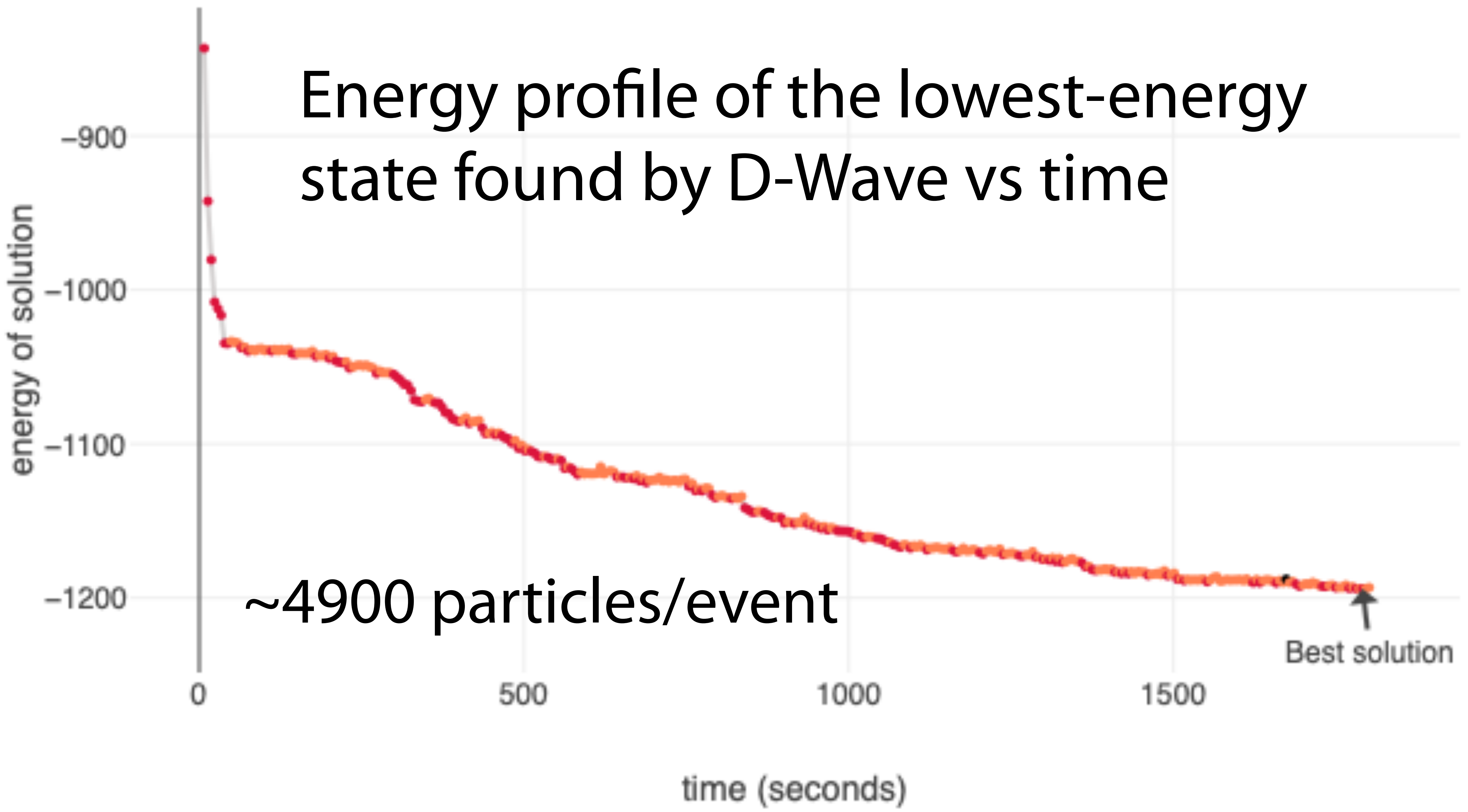




	2000Q	Advantage
Topology	Chimera	Pegasus
Qubits	2048	>5000
Couplers	>6000	>35000
Full connection	~64	~124

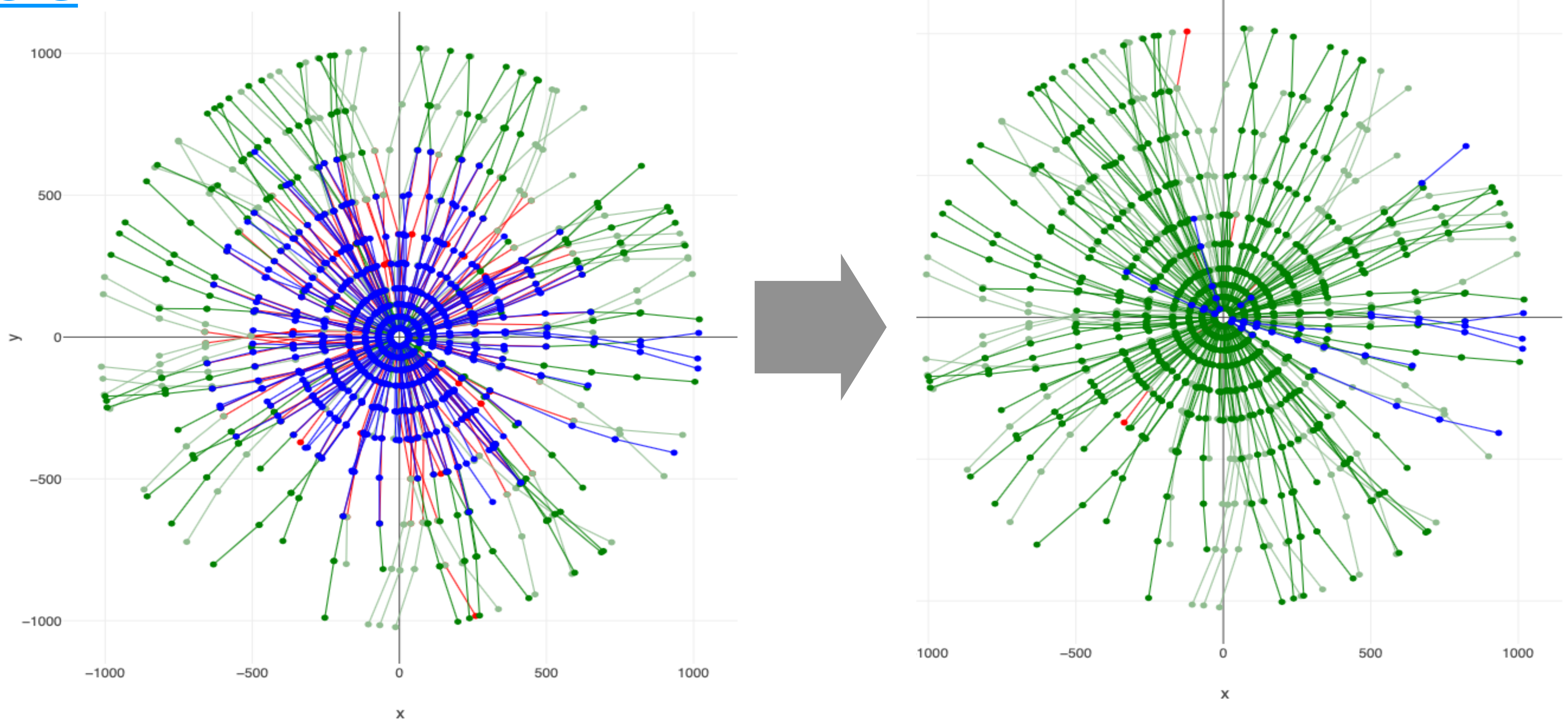
Track Finding with Quantum Annealing

Track finding studied using [TrackML Particle Tracking Challenge] dataset for HL-LHC



Iterating the annealing process until the lowest energy state is unchanged

Before annealing **After annealing**



Purity	37.2%
Efficiency	22.6%

Purity	98.5%
Efficiency	96.4%

- Many missing tracks or fake tracks before annealing (reconstruction by connecting nearby triplets)
- >95% of $p_T > 1\,\mathrm{GeV}$ successfully reconstructed after annealing

Exercise of Gate-based Charged Particle Tracking

Considered so far solving the QUBO problem by minimizing $O(b, T)$

$$O(b,T) = \sum_{i=1}^{N} b_{ii}T_i + \sum_{i=1}^{N} \sum_{j=1\ (i<j)}^{N} b_{ij}T_iT_j \quad T \in \{0,1\}$$

Can we solve this using gate-based quantum computer?

Exercise of Gate-based Charged Particle Tracking

Considered so far solving the QUBO problem by minimizing $O(b, T)$

$$O(b,T) = \sum_{i=1}^{N} b_{ii} T_i + \sum_{i=1}^{N} \sum_{j=1\ (i<j)}^{N} b_{ij} T_i T_j \quad T \in \{0,1\}$$

➡ Convert objective function to Hamiltonian that can be decomposed into Pauli observables

$$T_i = \frac{1}{2}(1 - s_i) \quad \Rightarrow \quad H(h, J, s) = \sum_{i=1}^{N} h_i s_i + \sum_{i=1}^{N} \sum_{j=1\ (i<j)}^{N} J_{ij} s_i s_j \ \ (+\,\text{constant})$$

$$s \in \{1, -1\}$$

Exercise of Gate-based Charged Particle Tracking

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$$s \in \{1, -1\}$$

$s \in \{1, -1\}$ can be obtained as expectation values of Pauli Z operator

➡ Possible to solve by minimizing the expectation values of the Hamiltonian using VQE!

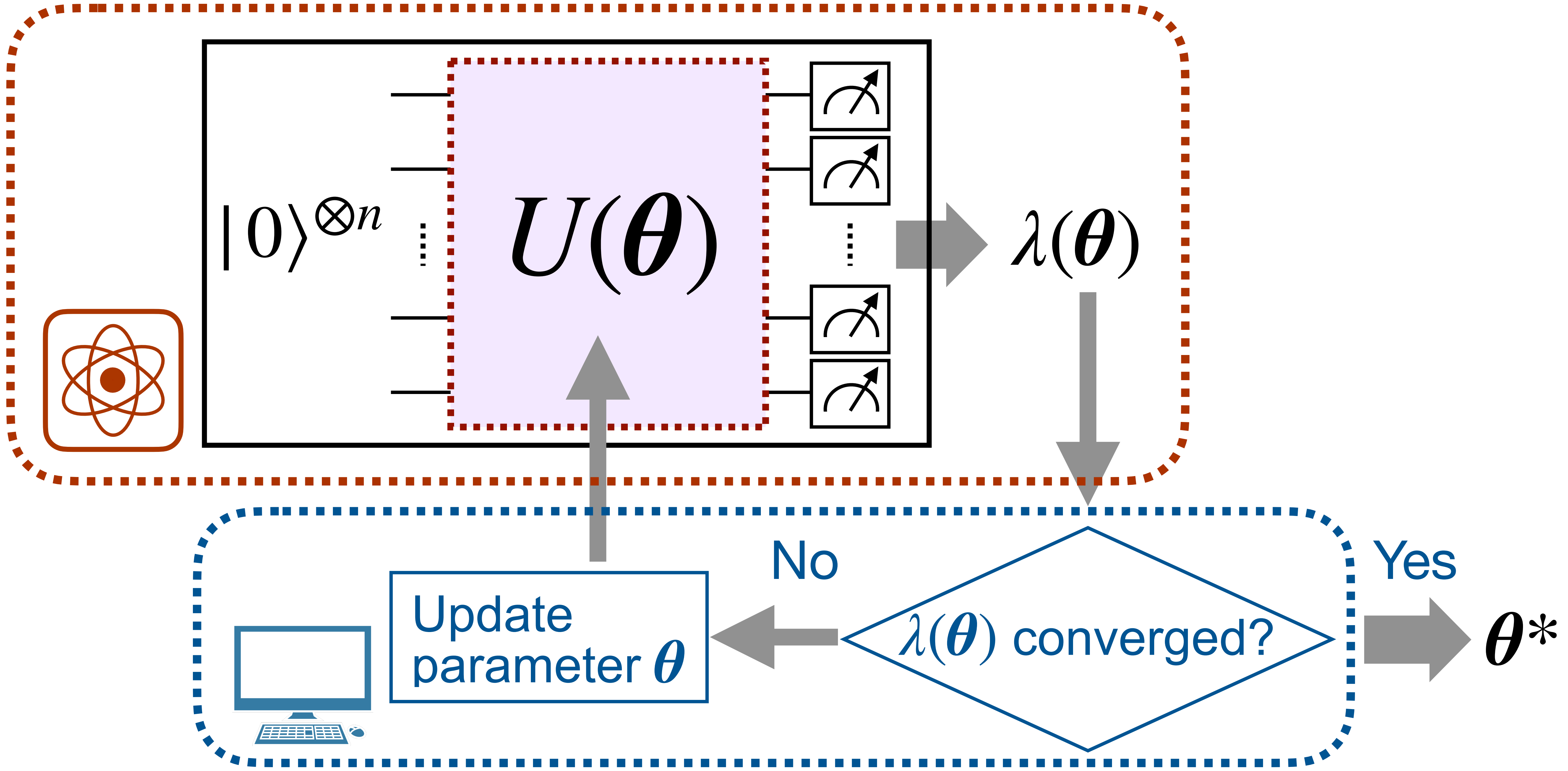
Implementation to VQE Circuit

Find the lowest-energy eigenstate of the Hamiltonian using VQE

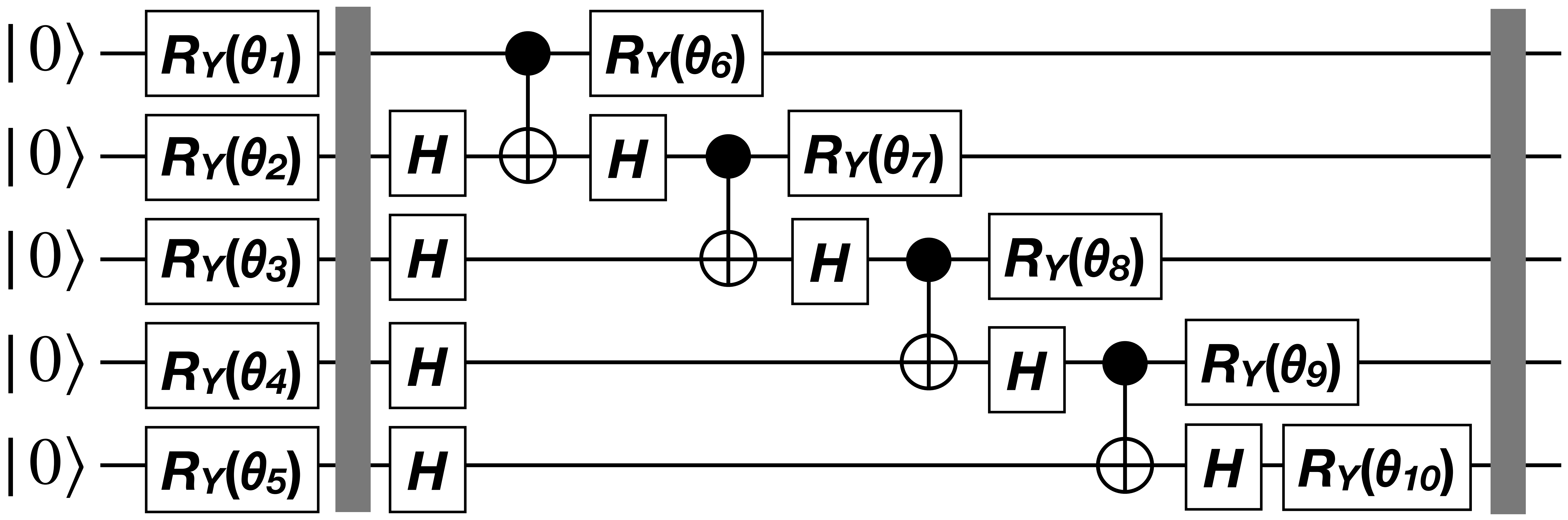
$$\lambda(\boldsymbol{\theta}) \equiv \langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle$$

$$\boldsymbol{\theta} \rightarrow \boldsymbol{\theta}^*$$

$$\Rightarrow \lambda(\boldsymbol{\theta}^*) \sim \langle \psi_{\min} | H | \psi_{\min} \rangle = \lambda_{\min}$$



R_Y and controlled-R_Z gates as $U(\boldsymbol{\theta})$ for $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|0\rangle$



Hands-on Exercise (III)

- Reconstruction of Charged Particles (Tracking) :
  - Tracking with annealing technique
  - Tracking with VQE-based approach

More recent perspectives on QML…

Conventional QNN Model

Conventional QNN Model

Important ingredients for successful QML model…

Barren Plateau

Hilbert space grows exponentially in number of qubits

Known that the training of variational quantum algorithm (parameterized quantum circuit) generally becomes difficult with the system size

J. R. McClean et al., Nat. Commun. 9, 4812 (2018)

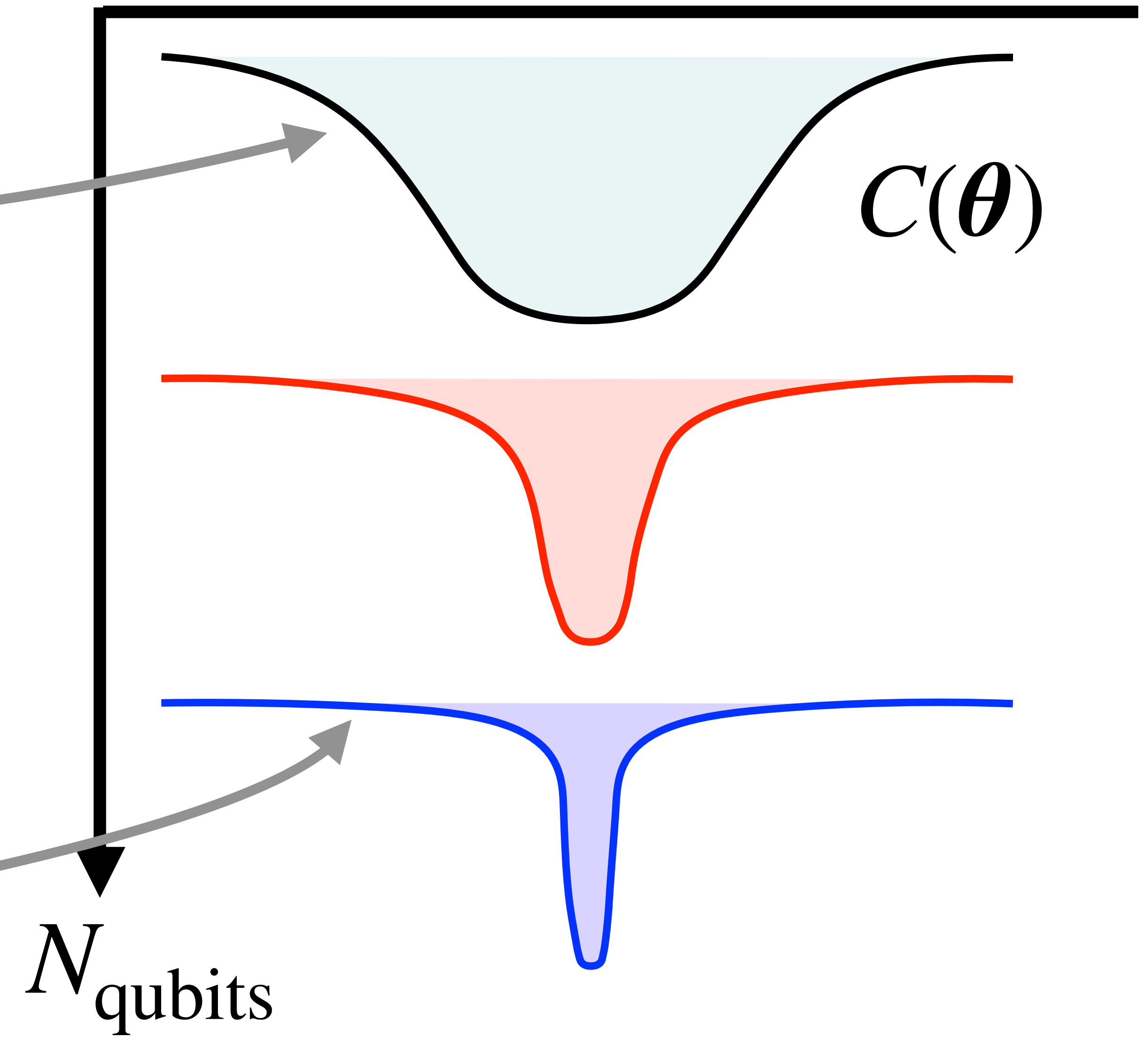
Cost function

$$C(\boldsymbol{\theta}) = \mathrm{Tr}[OU(\boldsymbol{\theta})\rho U^{\dagger}(\boldsymbol{\theta})]$$

$$\Rightarrow E_{\boldsymbol{\theta}\sim\mathrm{uniform}}\left[\frac{\partial C(\boldsymbol{\theta})}{\partial \theta_i}\right] = 0$$

$$V_{\boldsymbol{\theta}\sim\mathrm{uniform}}\left[\frac{\partial C(\boldsymbol{\theta})}{\partial \theta_i}\right] = \mathcal{O}(b^{-n}) \quad (b > 1)$$

Vanishing gradient

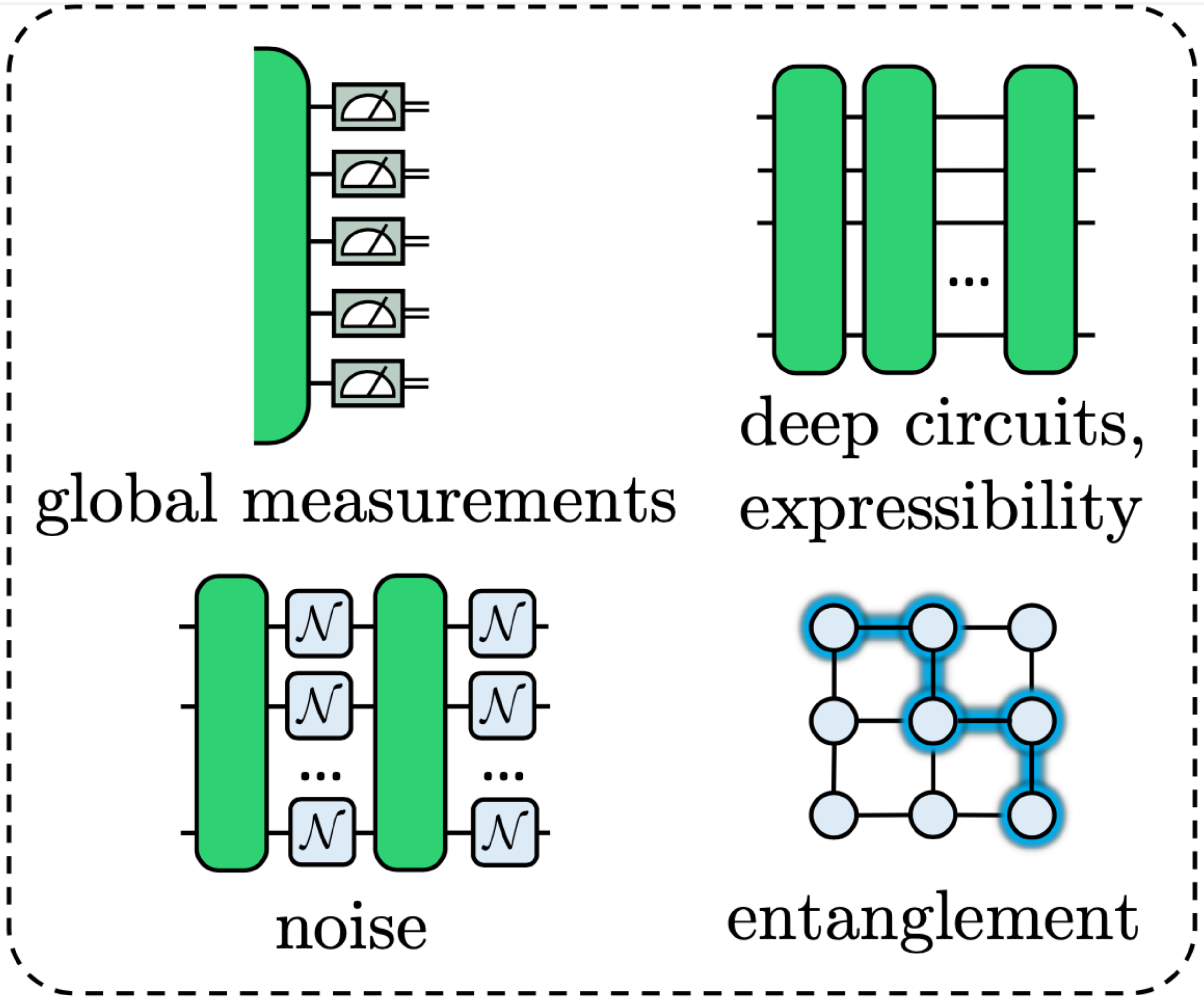


➡ **Barren Plateau** problem

Barren Plateau

Known that barren plateau can occur due to various reasons:

- *Expressibility of variational quantum circuit, Entanglement property, Cost function (global vs local), Noise, Data encoding, …*



S. Thanaslip et al., [Quantum Mach. Intell. 5, 21 (2023)]

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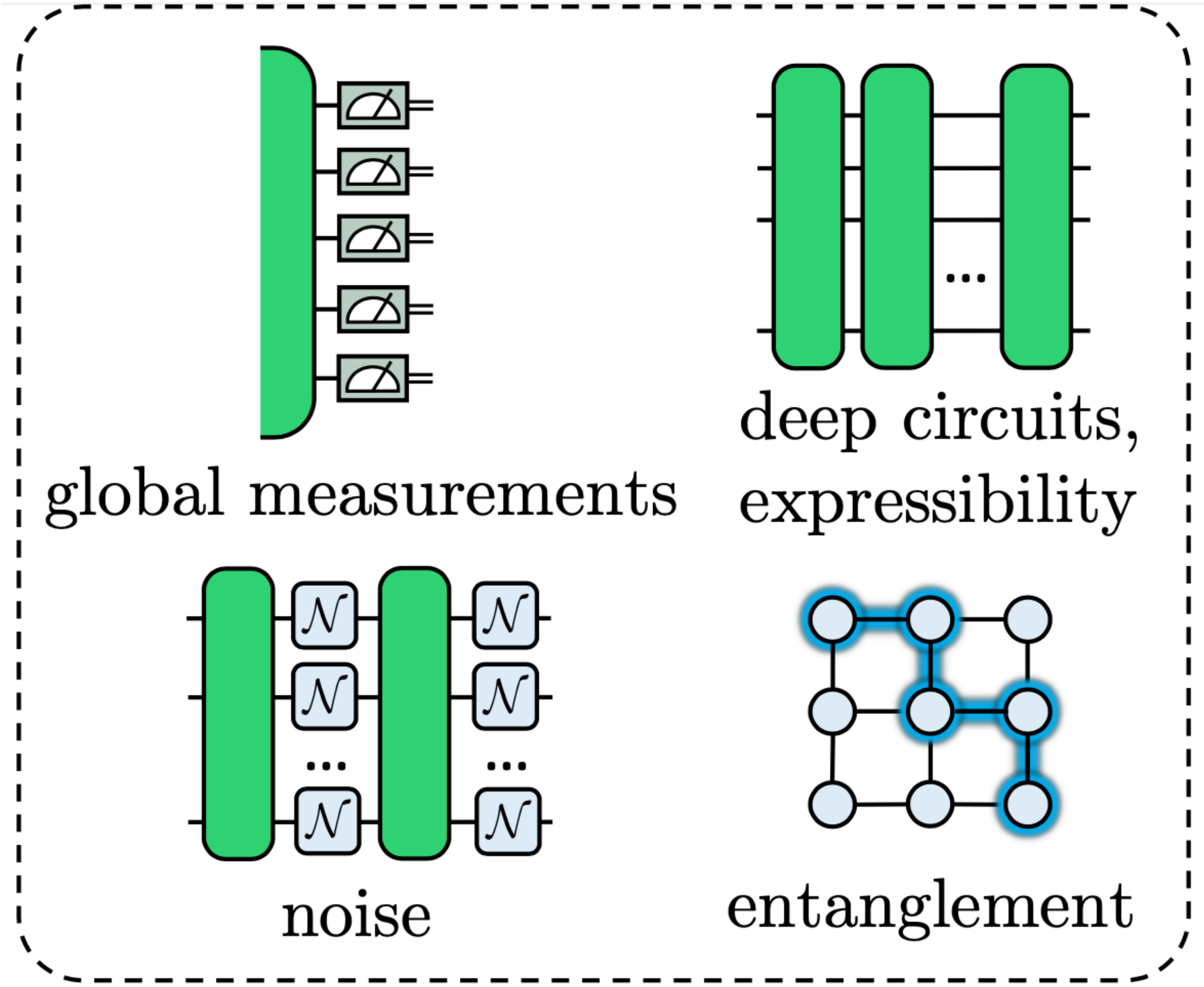
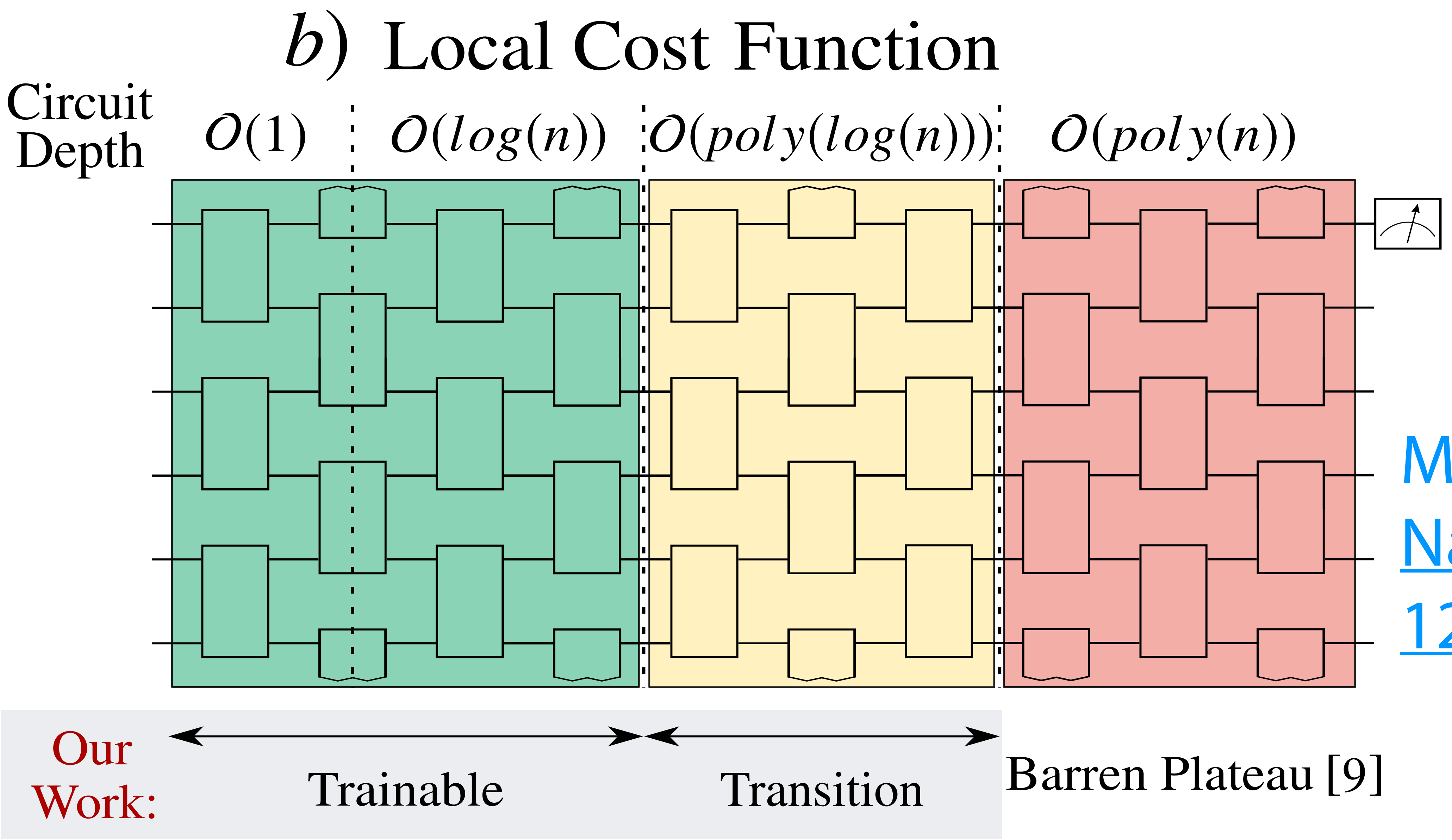


S. Thanaslip et al., [Quantum Mach. Intell. 5, 21 (2023)]

Very active field of research in quantum machine learning

- Generally tries to find model that one can avoid barren plateau



M. Cerezo et al., [Nat. Commun. 12, 1791 (2021)]

Should be further studied…

"We present strong evidence that commonly used models with provable absence of barren plateaus are also classically simulable, …"

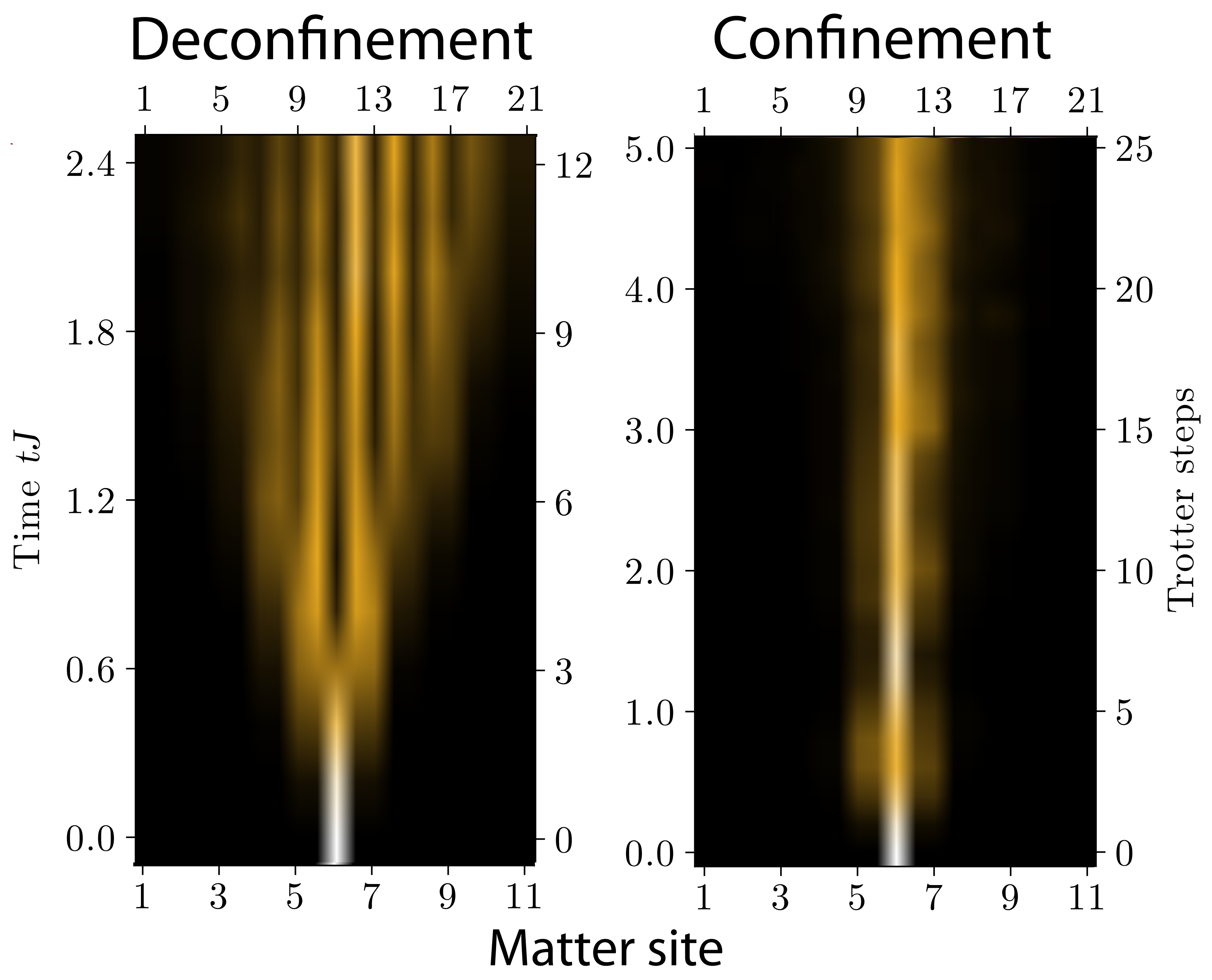
M. Cerezo et al., [arXiv:2312.09121]

Backup

QML Application to Quantum Data

Hamiltonian in $(1+1)d\ \mathbb{Z}_2$ lattice gauge theory

$$H(m,f) = -\frac{J}{2}\sum_{j=0}^{N_s-1}(X_j Z_{j,j+1} X_{j+1} + Y_j Z_{j,j+1} Y_{j+1}) - f\sum_{j=0}^{N_s-2} X_{j,j+1} + \frac{m}{2}\sum_{j=0}^{N_s-1}(-1)^j Z_j$$



Confinement ($f \neq 0$) and Deconfinement ($f = 0$) phases depending on the presence of background electric field

Recognize (de)confinement phases as a function of m from a time-evolved state $|\psi(m,f)\rangle = e^{-iH(m,f)T}|\psi_0\rangle$ using QCNN