Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

QUANTUM COMPUTATION FOR HEP

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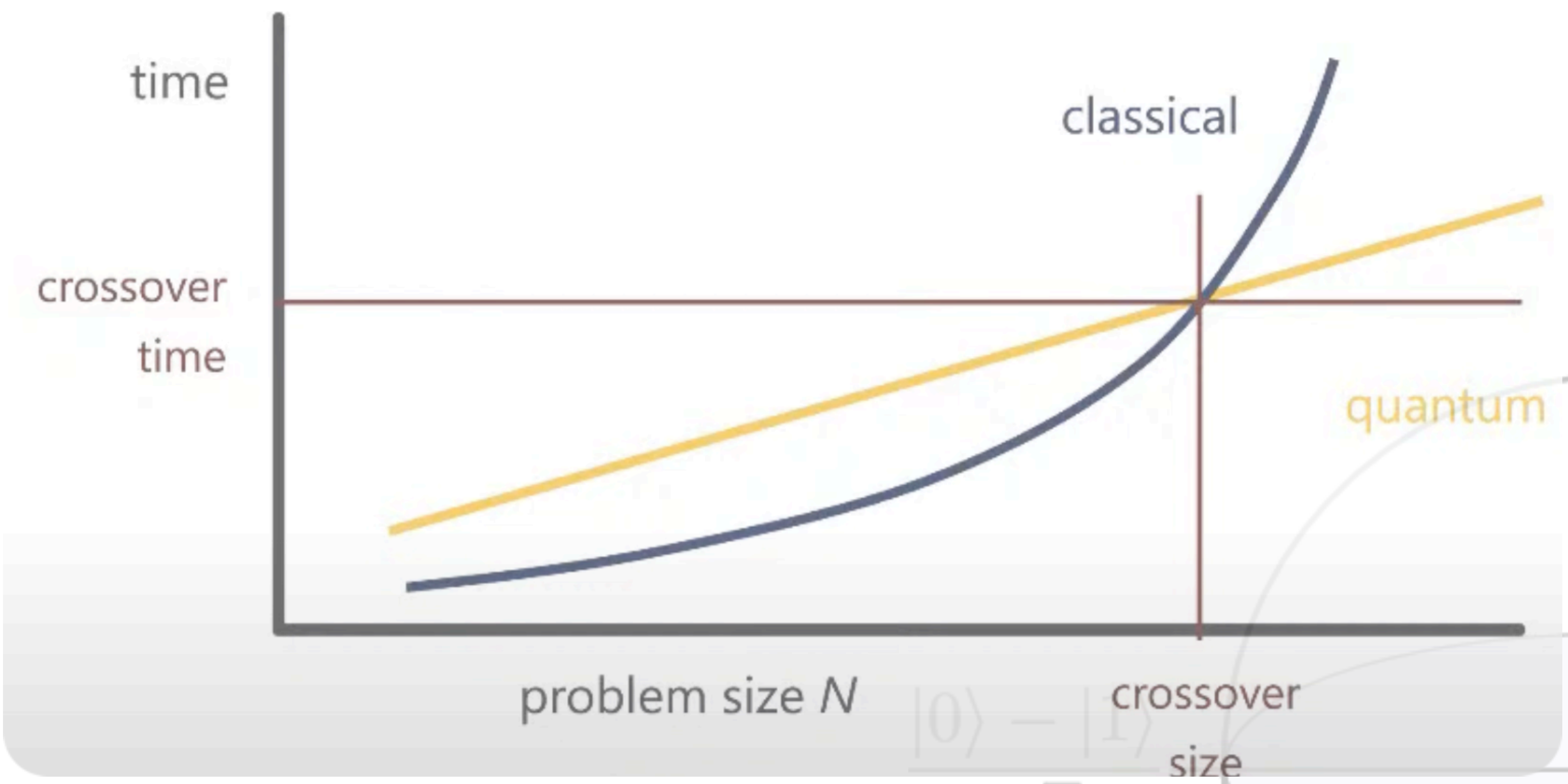
INTRODUCTION

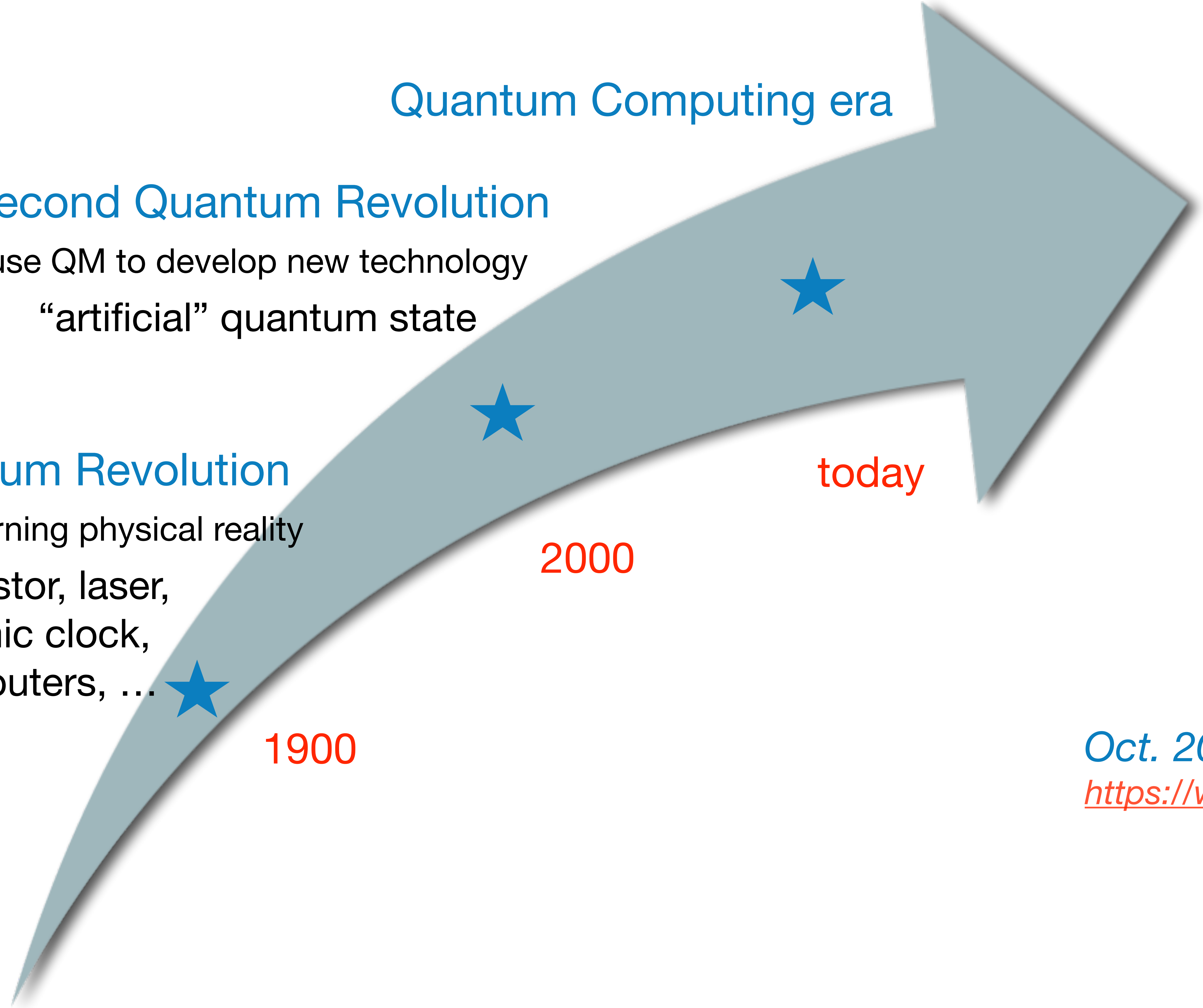
- quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences, with the potential for achieving a significant speed-up of numerical simulations



- high energy physics can both leverage and help realising this potential through a source of formidable challenging computational problems
  - Quantum Computing & Quantum Machine Learning
  - Example applications in HEP
  - The road ahead & summary

Recent reviews on QC in HEP:
- C.W. Bauer et al, Quantum Simulation for High-Energy Physics, PRX QUANTUM 4, 027001 (2023)
- A. Di Meglio et al, Quantum Computing for High-Energy Physics, Summary of the QC4HEP Working Group, arXiv:2307.03236 [quant-ph]
- QT4HEP 2022 - CERN, Nov 2022
- QTML 2023 - CERN, Nov 2023

QC (R)EVOLUTION AND EFFORT WORLDWIDE



Quantum Computing era

Second Quantum Revolution

use QM to develop new technology

"artificial" quantum state

First Quantum Revolution

QM: rules governing physical reality

transistor, laser, atomic clock, computers, …

1900

2000

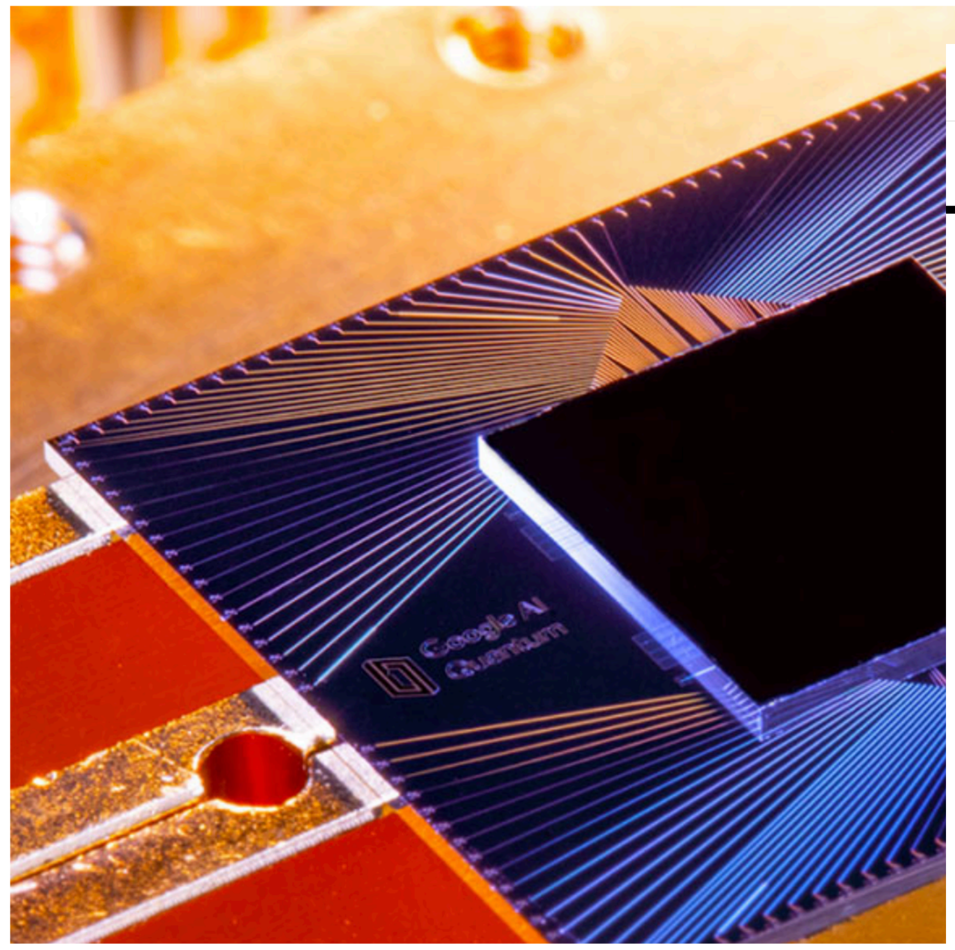
today

Dowling & Milburn, Quantum technology: the second quantum revolution. Phil, Trans. of the Royal Society of London. Series A 361.1809 (2003): 1655-1674

NEWS QUANTUM PHYSICS

Google officially lays claim to quantum supremacy

A quantum computer reportedly beat the most powerful supercomputers at one type of calculation



Oct. 2019: sciencenews.org

https://www.nature.com/articles/s41586

nature

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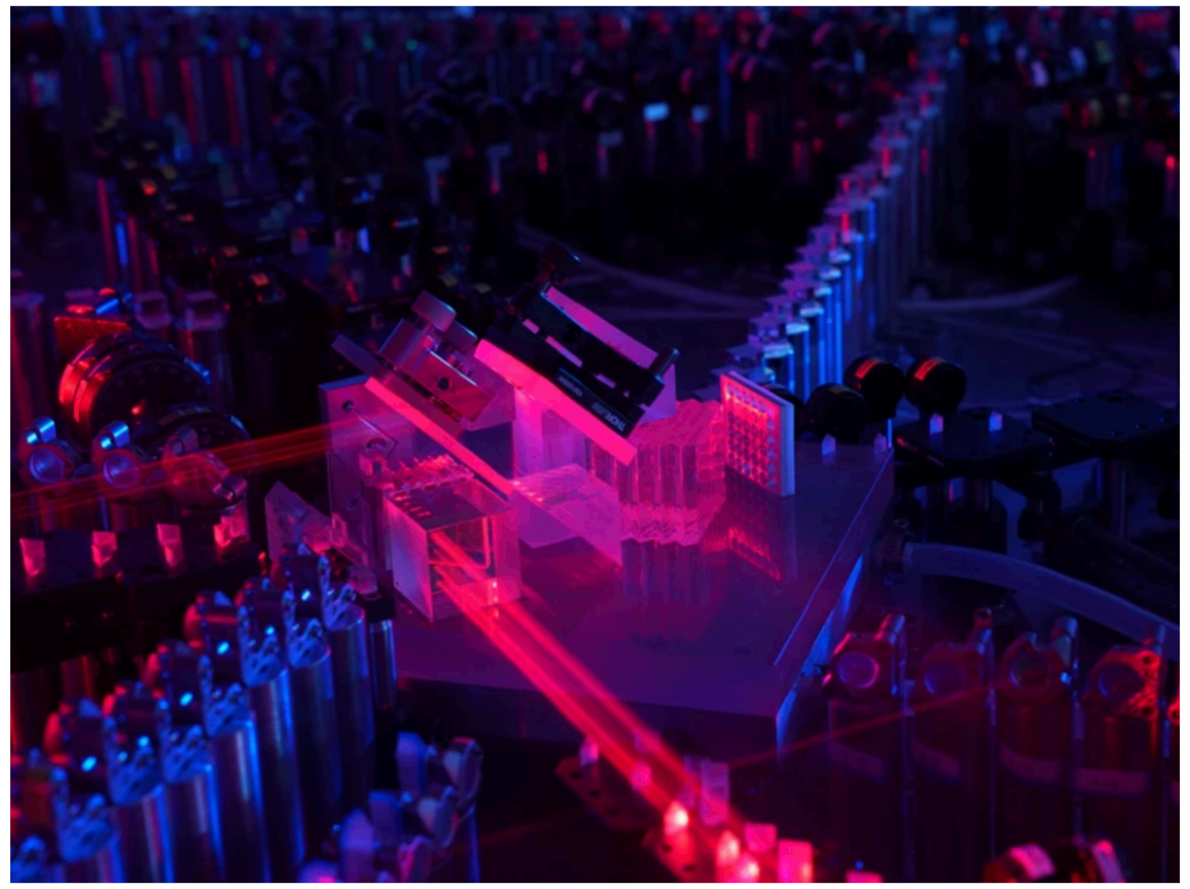
NEWS | 03 December 2020

Physicists in China challenge Google's 'quantum advantage'

Photon-based quantum computer does a calculation that ordinary computers might never be able to do.

Philip Ball



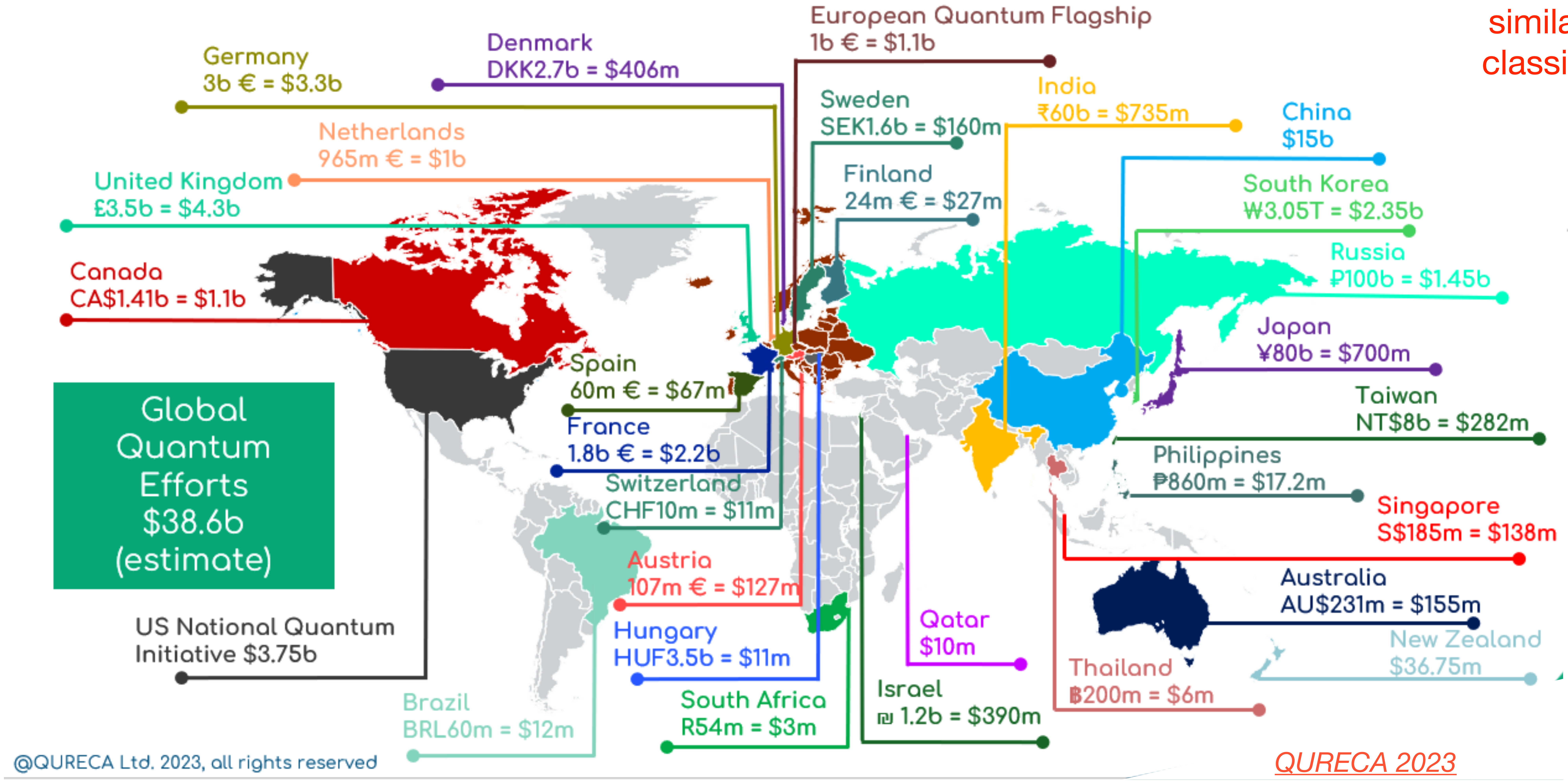
This photonic computer performed in 200 seconds a calculation that on an ordinary supercomputer would take 2.5 billion years to complete. Credit: Hansen Zhong

Dec. 2020:

https://www.nature.com/articles/d41586-020-03434-7

QC (R)EVOLUTION AND EFFORT WORLDWIDE

quantum initiatives ongoing today in >29 countries
global Q-Tec market projected to reach $106b by 2040

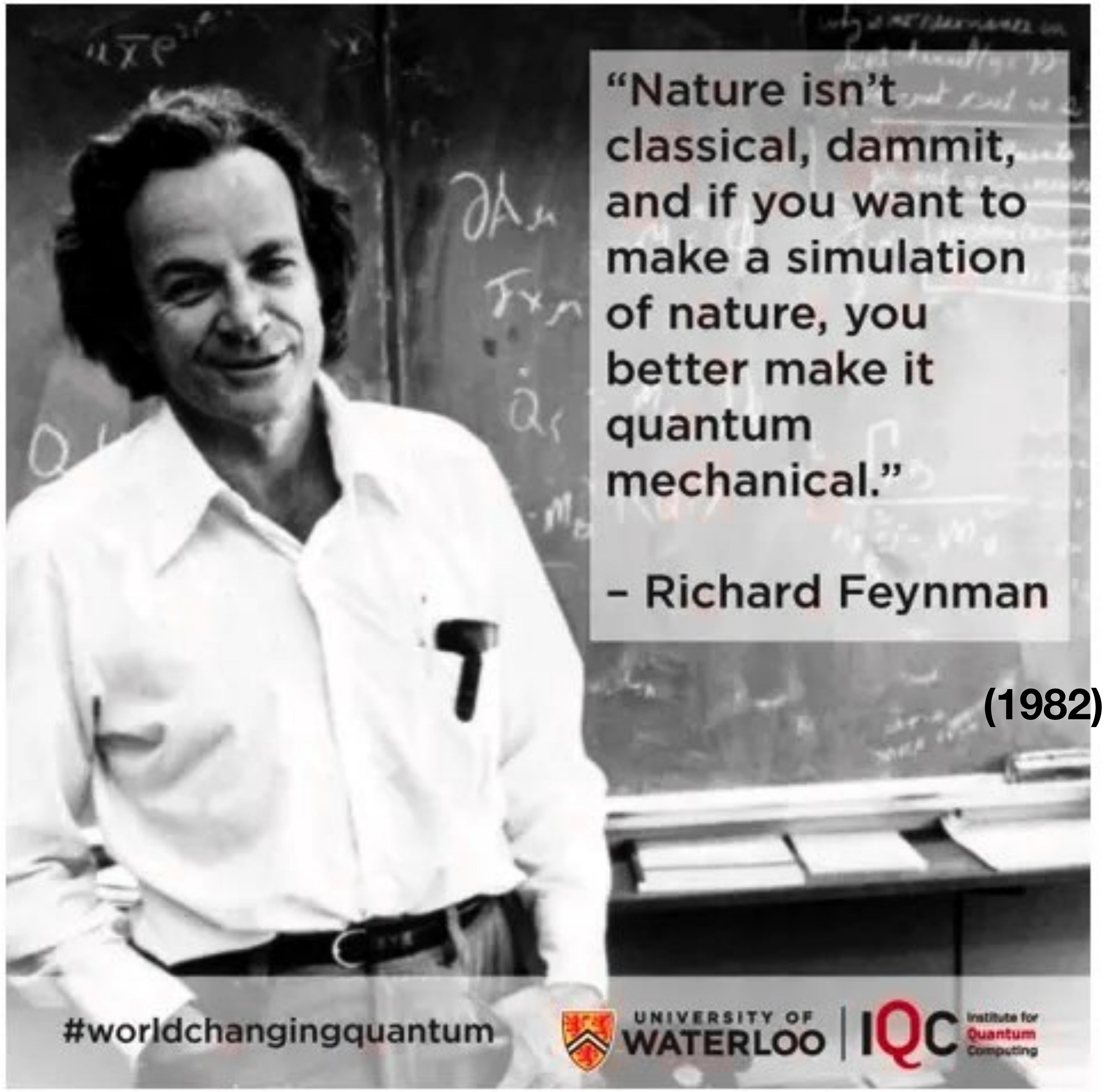


but:

for practical applications, quantum computing today is at a similar stage of development as classical computers in the '50 …

QURECA 2023

WHY QUANTUM COMPUTING IN HEP?



(1982)

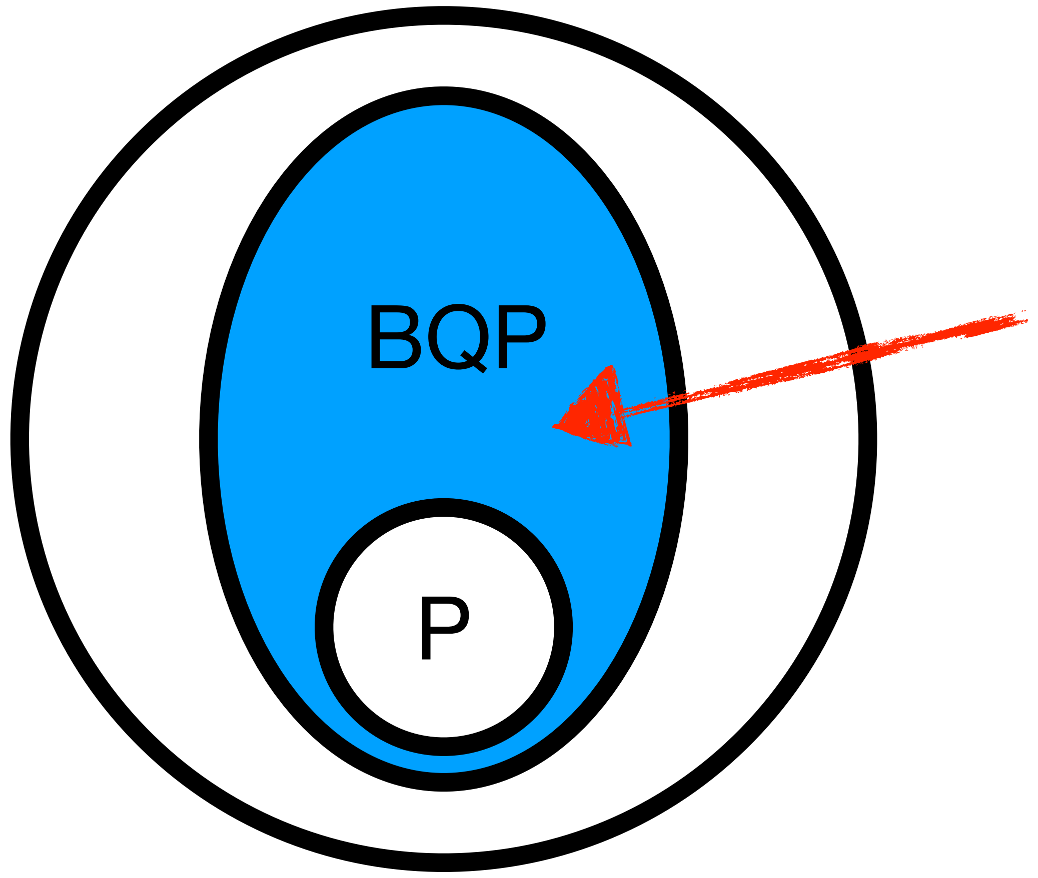
Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

HEP is inherently quantum mechanical, thus simulating and analysing hep data with quantum computers seems a very good idea

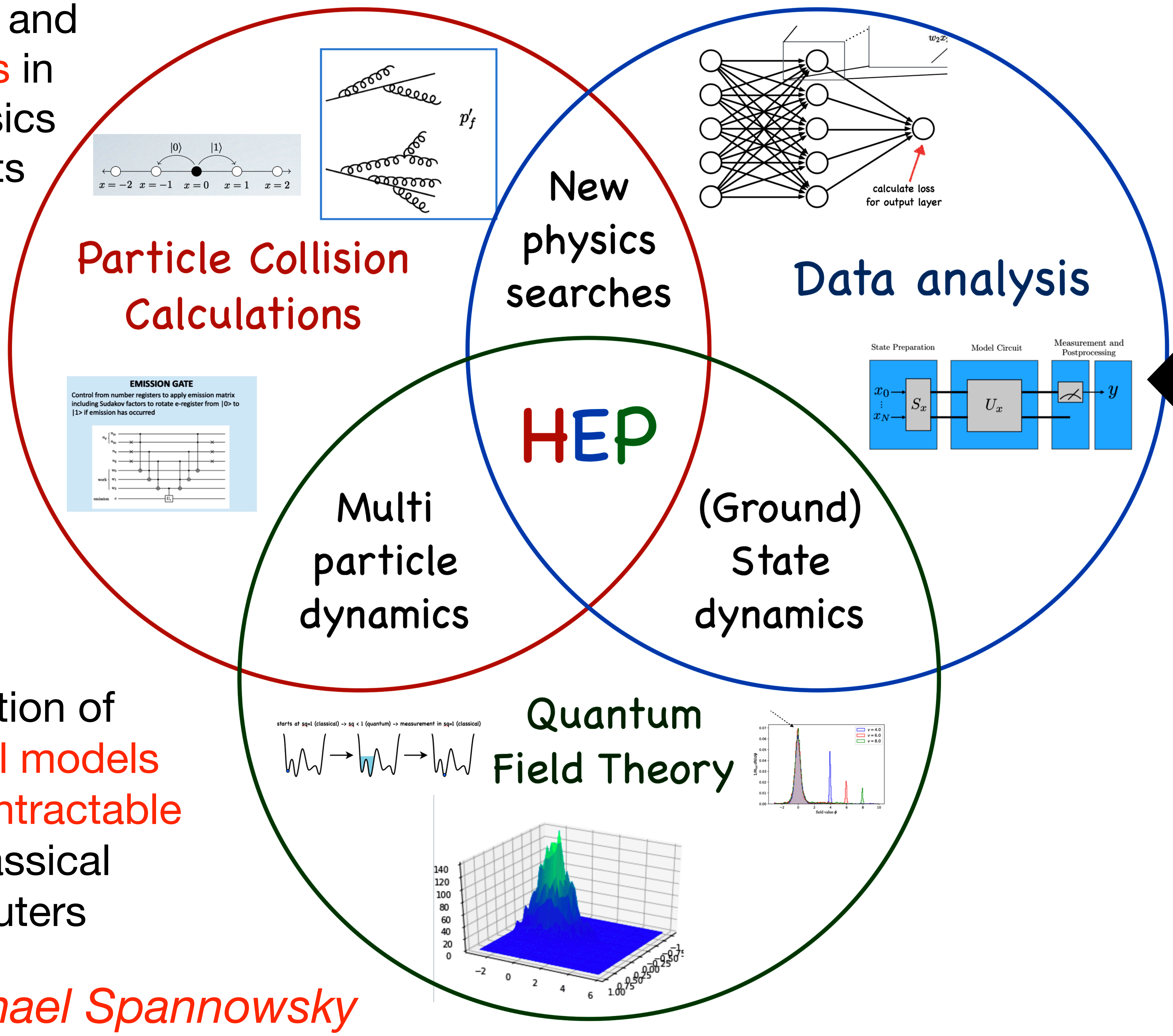


many
HEP problems
live here

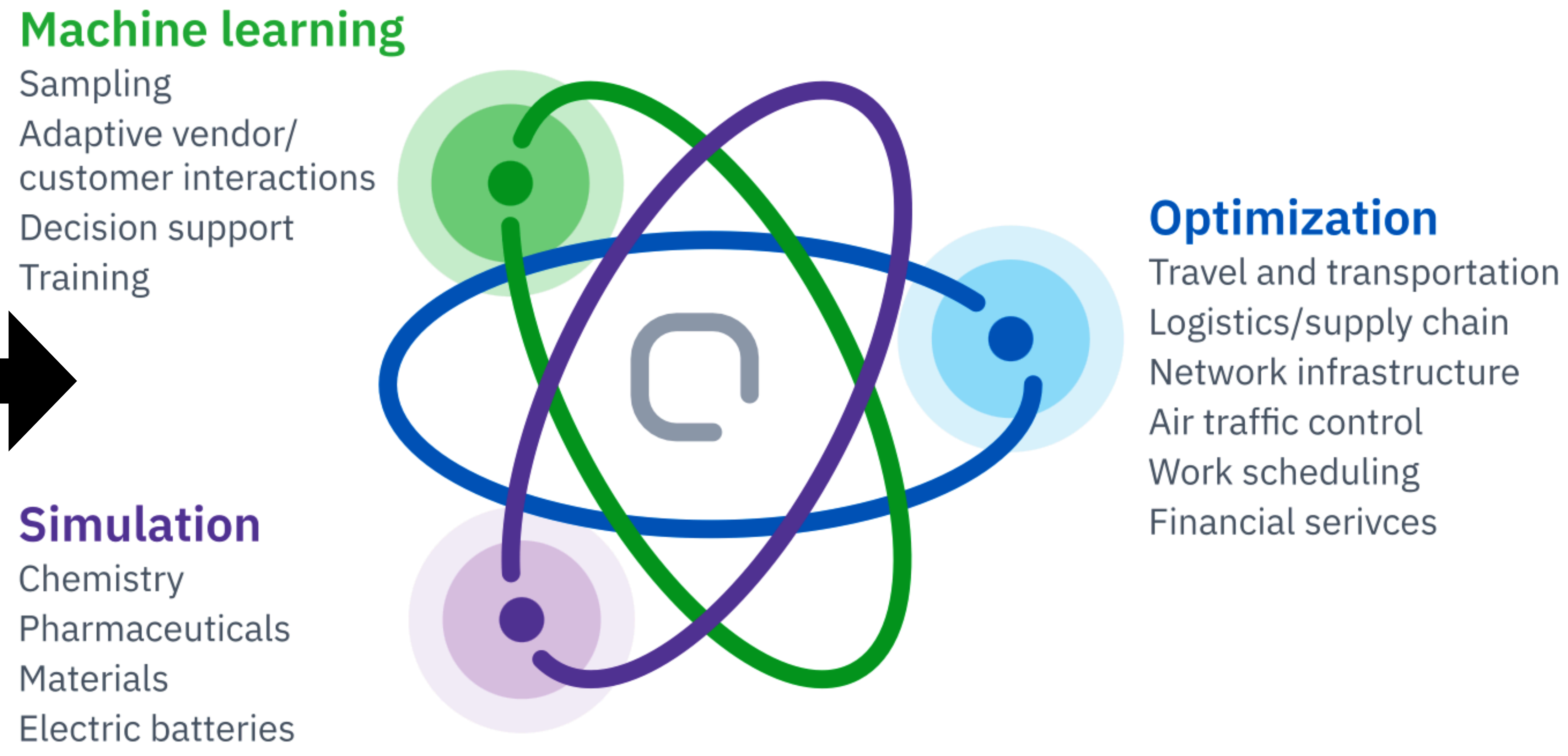
HIGH ENERGY PHYSICS AND QC

three major application areas in HEP
that may benefit from QC

simulation of particle collisions and and data analysis in particle physics experiments



exploration of theoretical models which are intractable with classical computers



QC use-cases in 2023 for IBM

credit: Michael Spannowsky

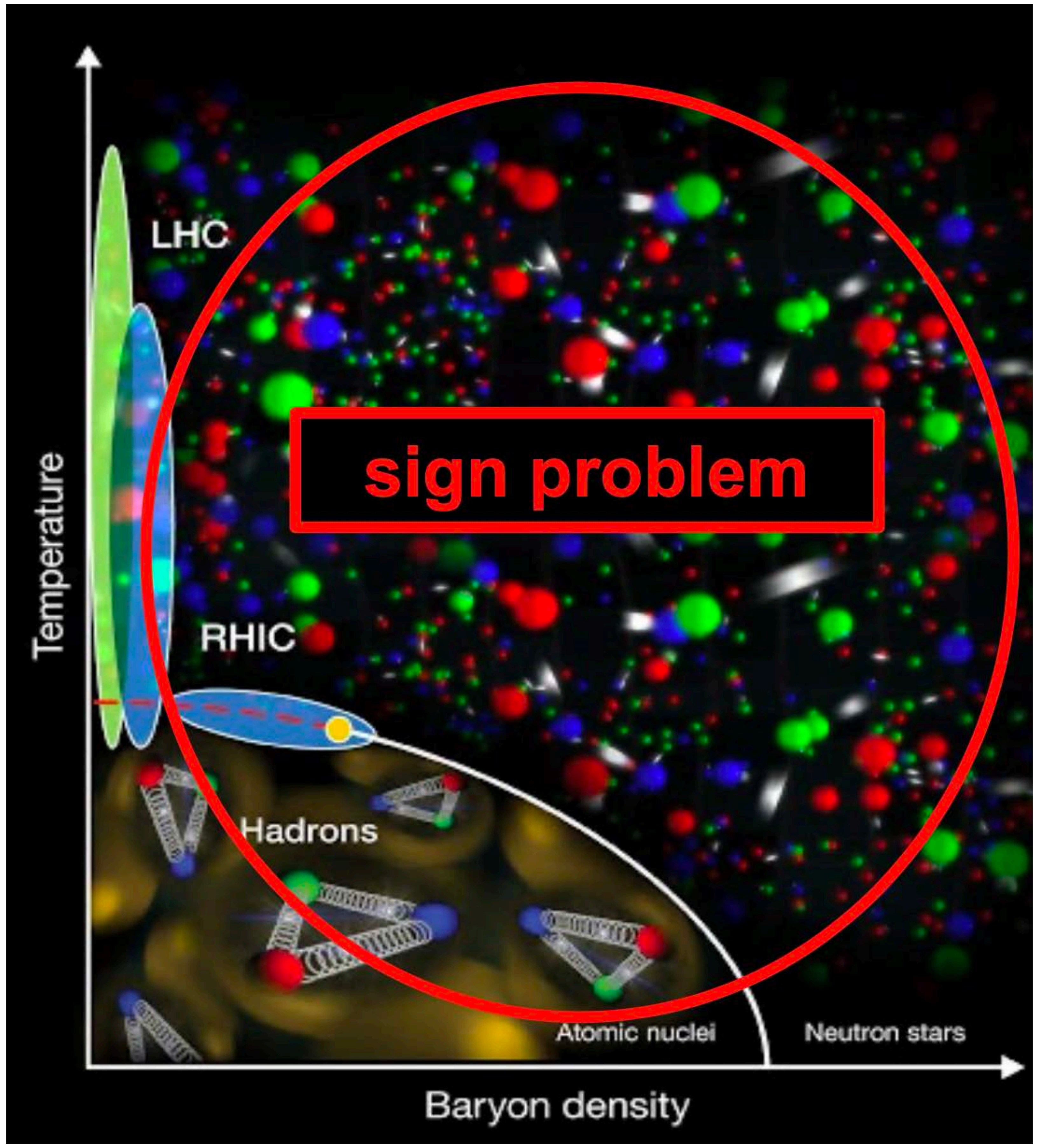
EXPERIMENTAL DATA CHALLENGE AT HL-LHC

example ATLAS:

CPU consumption x5÷10 wrt today

Data volume ~1.5-2.5 EttaByte by the end of Run-4 in 2033

AND THEORY CHALLENGES …



credit: Michael Spannowsky

despite the great success of classical lattice field theory simulations out-of-equilibrium and real-time dynamics (e.g., of particle collisions, thermalization phenomena, etc), remain out of reach for euclidean path-integral Monte Carlo simulations

rooted in the notorious sign-problem: highly oscillatory behaviour of the path integrals arising in real-time phenomena, implies an exponentially growing sampling run-time complexity with an increasing number of lattice sites

to circumvent the problem:

- describe lattice fields theories in the equivalent Hamiltonian formalism
- leverage exponential representation advantage of QC to cope with the memory scaling required to store the full wave function on the lattice

several examples in recent literature:

- Araz, Ahenk, Spannowsky: arXiv:2210.03679 (sigma model)
- Lewis, Woloshyn: arXiv:1905.09789 (U(1))
- Kico, Stryker, Savage: arXiv:1908.06935 (SU(2) (1d))
- Haase et al: arXiv:2006.14160 (lattice gauge theory)
- Fromm, Philipsen, Spannowsky, Winterowd: arXiv:2306.06057 (Z2 lattice gauge theory)

EXAMPLE OF APPLICATION: SIMULATING COLLIDER PHYSICS ON QC USING EFT

- Simulating the full dynamics of a quantum field theory over a wide range of energies requires exceptionally large quantum computing resources not available in today's quantum computers
- idea: to cope with this limitation, use QC only for the low energy (non-perturbative) dynamics, leveraging EFT to separate short and long distance physics from one another

example: Soft-Collinear EFT (SCET) provides a method to determine the dynamical properties in scattering process

$$d\sigma = H \otimes \underbrace{J_1 \otimes \ldots \otimes J_n}_{} \otimes S$$

credit: C.W. Bauer

hard object describe short distance scattering

jets functions objects: describe how single energetic particles sprays

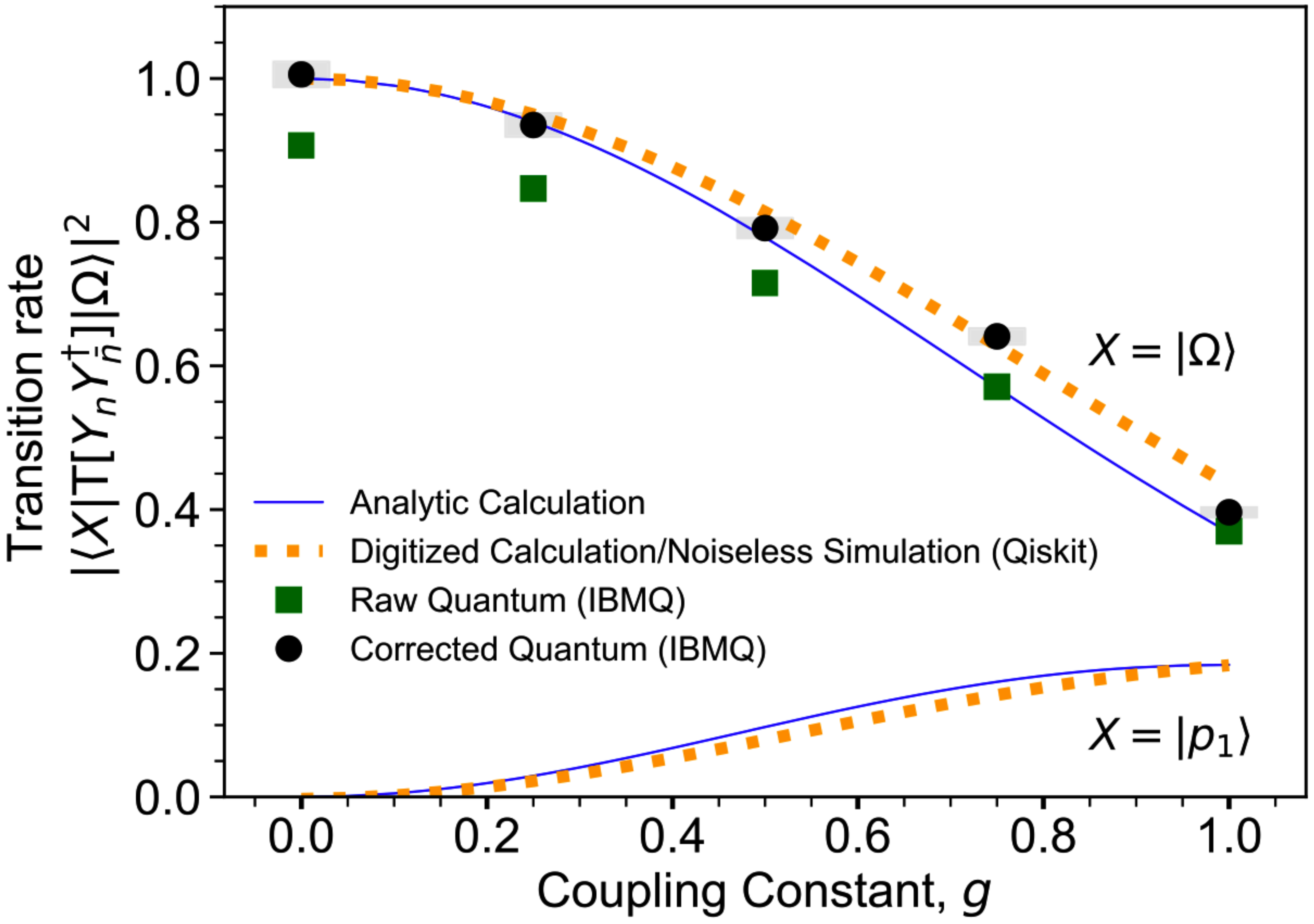
Soft function object: describe how jets interact one with the other (non-perturbative object, no known way to compute it)

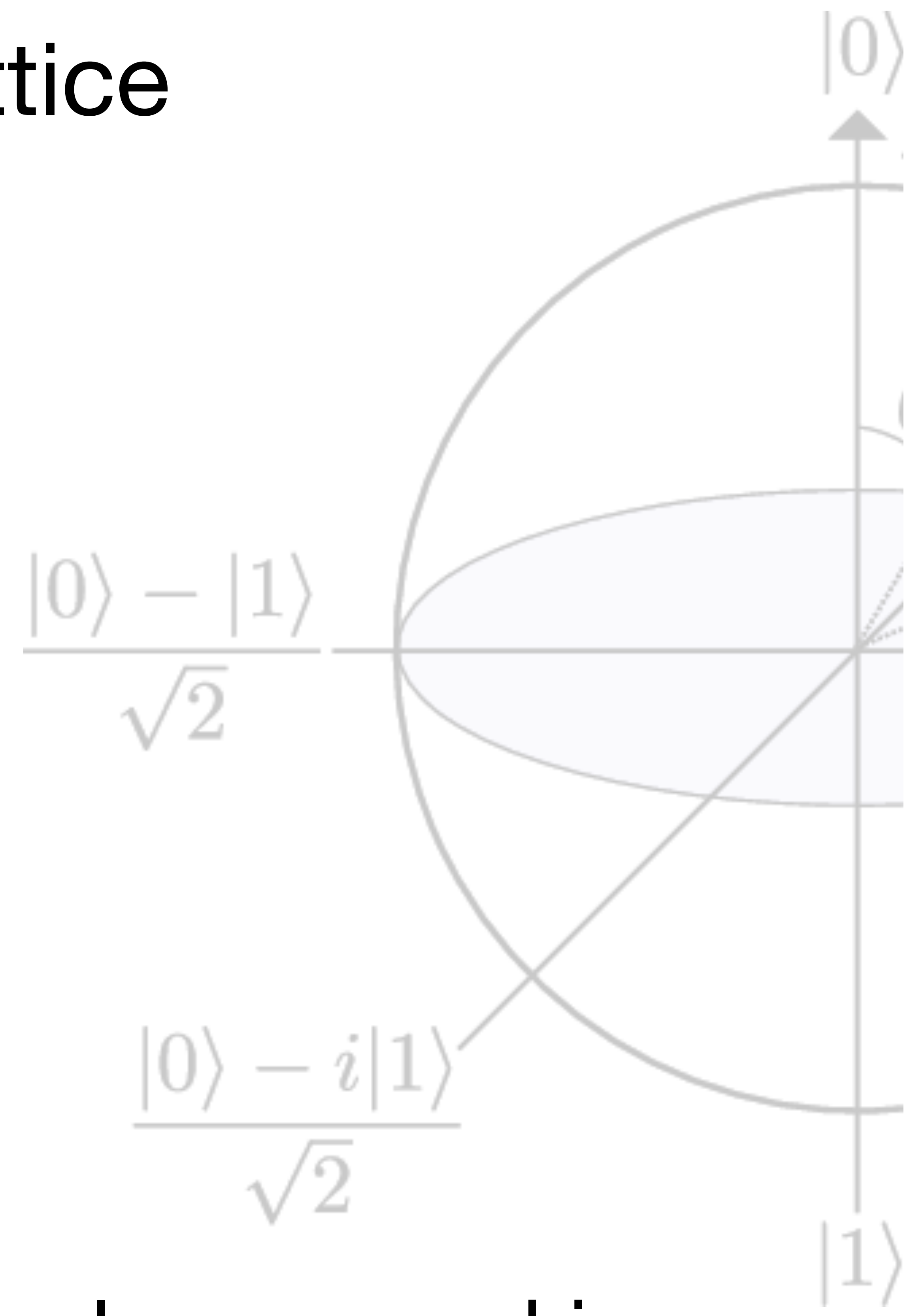
we can use quantum computers to perform first principle calculation of soft functions …

C.W.Bauer, B.Nachman, M.Freytsis, PRL 127, 212001 (2021)

EXAMPLE OF APPLICATION: SIMULATING COLLIDER PHYSICS ON QC USING EFT

- proof of principle: very simple 1D scalar field theory with 3 site lattice





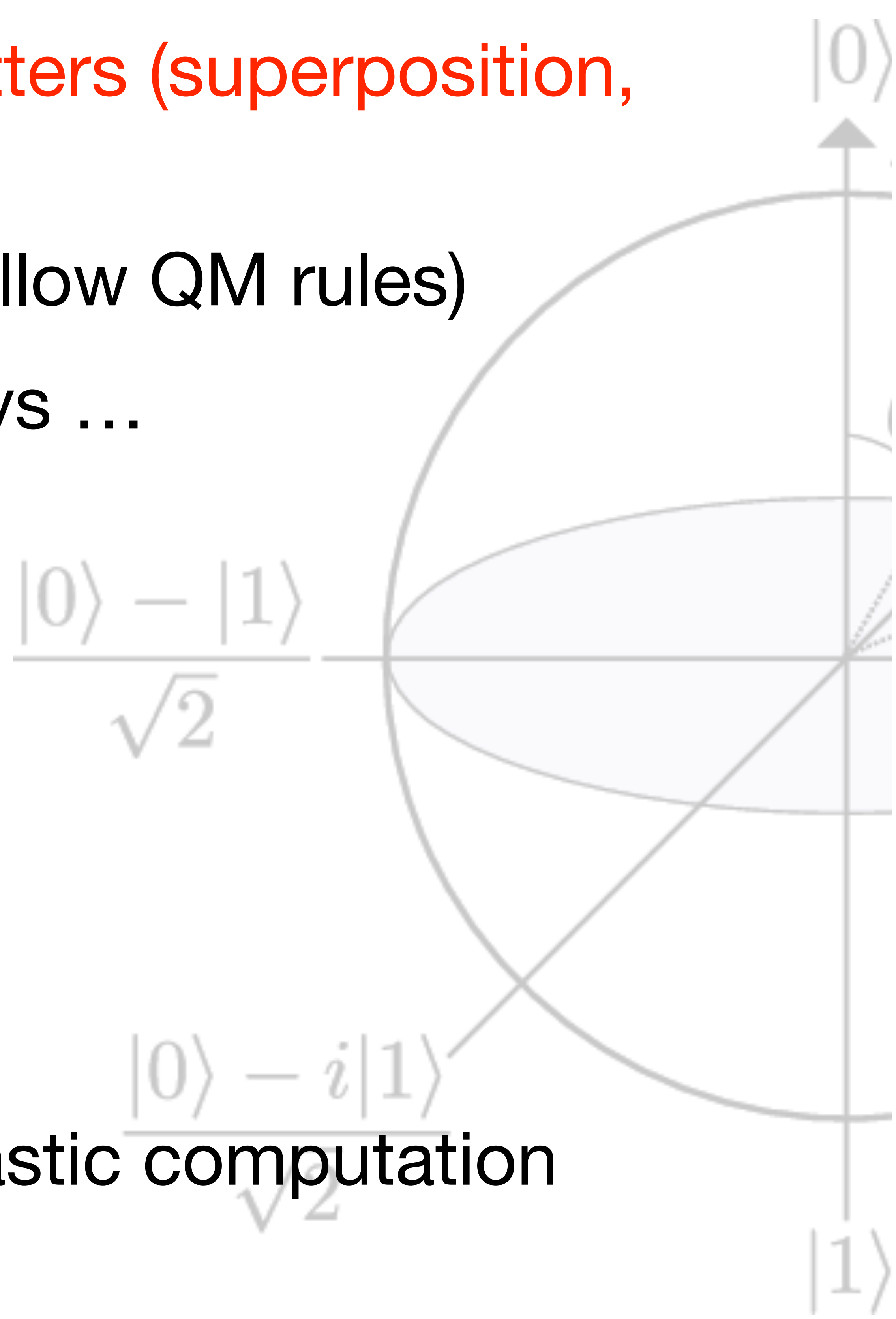
people now working on realistic use-cases (gauge theories & non-abelian GT)

C.W.Bauer, B.Nachman, M.Freytsis, PRL 127, 212001 (2021)

QUANTUM COMPUTING

- QC is a computing paradigm that explicitly leverage quantum mechanical properties of matters (superposition, interference and entanglement) to perform calculations
  - in contraposition to CC where QM enters only indirectly (eg. semiconductors in CPUs follow QM rules)
  - QC are not “faster” computers wrt CC, but systems that do computation in different ways …

- Principles of quantum mechanics that may enhance/affect computations:
  - **Superposition** leads to parallelism → exponential speed up
  - **Entanglement** → non linear correlations
  - **Quantum operations** (gates) are unitary transformations → reversible computing
  - Output is the result of a **quantum state measurement** according to Born rule → stochastic computation
  - **No-cloning** theorem → information security
  - **Quantum state coherence and isolation** → computation stability and errors
  - **Qubit state collapse** → reproducibility



ELEMENTS OF A QUANTUM CIRCUIT MODEL OF COMPUTATION

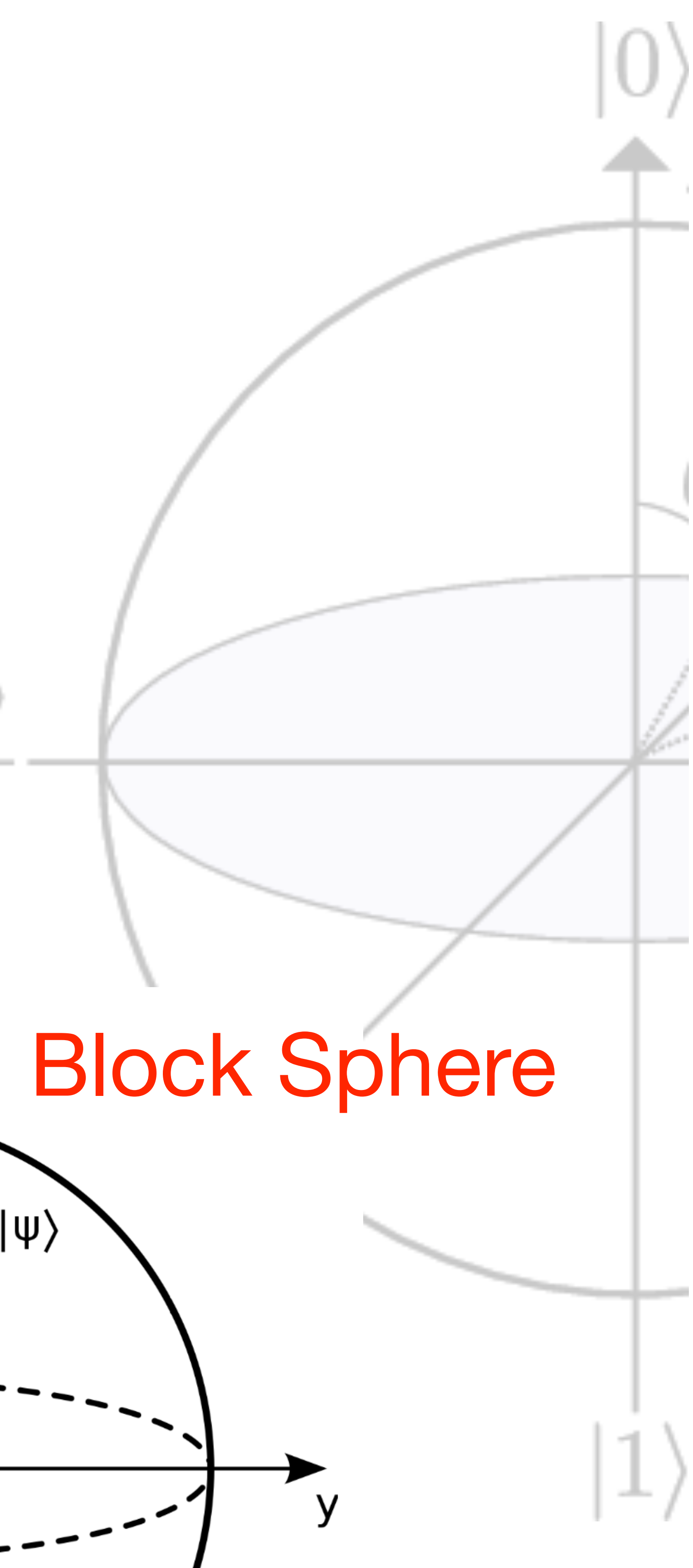
- in a general way any computation (classical or quantum) is based on three fundamental elements:

input data → operations on data → output results

- in a quantum circuit these elements are described by:
  - **qubits** (quantum bits): basic unit of quantum information
    - similar role as a bits in terms of storing information, but behave differently tanks to the quantum properties
  - **quantum logic gates**: operators that transform quantum data
    - the building blocks of QC, like classical logic gates for classical computers
  - **quantum measurement**: the operation that allows to access classically the resulting quantum state
    - reading out information from a quantum system generally change the state and destroy the computation that we are performing
    - impossible to predict the exact outcome of a quantum measurement, due to the probabilistic nature of QM all we can predict are only likelihood

QUBIT: QUANTUM BIT

- basic unit of quantum computation representation
  - **classical bit**: binary (“0 or 1”)
  - a generic quantum state (**qubit**) $|\psi\rangle$ can be written in a superposition of a Hilbert space basis: can “take” infinitely many different values, it is continuous (but when we read it we always find 0 or 1)



classical bit

○ 0

○ 1

computational basis typically used as canonical basis:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = a_0 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + a_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} = a_0|0\rangle + a_1|1\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

\

qubit

Block Sphere

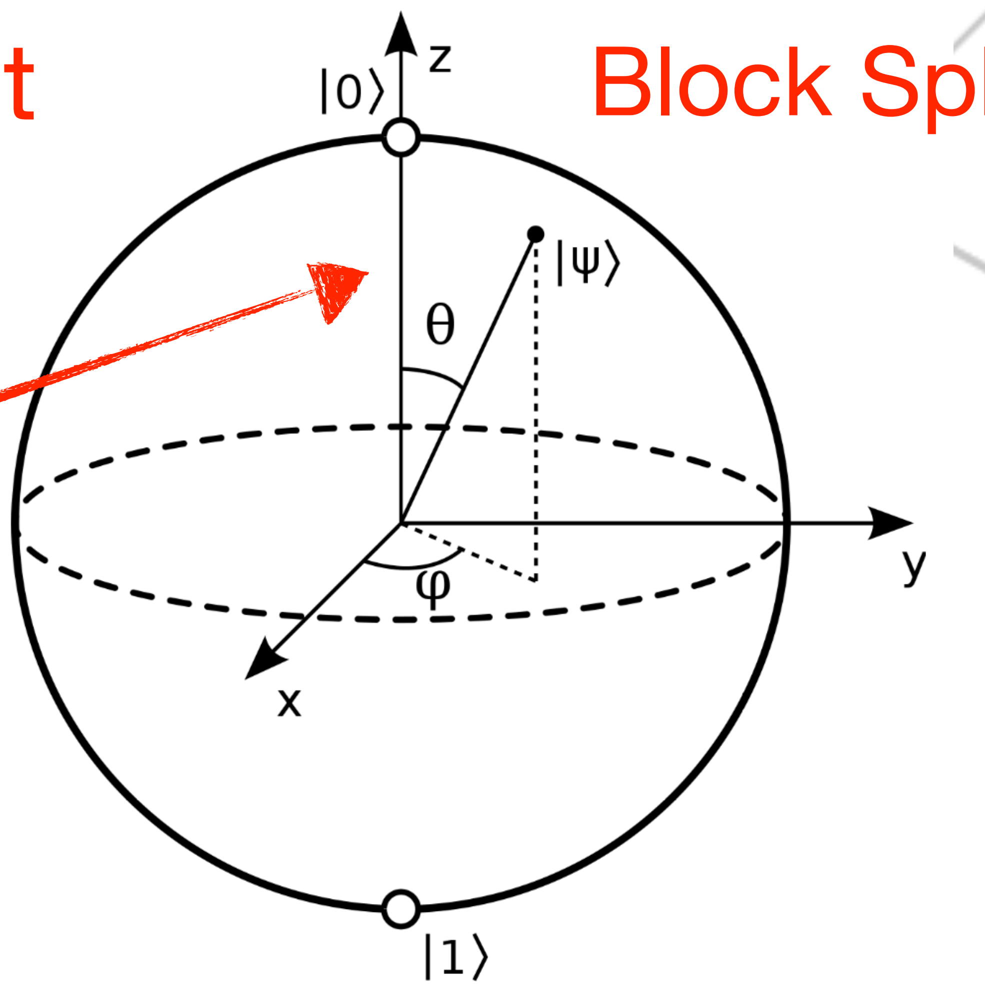
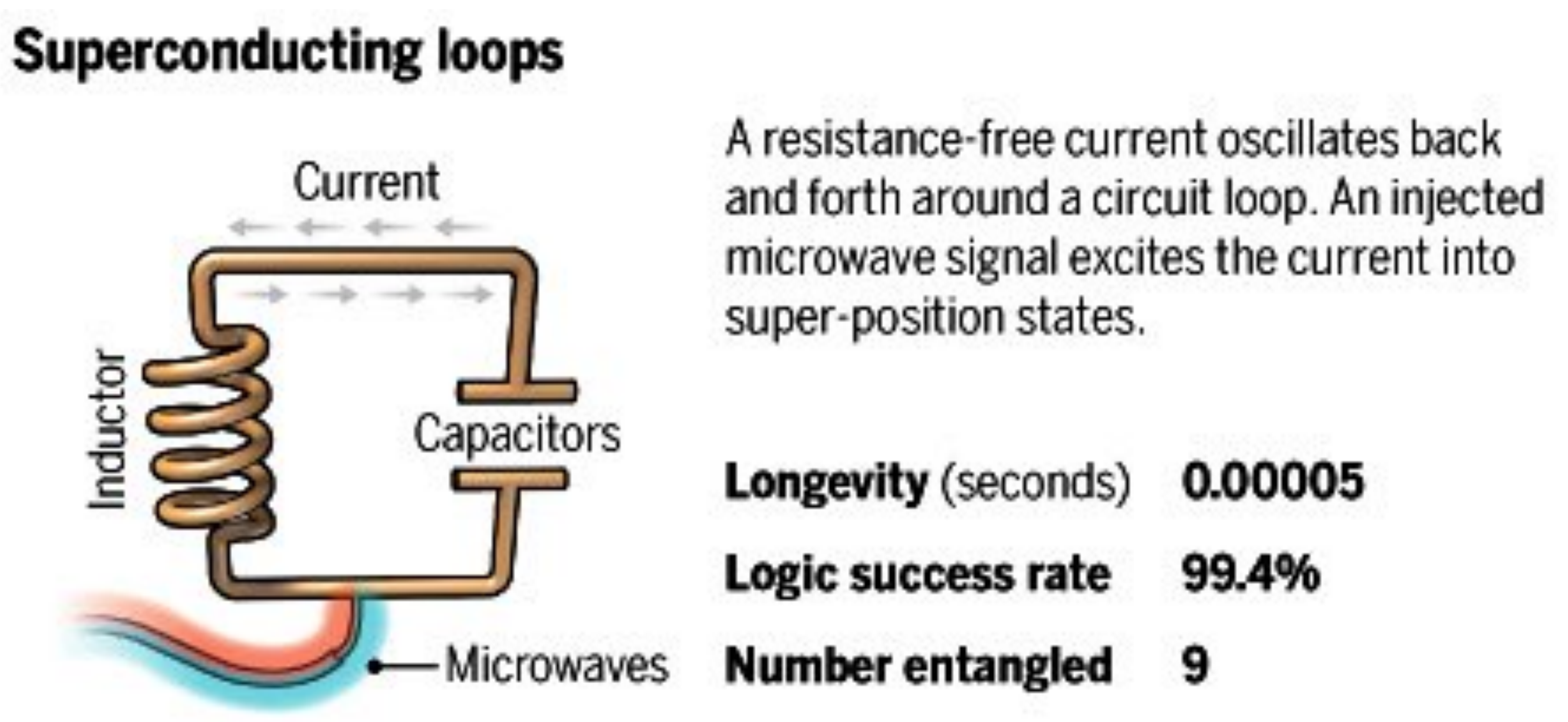


Image credits: wikipedia.org

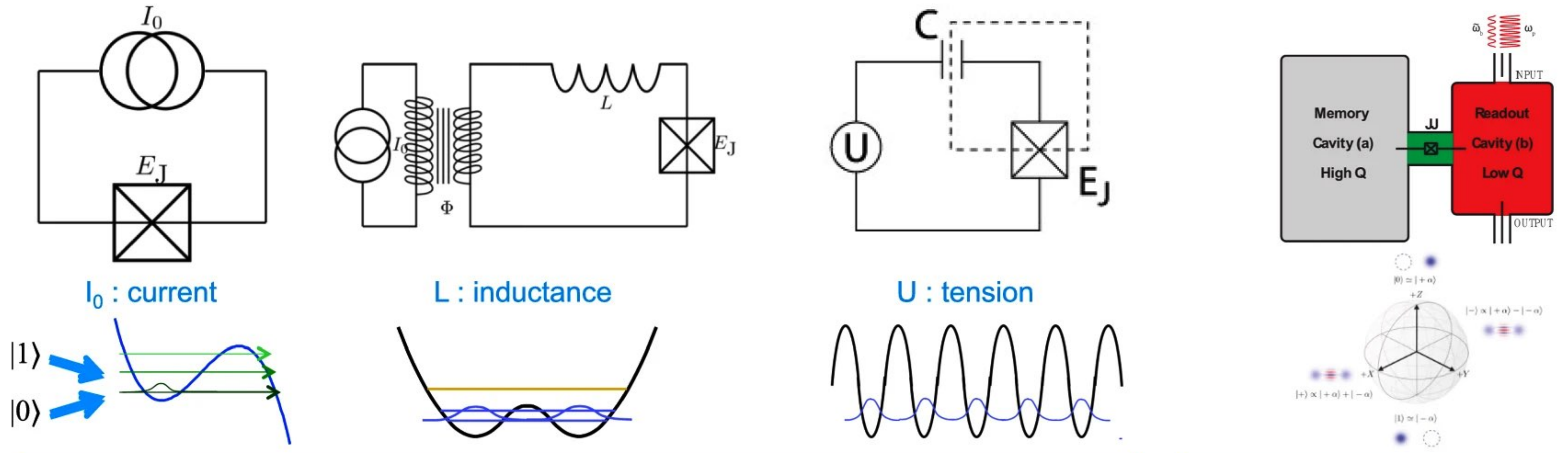
Extending this to a system of n qubits forms a 2^n-dimensional Hilbert Space

TECHNOLOGIES FOR QUANTUM COMPUTERS

- not yet a standard way to implement qubits, unlike for classical bits encoded in transistors
  - physically, qubits can be any two-level systems: the spin of an electron, the polarization of a proton, …
  - current leading technology in the quantum computing commercial space: superconducting qubits



phase qubit | flux qubit | charge qubit - transmon | cat-qubits



	phase qubit	flux qubit	charge qubit - transmon	cat-qubits
	Josephson junctions handle the qubit degree of liberty			Josephson junctions prepare, couple and correct the cat-qubits
|0⟩ and |1⟩ qubits	two energy levels in a potential well	two superconducting current directions	two levels of charge of Cooper pairs	pairs of entangled microwave photons in a cavity
quantum gates	micro-waves	magnetic field	micro-waves	micro-waves
qubits readout	resonator and micro-waves	magnetometer (SQUID)	resonator and micro-waves	resonator and micro-waves
commercial vendors	abandonned	D-Wave The Quantum Computing Company, rigetti, QILIMANJARO Quantum Tech, Alibaba, bleximo, Atlantic Quantum	IBM, Google, IQM, OQC	ALICE & BOB, qci, amazon

⊕ **Pros** — fast operation (ns), built on existing semiconductor industry

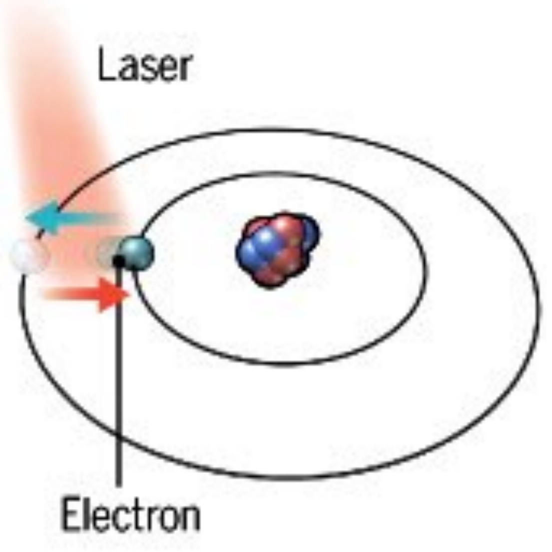
⊖ **Cons** — quickly experience decoherence so requires error correction, have to be kept cold (T<100 mK), only 2D topology (swaps)

O.Ezratty, Eur. Phys. J. A 59, 94 (2023)

TECHNOLOGIES FOR QUANTUM COMPUTERS

- multiple other technologies used to implement current quantum processing units

Trapped ions or neutral atoms arrays

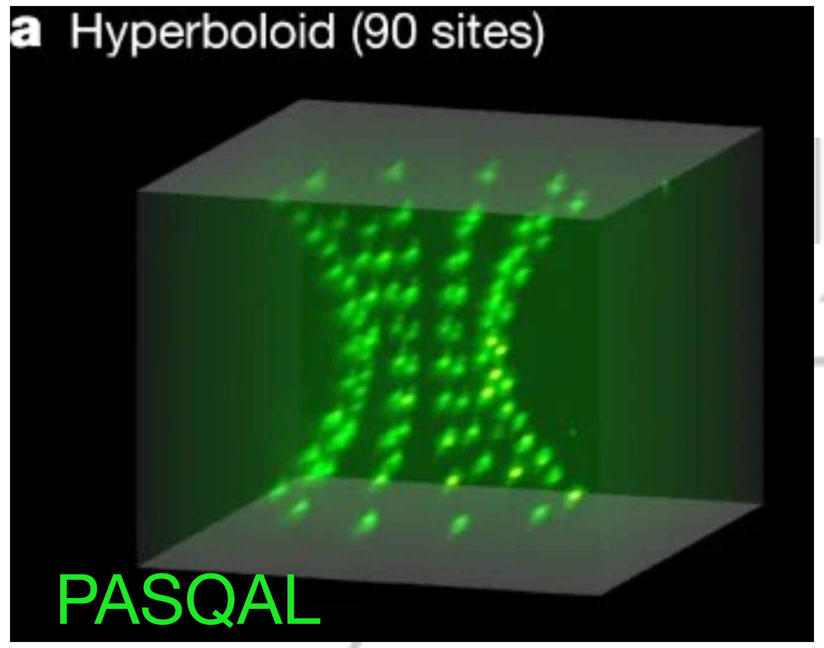


use the energy levels of electrons in neutral atoms or ions as qubits. In their natural state, these electrons occupy the lowest possible energy levels. Using lasers, we can “excite” them to a higher energy level. We can assign the qubit values based on their energy status

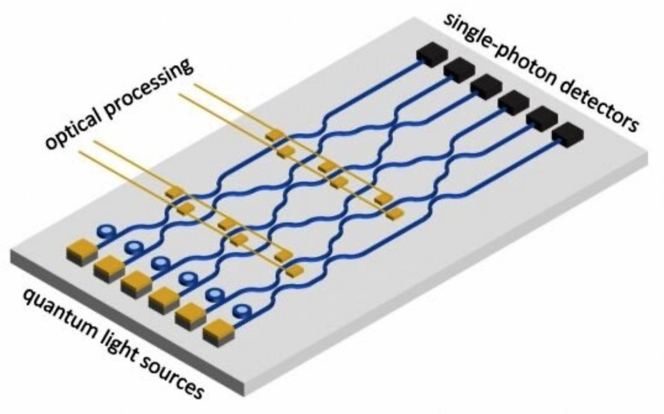
Company support
IonQ, PASQUAL, AQT, Atom Computing, …

⊕ **Pros** very stable, longer decoherence time, high gate fidelity, 2D and 3D, many qbits

⊖ **Cons** slow operations, hard to program, many and sophisticated laser technology needed



Linear / non-linear optical QC

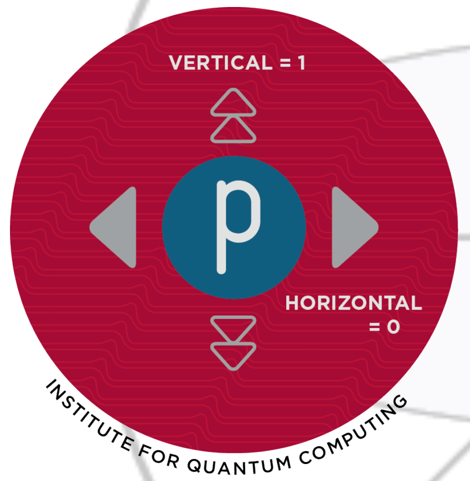


use particles of light to carry and process information. Qubits realised by processing states of different modes of light through both linear (mirrors, beam splitters, phase splitters, …) and nonlinear element (quantum microprocessor based on laser photonics at room temperature)

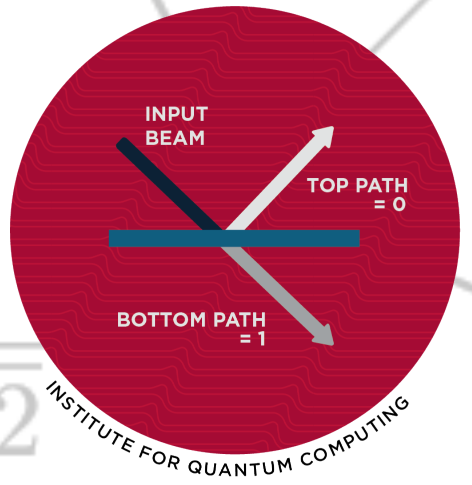
Company support
Xanadu, PsiQuantum, …

⊕ **Pros** can operate at room temperature, photons much less sensitive to the environment, longer decoherence time

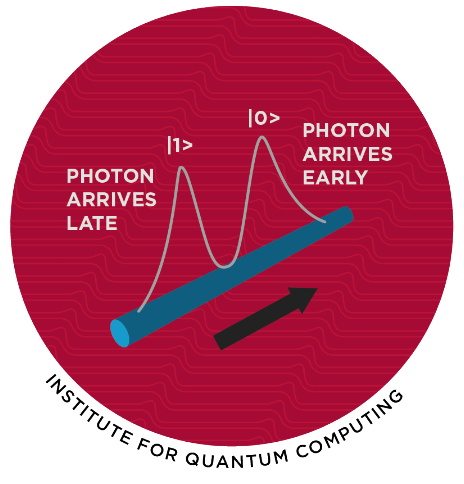
⊖ **Cons** emerging technology, difficult to construct large numbers of gates and connect them in a reliable fashion to perform complex calculation, photons cannot be stored



POLARIZATION QUBIT



PATH QUBIT



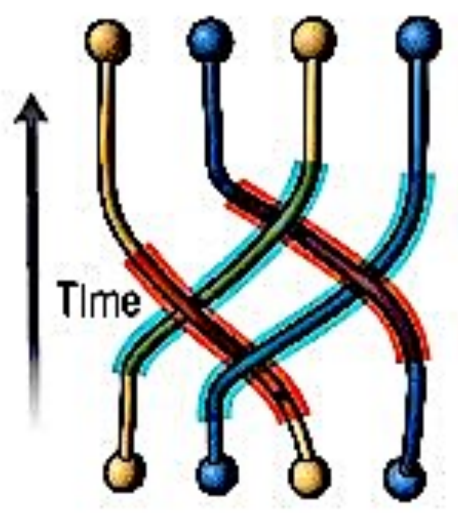
TIME QUBIT

Silicon quantum dots

These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.

Company support
Intel, SQC, HRL, …

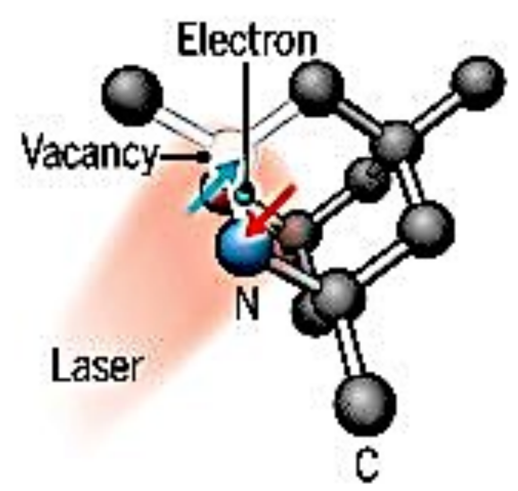
Topological qubits



Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures. Their braided paths can encode quantum information.

Company support
Microsoft

Diamond vacancies



A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.

Company support
Quantum Diamond Technologies

images/text adapted from: C. Bickle/G. Popkin

EXAMPLES OF QUANTUM COMPUTERS

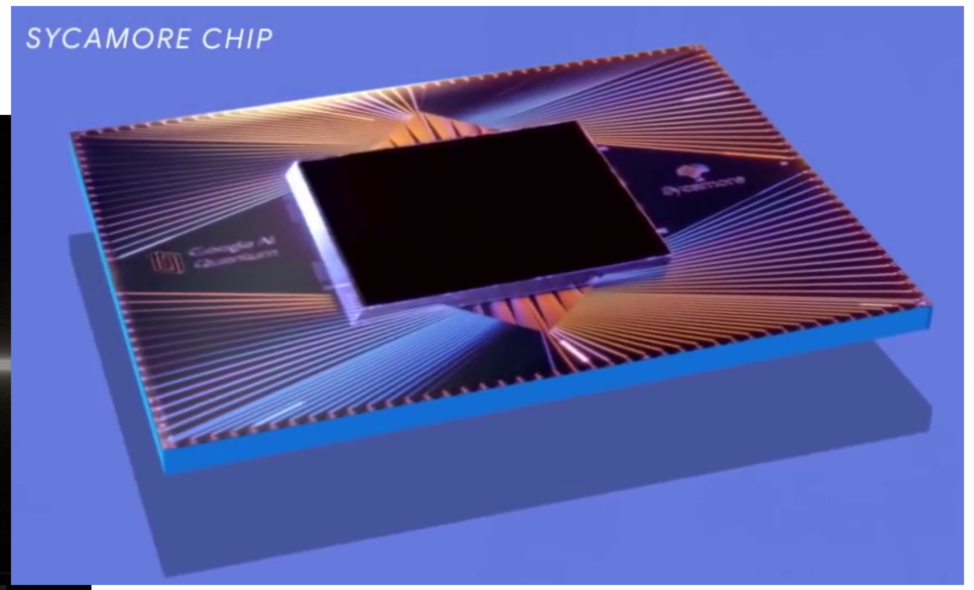
IBM Q

433 qubits today
1000+ near-term

actual quantum processor is just O(2x2 cm^2)
needs cooling&protection from environment to
preserve the quantum capabilities

source: IBM

Google
54 qubits



PASQAL
300+ qubits today
~1000 near-term

DWAVE
5000+ qubits today
(quantum annealers)

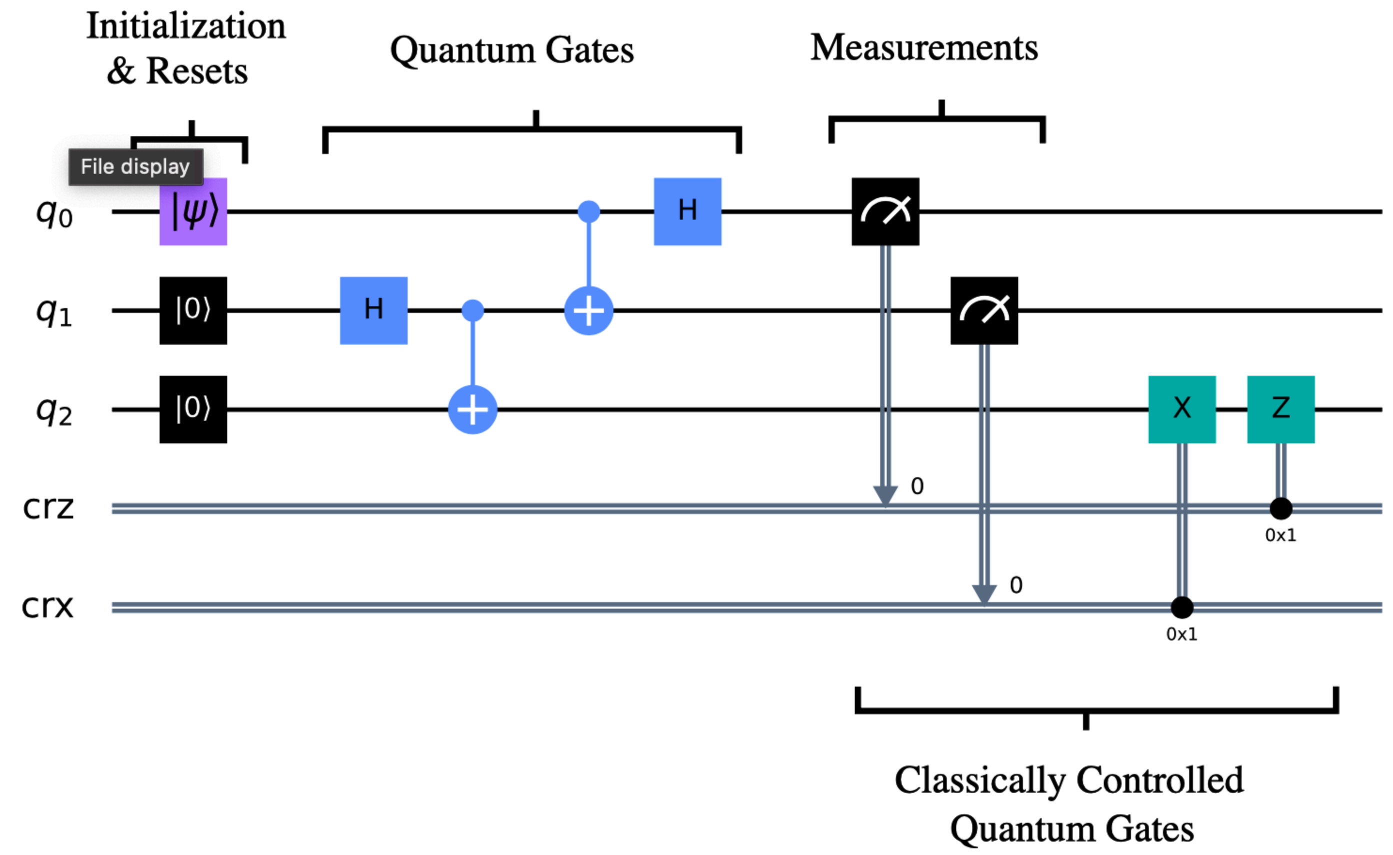
IONQ
35 qubits today
60+ near-future

OPERATIONS OVER QUBITS: QUANTUM GATES&CIRCUITS

- quantum computation proceeds by applying physical operations on the quantum state of qubit inducing a change in the state, in a similar way as we operate on classical bits through logical operations
- a state-changing operator is called a quantum gate, and it is represented by a complex unitary matrix, eg length-preserving, linear transformation matrix, which represent a rotation on the Bloch sphere:

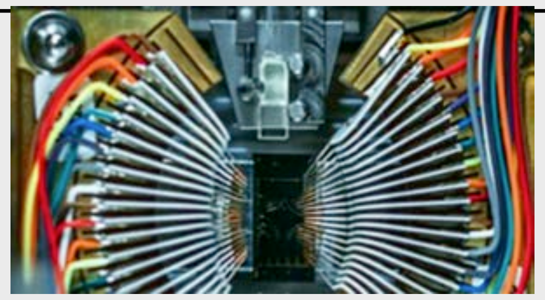
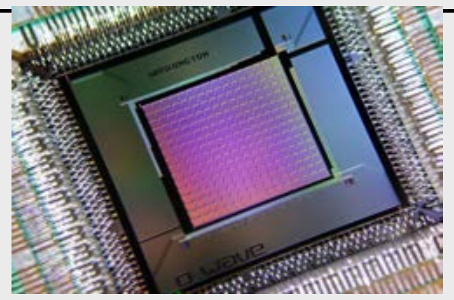
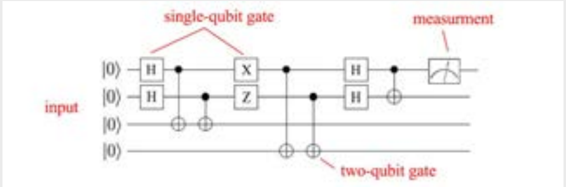
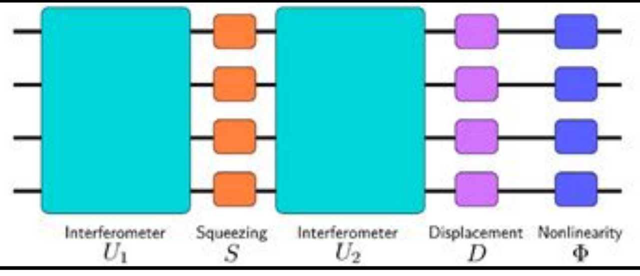
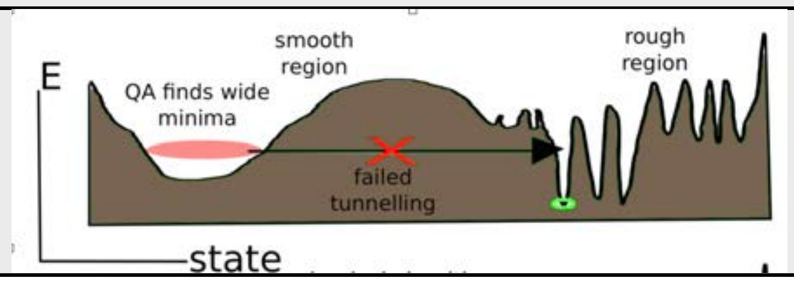
$$|\psi'\rangle = U|\psi\rangle \quad \text{with } U \text{ unitary matrix:} \quad U : U^{\dagger}U = I$$

- quantum circuit = a collection of quantum gates that operates on qubits
- quantum software is programmed by building these circuits
- NOTE: when ported to the real quantum hardware they can look very different from the initial design (circuit adaptation to the quantum hw: transpiling)



Operator	Gate(s)	Matrix
Pauli-X (X) (NOT gate)	X, ⊕	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix}1 & 0\\0 & e^{i\pi/4}\end{bmatrix}$
Controlled Not (CNOT, CX)	●–⊕	$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix}$
Controlled Z (CZ)	●–Z, ●–●	$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & -1\end{bmatrix}$
SWAP	×–×	$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\end{bmatrix}$
Identity/idle	I	$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$

QC PARADIGMS

<table>
<tr><th>Type</th><th>Discrete Gate
(DG)</th><th>Continuous Variable
(CV)</th><th>Quantum Annealer
(QA)</th></tr>
<tr><td>Computing</td><td>Digital</td><td>Digital/Analog</td><td>Analog</td></tr>
<tr><td>Property</td><td>Universal (any quantum algorithm can be expressed)</td><td>Universal
-
GBS non-Universal</td><td>Not universal — certain quantum systems</td></tr>
<tr><td>Advantage</td><td>most algorithms and tech support</td><td>uncountable Hilbert (configuration) space</td><td>continuous time quantum process</td></tr>
<tr><td>How?</td><td>IBM - Qiskit
~500 Qubits</td><td>Xanadu</td><td>DWave - LEAP
~7000 Qubits</td></tr>
<tr><td>What?</td><td></td><td></td><td></td></tr>
<tr><td></td><td>
</td><td>
</td><td>
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- universal gate-based quantum computers designed to tackle a wide range of problems
- Quantum Annealers designed specifically for optimization problems
- uses a network of qubits and couplers arranged to efficiently map optimization problems onto the quantum hardware
- allows for the effective translation of optimization problems into Hamiltonian equations and the subsequent minimization of these equations by applying an annealing process

credit: Michael Spannowsky

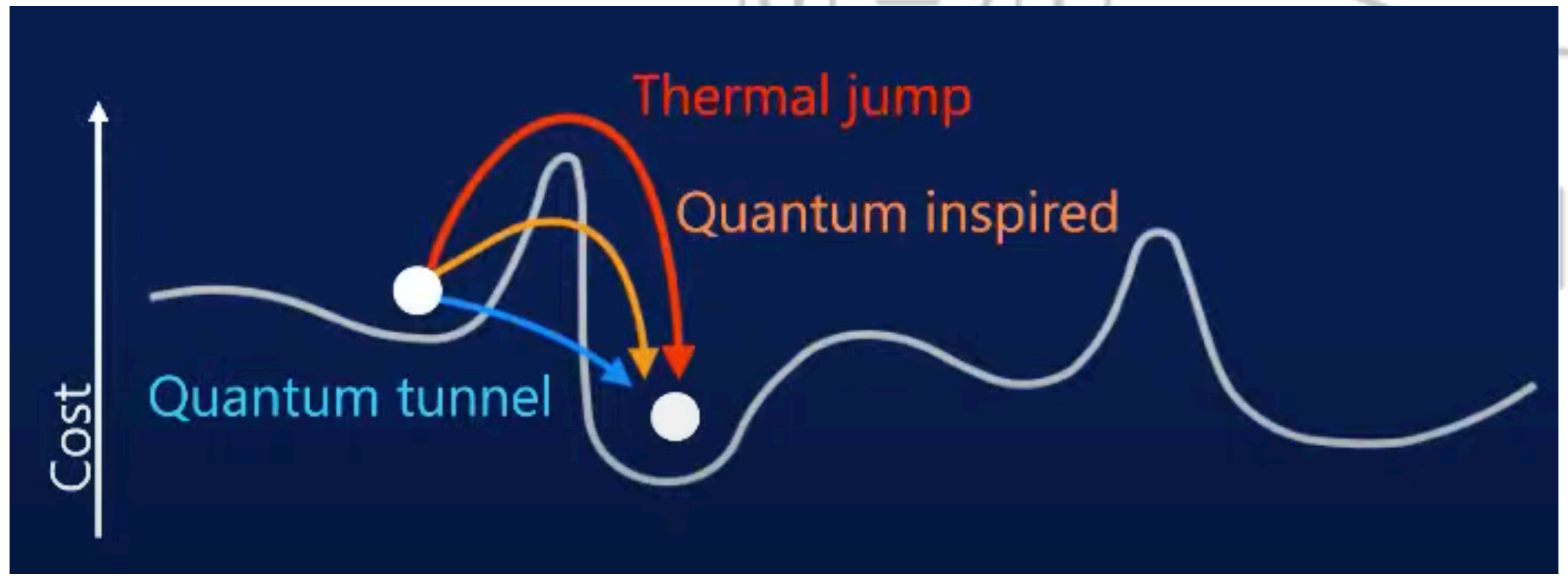
QUANTUM ALGORITHMS

- traditionally designed assuming the availability of fault-tolerant quantum processors supporting a large number of qubits and quantum gates
- in this context an entire zoo of sophisticated quantum algorithms that can offer exponential speedups over classical algorithms has been studied and proposed in literature:

60+ quantum algorithms with quantum speedup
https://quantumalgorithmzoo.org/

  - Shor's Algorithm: Factoring large integers, a crucial step in certain cryptographic protocols, in polynomial time
  - Grover's Algorithm: Searching an unsorted database for a specific item, dramatically improving upon classical search algorithms
  - Quantum Monte Carlo: Simulating physical systems at low temperatures and high energies, inaccessible to classical computers
  - Quantum Fourier Transform
  - …

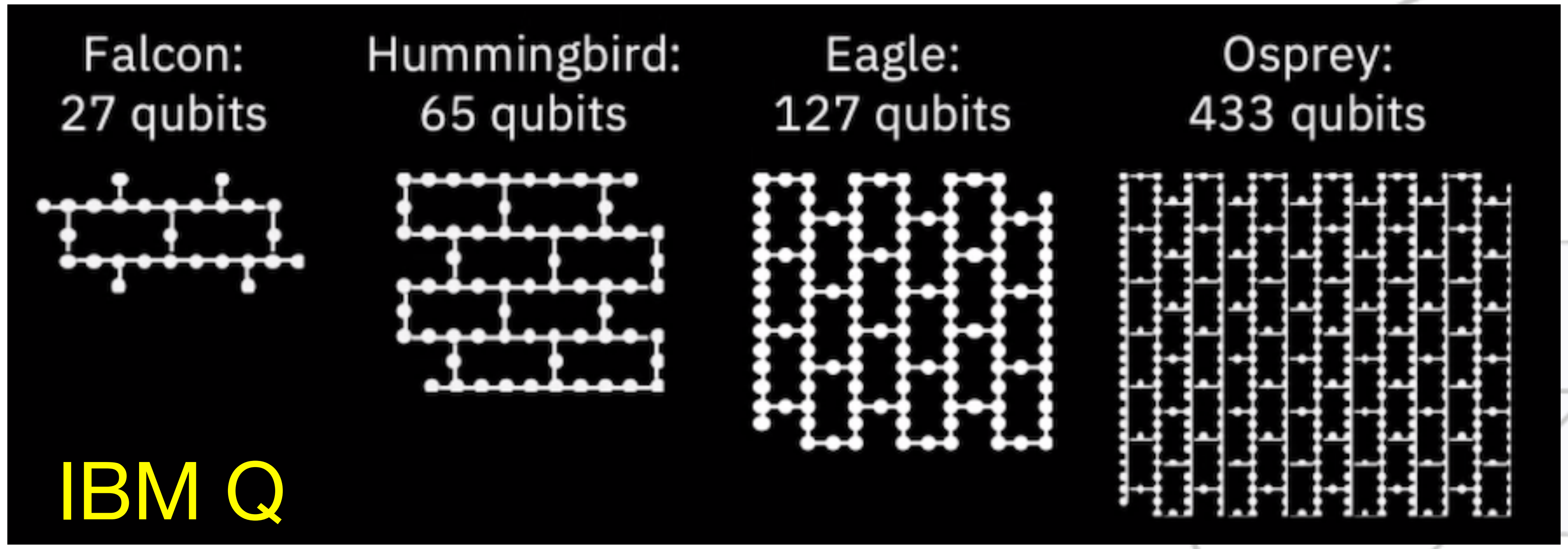
- In the meantime:
  - Quantum-inspired algorithms: classical algorithm designed to emulate quantum effects to achieve faster solutions (ex. quantum annealers, tensor networks, …)
  - Quantum Machine Learning …



credit: M.Troyer - Quantum Colloquium 2021 - Simons Institute

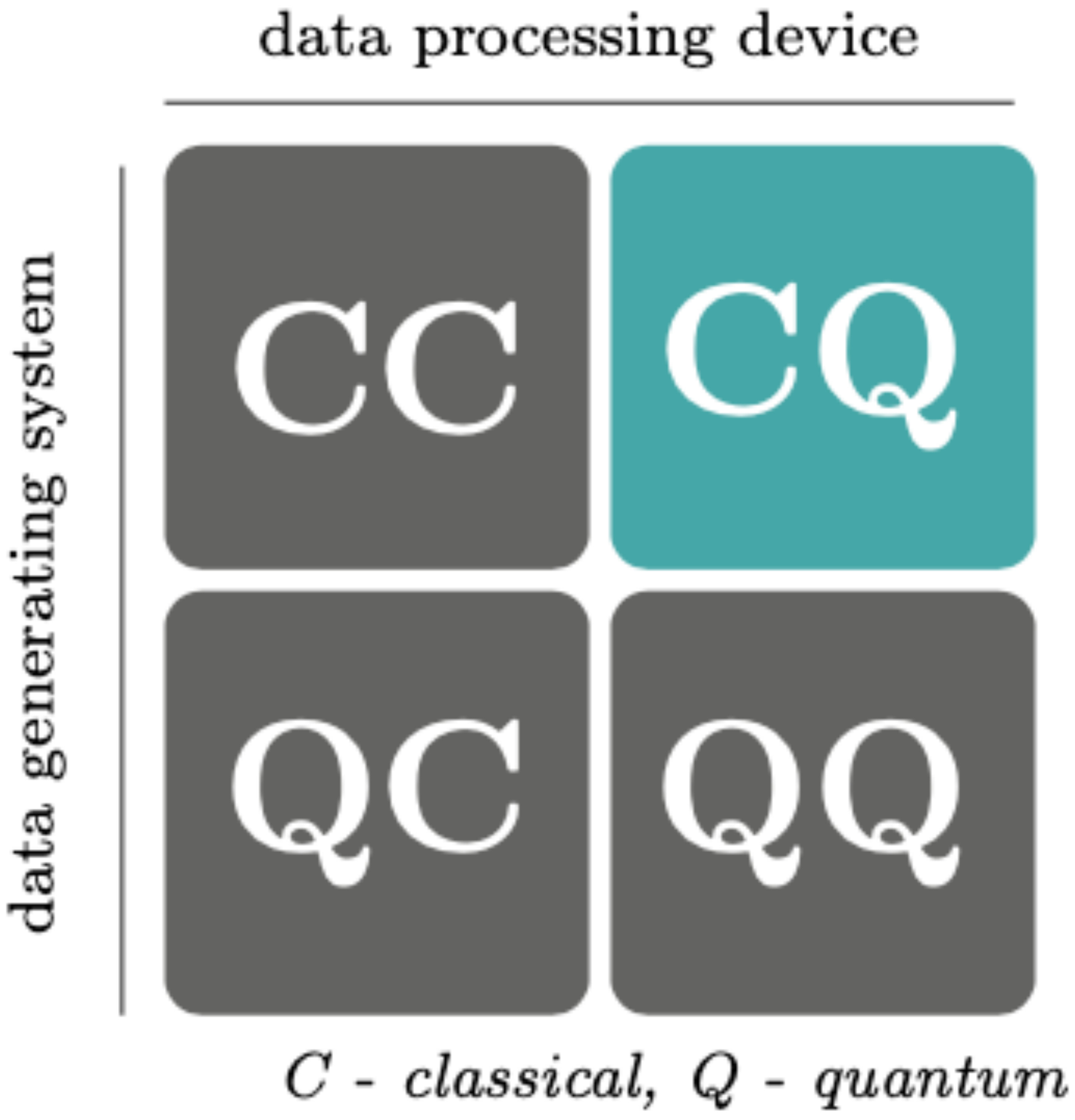
NEAR TERM QUANTUM CIRCUITS & QML

- current quantum computers support only $O(10^1 \div 10^2)$ qubits, and in the near term this number will not exceed $O(10^3)$ and not all necessarily able to interact with each others: these are the so called noisy intermediate-scale quantum devices (NISQ):
  - no error correction: produce only approximate results of computations
  - algorithms limited to use only a few qubits and gates with deep impact on quantum algorithmic design and achievable performance



- interesting to find computational problems that can be solved by NISQ device while possibly exhibiting some kind of advantage wrt classical algorithms: ML and Optimisation are two of such problems
- QML: emerging design paradigm that follows a two-step methodology akin to classical ML:
  - fix a priori a, possibly generic, parametric architecture for the quantum gates that define the quantum algorithm
  - choose the parameters of the architecture via classical optimization techniques based on data examples and on measurements of the outputs of the circuit (as is in classical ML)

APPROACHES TO COMBINE QC AND ML



different possibilities:

- CC: classical data being processed classically but with methods inspired by QC algorithms (like tensor networks)

- QC: quantum data processed with classical algorithms, eg use classical ML to help preparing and use QC (describe quantum state in a compact manner, state preparation, qubit error correction, …)

- CQ: classical data processed with quantum devices: eg QML

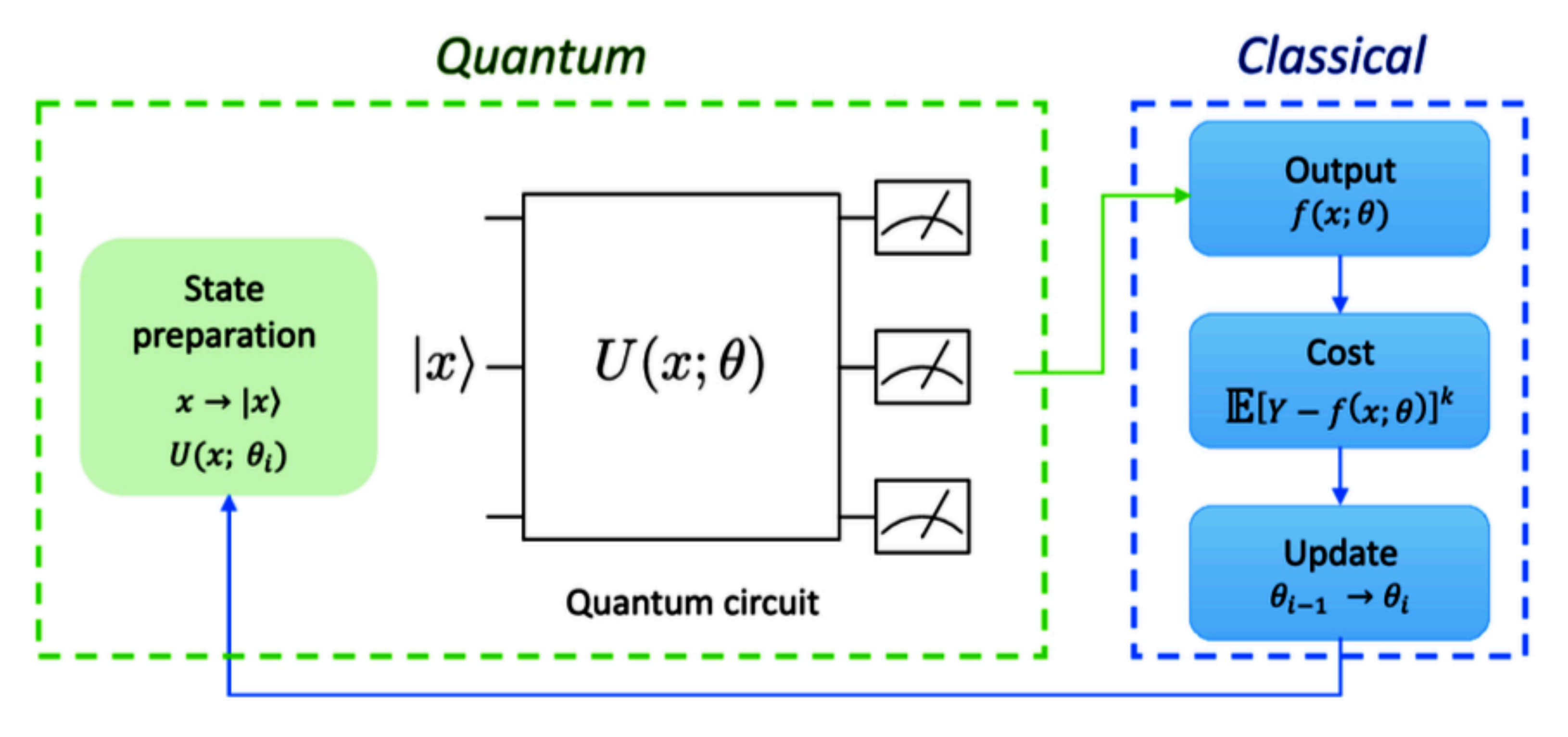
- QQ: quantum data being processed by a quantum computer. Connected to CQ (just change the input data), becomes interesting with the development of quantum sensing

E.A. Gilles Brassard, S. Gambs: Machine learning in a quantum world. In: Advances in Artificial Intelligence, pp. 431–442. Springer (2006)

QML MODELS

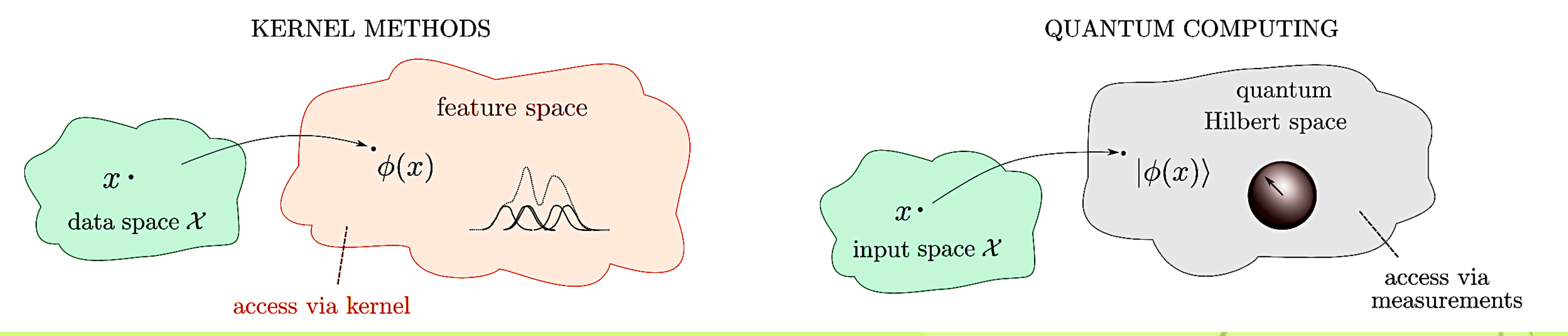
Variational Algorithms

ex. Quantum-NN



Kernel Methods

ex. Quantum-Support Vector Machines



$$K(x, x') = \phi(x)^T \phi(x')$$

$$|\phi(x)\rangle = U_\phi(x)|0\rangle$$

$$|\phi(x')\rangle = U_\phi(x')|0\rangle$$

$$|\langle \phi(x) | \phi(x')\rangle|^2 = K(x, x')$$

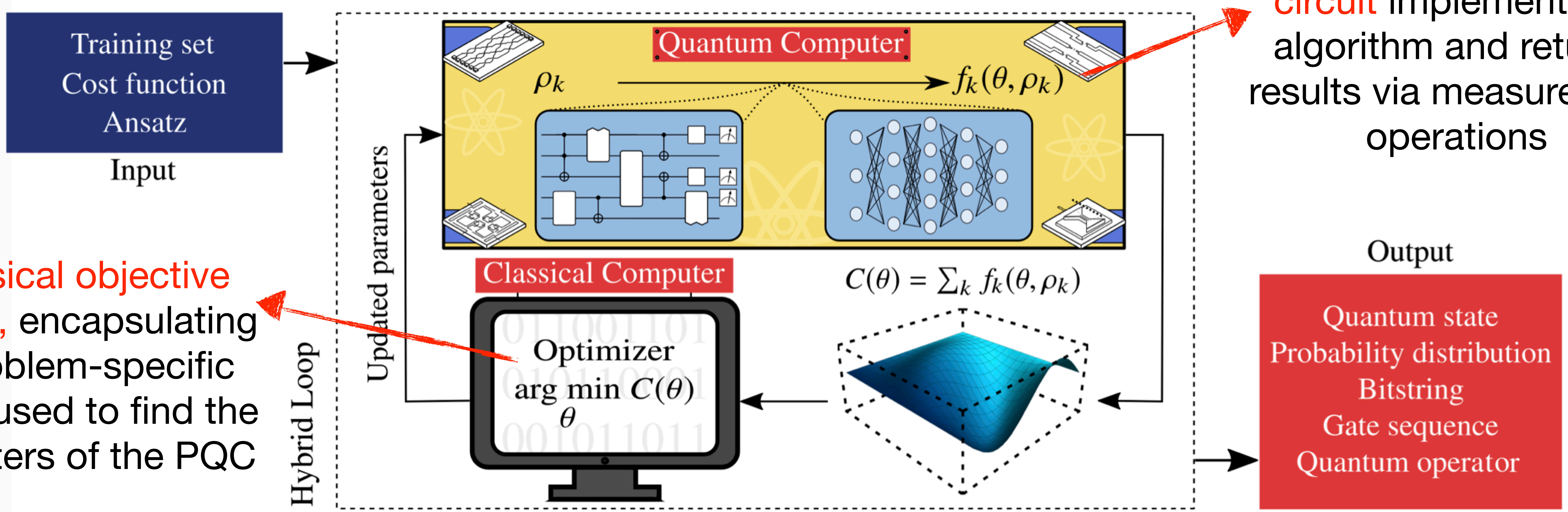
Energy Based Methods

Build network of stochastic binary units and optimise their energy
ex: Quantum-Botzman Machines have quadratic energy function that follows the Boltzman distribution (Ising Hamiltonian)

VARIATIONAL QUANTUM MODELS

- variational quantum models: are hybrid algorithms that uses both classical computers and quantum to find the solution of a given problem

a parametric quantum circuit implements an algorithm and returns results via measurement operations



a classical objective function, encapsulating the problem-specific goal, is used to find the parameters of the PQC

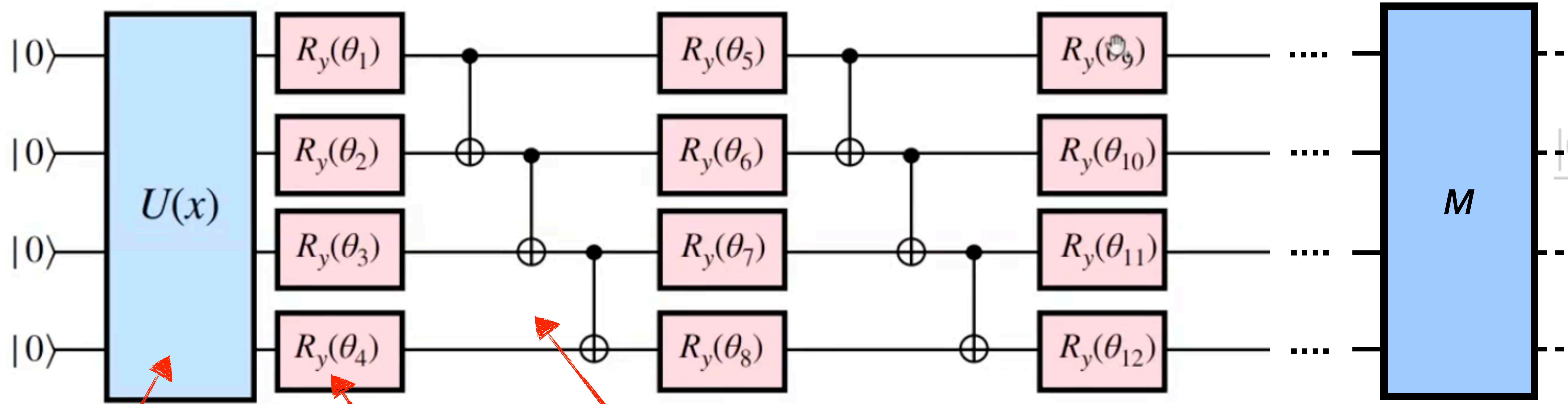
cordit: Cerezo et al

- loss, gradients, and parameter updates are calculated on a classical processor (GPU)
- advantages of VQM: one circuit can represent an entire family of different circuits, less sensitive to noise

QUANTM NEURAL NETWORKS

- **a typical example of a QNN:**

$$\hat{y} \doteq f(x,\theta) = \langle M \rangle =$$
$$= \langle x | V^{\dagger}(\theta) M V(\theta) | x \rangle$$



$\hat{y}$

$L(y, \hat{y} | \theta)$

parametrised rotations
(along y in this example)

repeated N-times (N-layers) to increase
expressibility

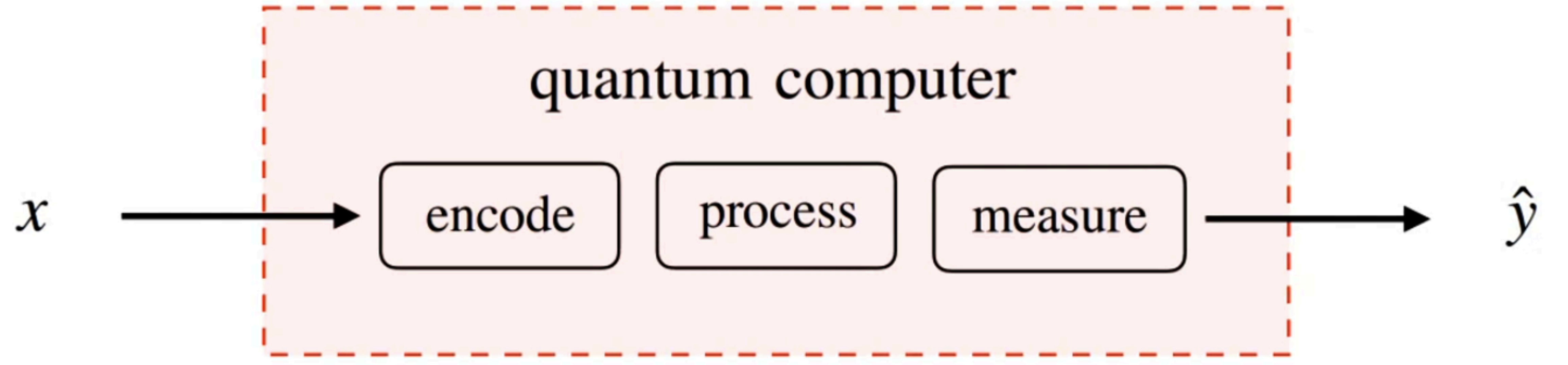
entanglement block
via CNOT gates
creates non-classical correlations that hopefully will increase the
expressibility of the circuit

encoding
classical
input x

$$\theta^* = \arg\min \sum_{i \in D} L(y_i, f(x_i, \theta))$$

ENCODING CLASSICAL DATA

- encoding of classical data is a crucial step in implementing a QML algorithm

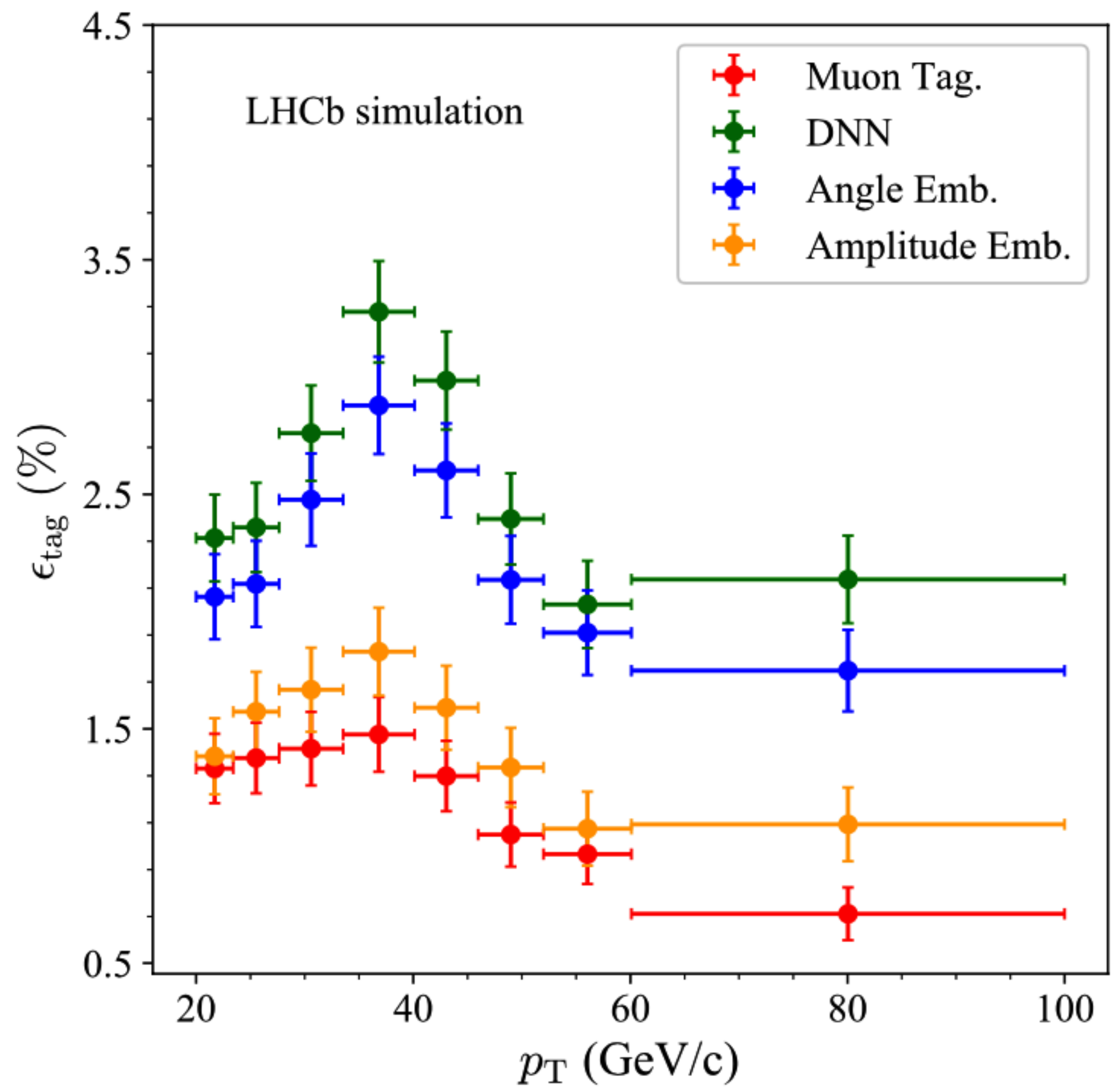


- several way to do it, ranging from conceptually simple but resources hungry (# qubits), to more efficient but also more complex (tradeoff between compression and circuit depth)

- example: amplitude encoding

$$x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \rightarrow |x\rangle = \frac{1}{||x||}(x_0|0\rangle + x_1|1\rangle) = \frac{1}{||x||}\sum_{i=0}^{N} x_i|i\rangle$$

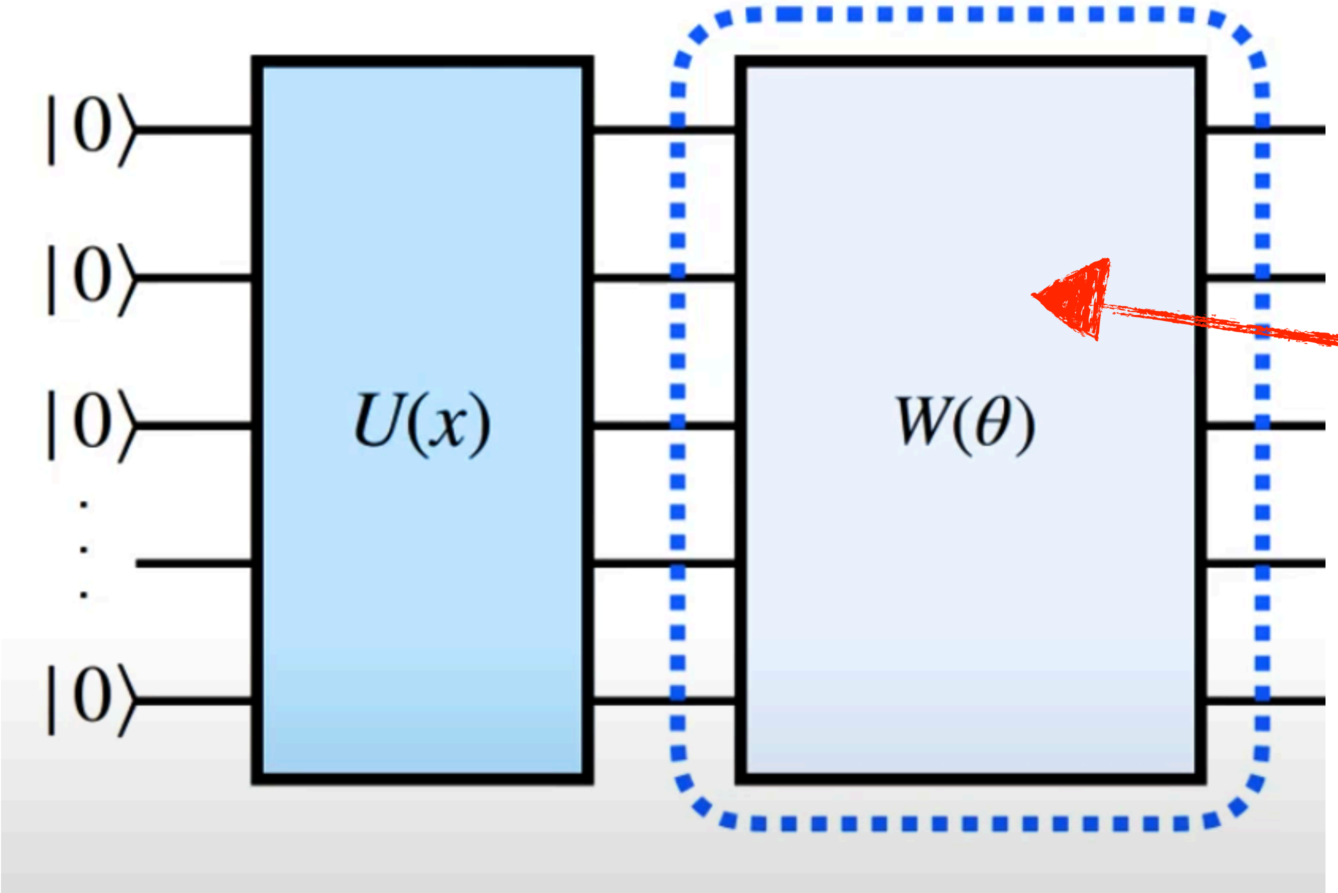
  - fewer qubits needed: exponential compression $n_q \propto O(\log N)$
  - more complex preparation and readout: # of gates $n_g \propto O(\text{poly}(N))$



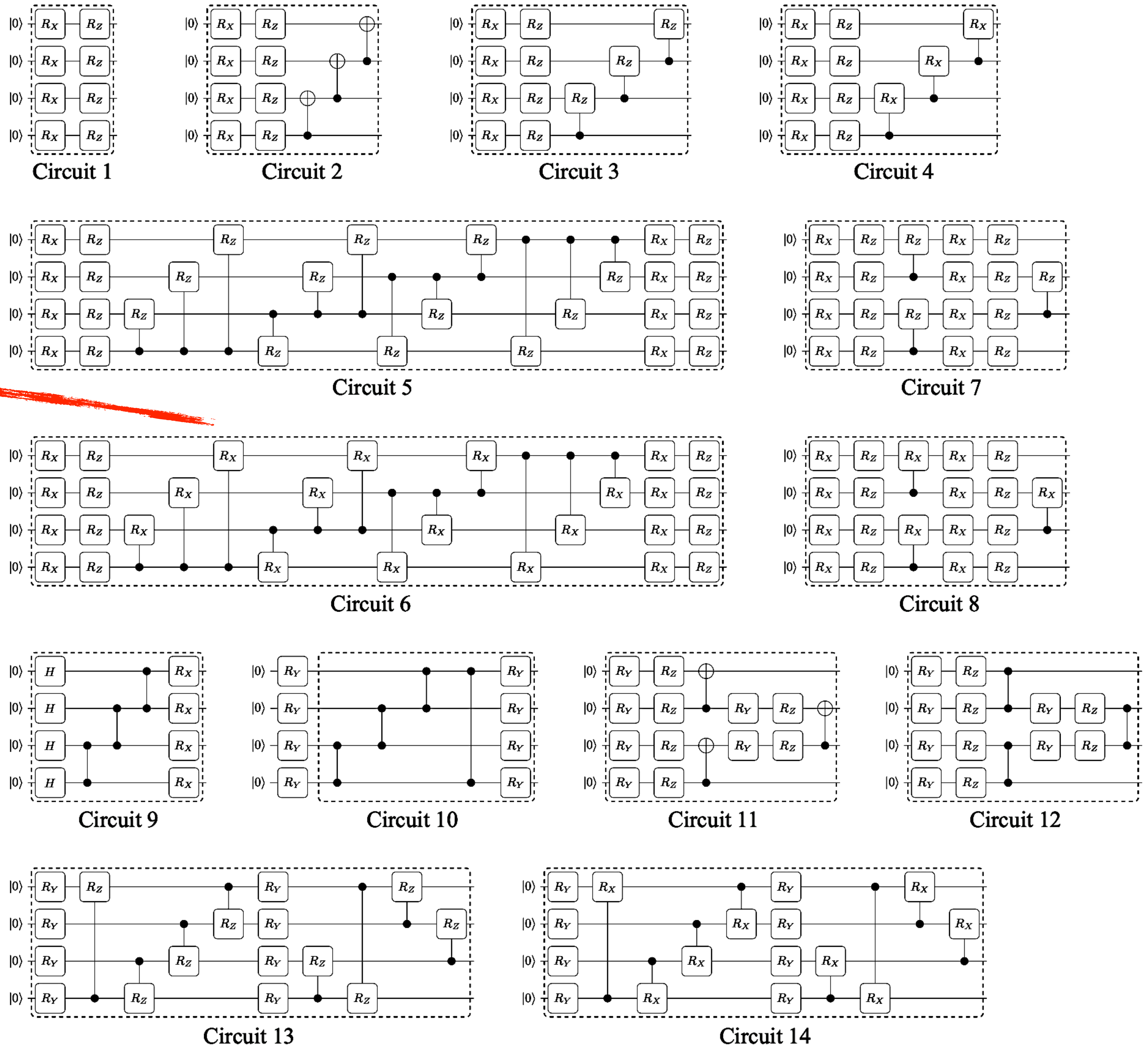
A.Gianelle et al, JHEP 2022, 14

EXPRESSIVE POWER OF PARAMETRIZED QUANTUM CIRCUITS

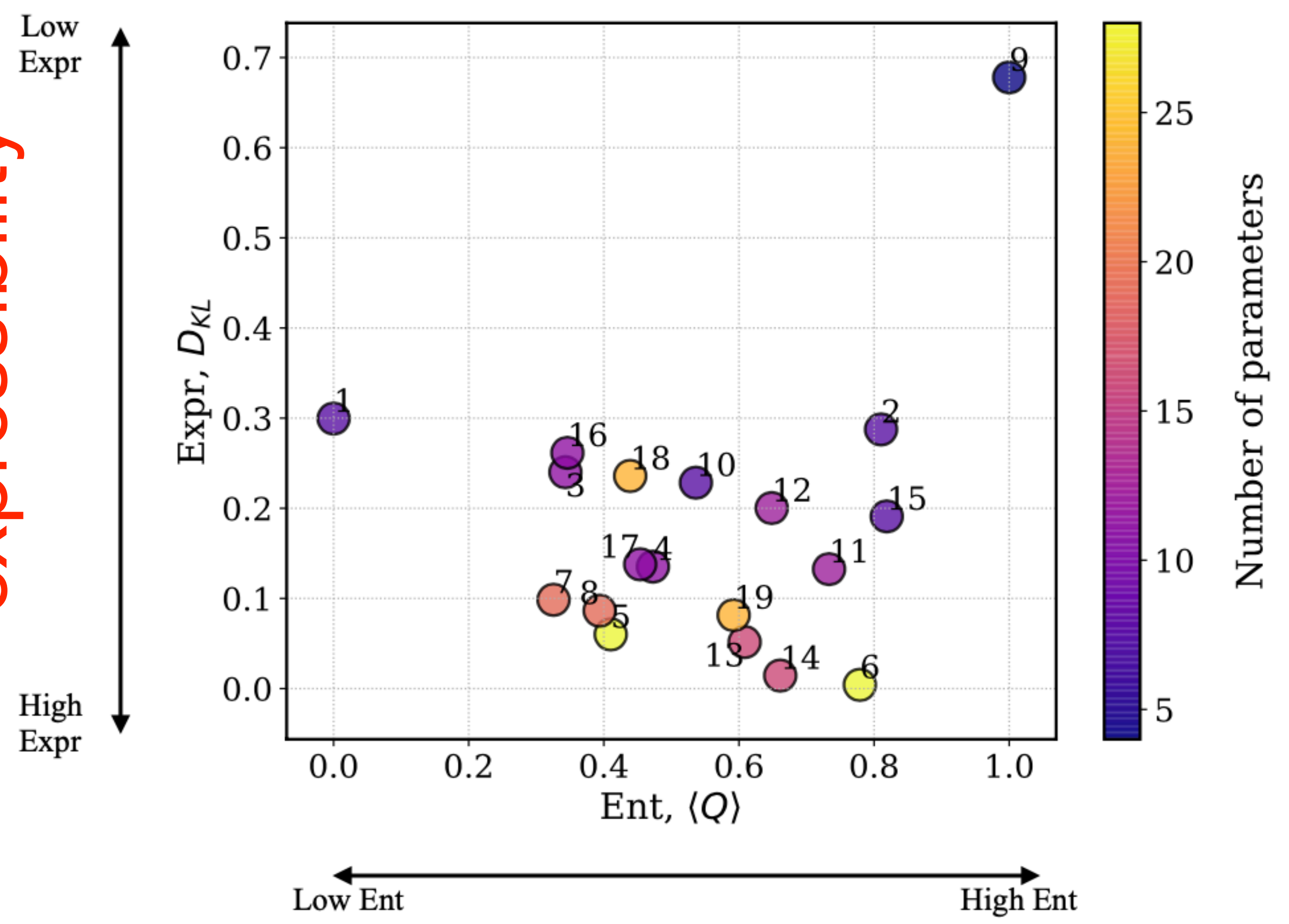
- several studies in literature on how to choose the circuit ansatz in order to maximise expressibility and entangling capabilities (eg ability to efficiently represent the solution space for the tasks at hand and to capture non-trivial correlation in the quantum data)



encoding PQC



expressibility



entangling

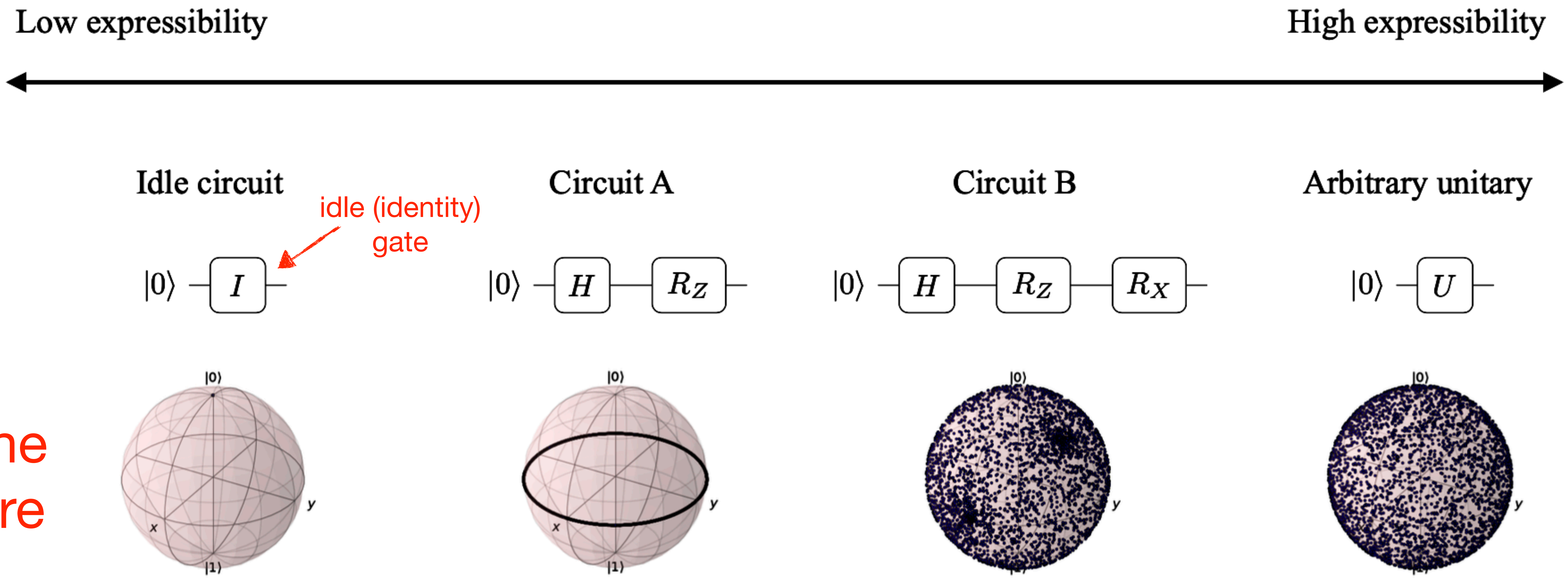
S. Sim et al: arXiv:1905.10876

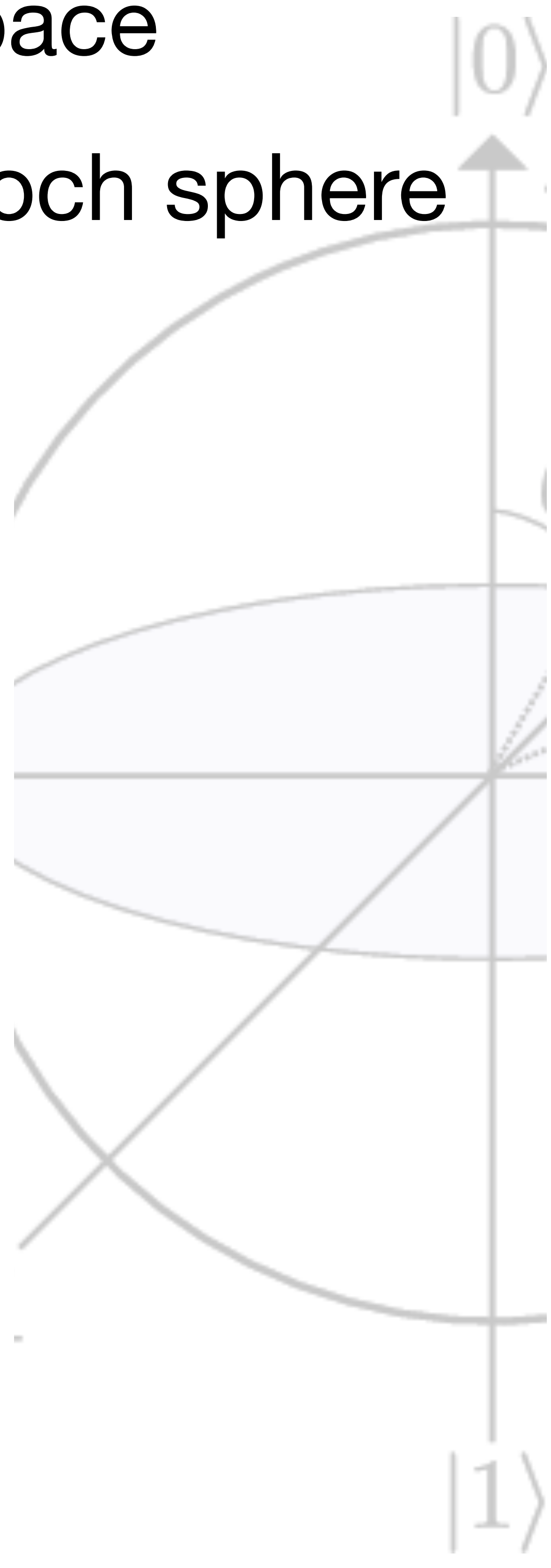
EXAMPLE: EXPRESSIBILITY FOR A SINGLE QUBIT

- expressibility: circuit's ability to generate (pure) states that are well representative of the Hilbert space
- in the case of a single qubit, the expressibility corresponds to the circuit's ability to explore the Bloch sphere

circuit

points on the block sphere





S. Sim et al: arXiv:1905.10876

TRAINABILITY AND BARREN PLATEAUS PROBLEM

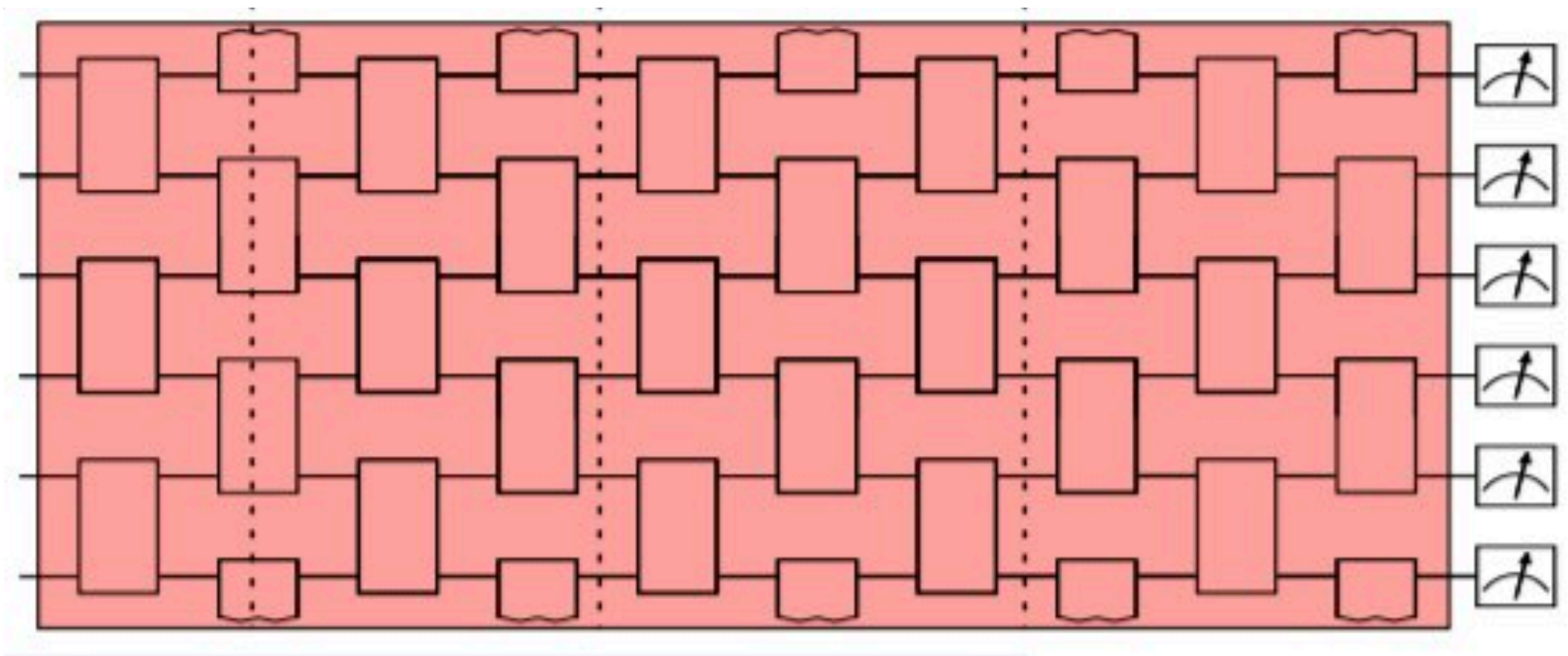
- variational circuits can be affected by presence of large regions of the cost function's parameter space where the variance of the gradient is almost 0 (flat loss landscape)
- a variational circuit initialised in one of these areas will be untrainable using any gradient-based algorithm
- it can be shown that using a deep random parametrised circuit, with a random initialisation of the parameters the gradient's variance will exponentially decrease with the # of qubits

$$\langle \partial_\theta L \rangle \simeq 0$$

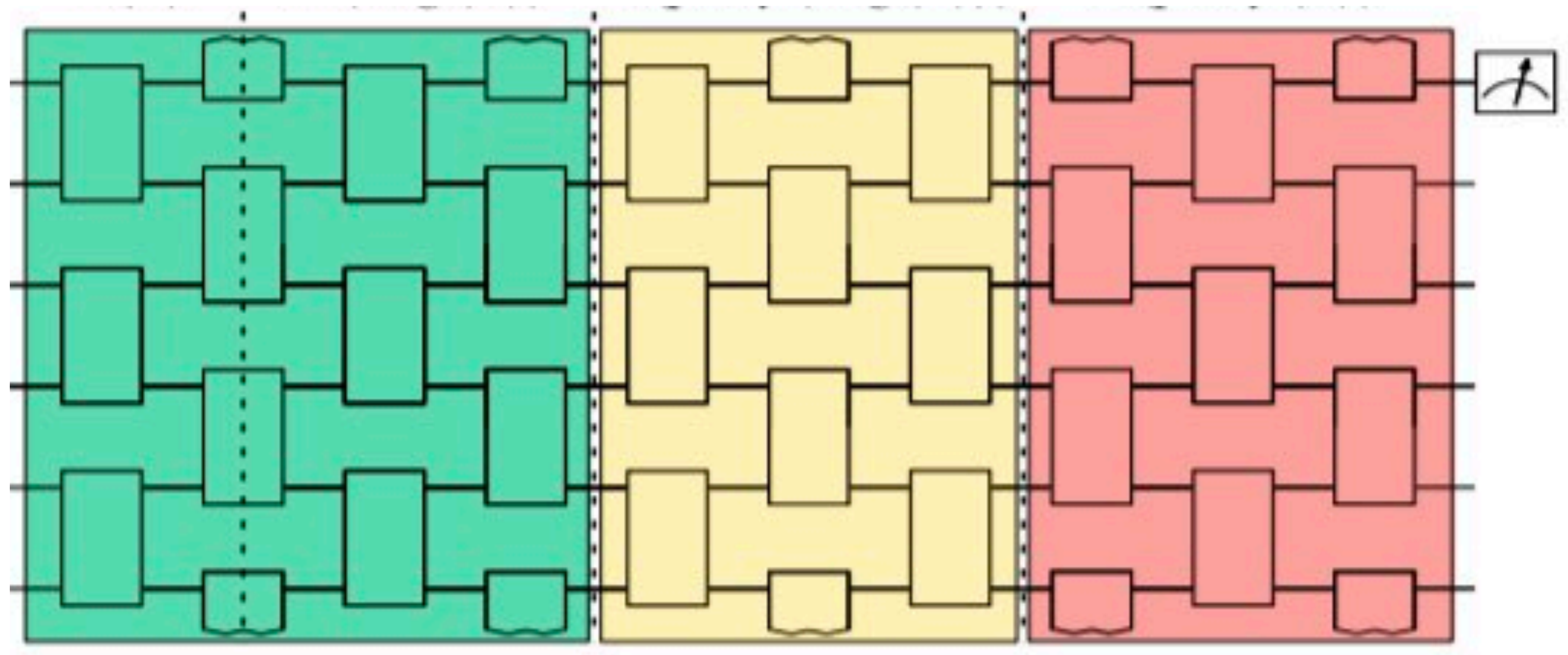
$$\text{Var}[\partial_\theta L] \sim 2^{-n}$$

J.R. Mc Clean et al., Nat. Comm.

- a possible mitigation strategy: use local cost functions that only have information from part of the circuit coupled with not too-deep circuits and not too much entanglement



global loss



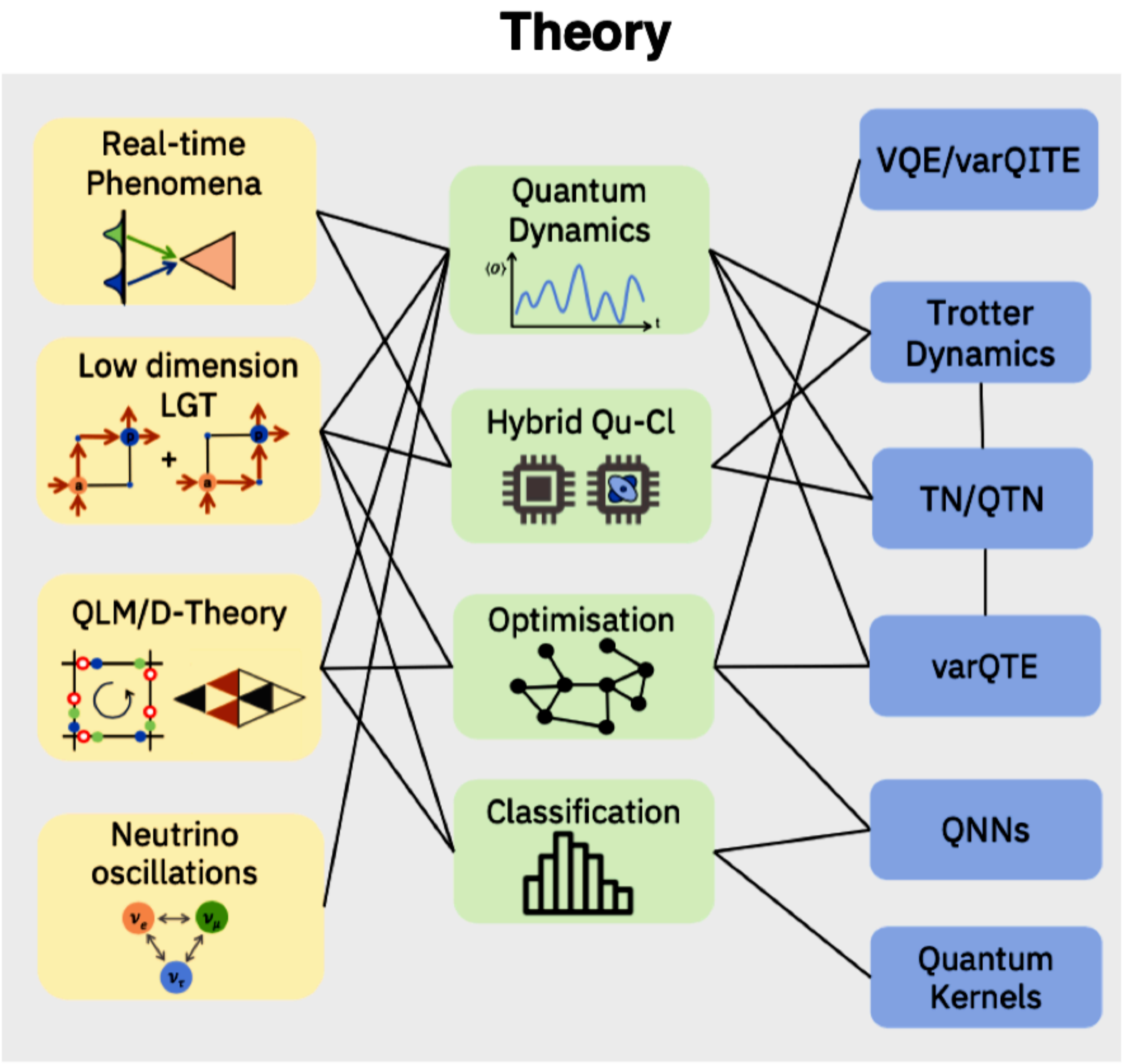
local loss

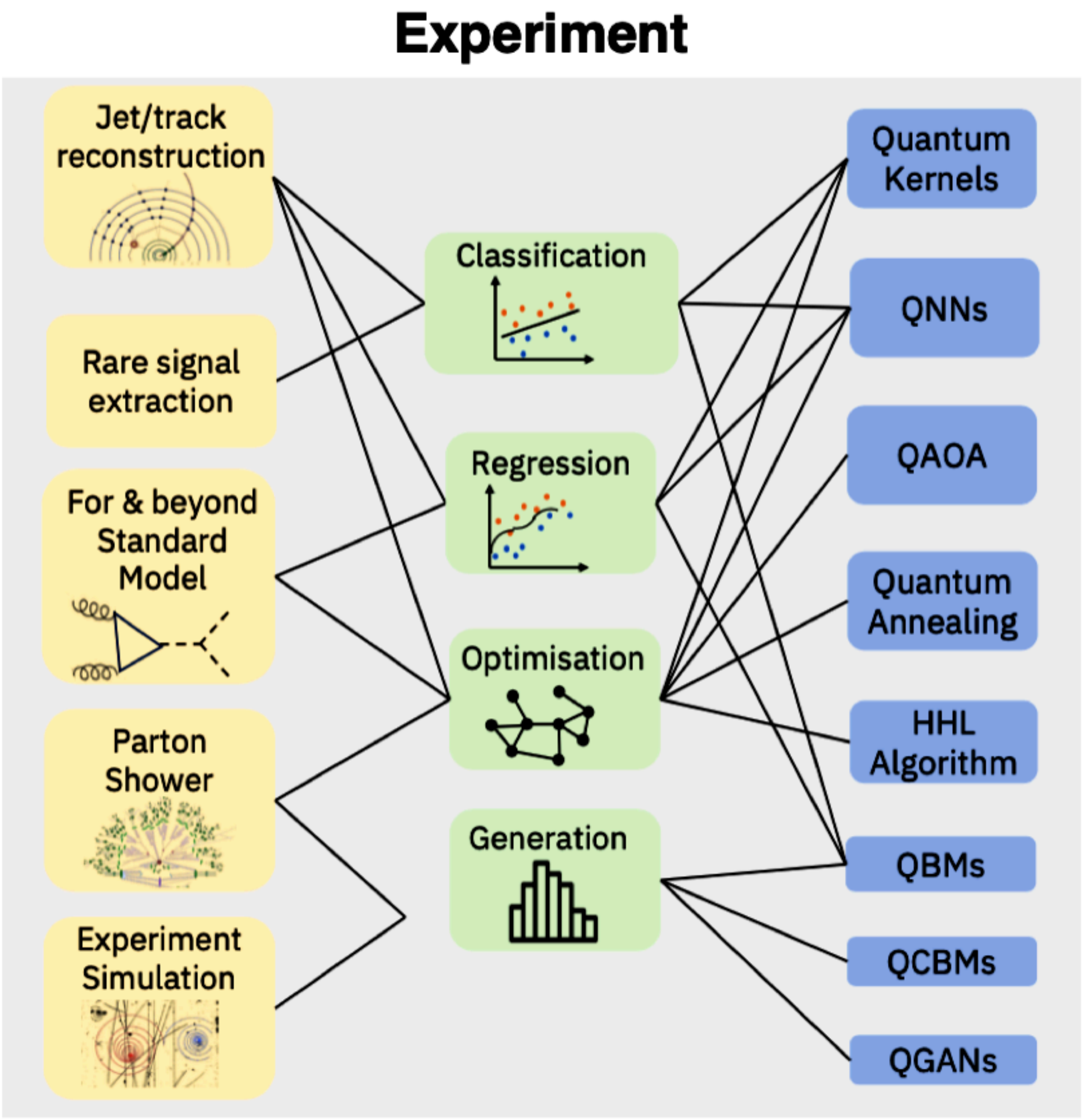
$$\text{Var}[\partial_\theta L] \geq \text{Lower Bound}(L) \sim$$

$$\sim \text{poly(n)}^{-1}$$

Cerezo et al: arXiv:2001.00550

QML APPLICATIONS IN HEP





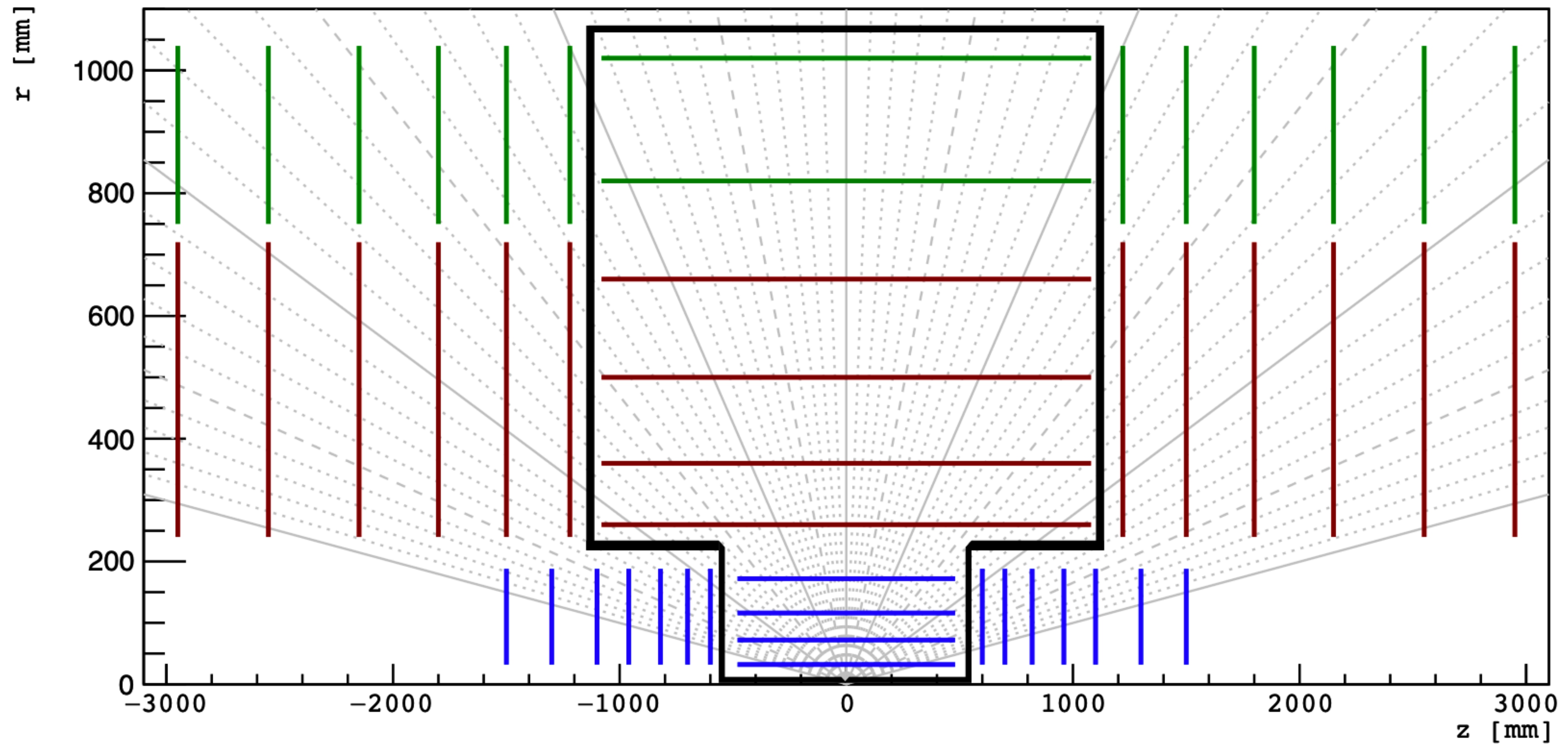
A. Di Meglio et al: arXiv:2307.03236 [quant-ph]

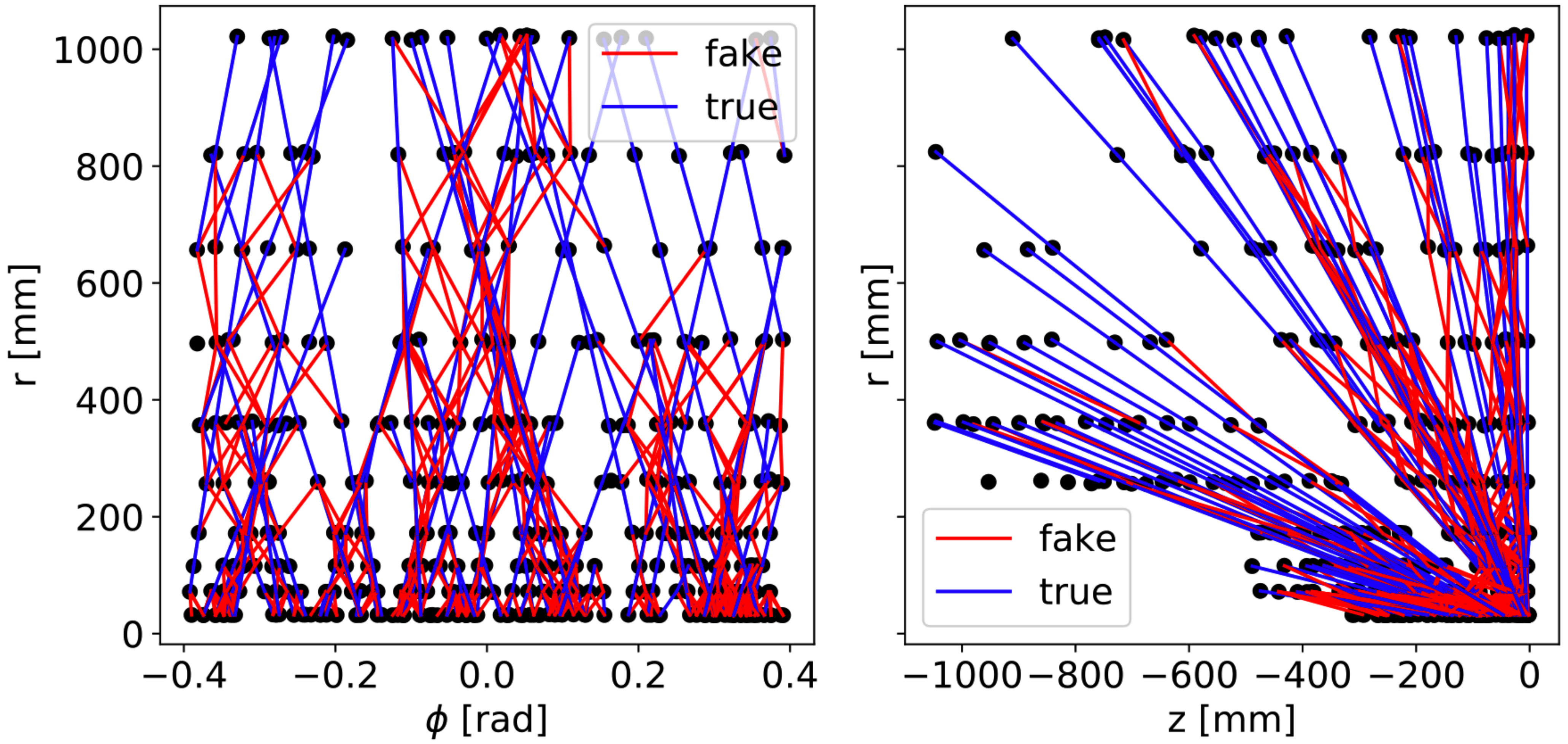
QML IN HEP: TRACKING RECONSTRUCTION WITH QGNN

- Implements an hybrid classical-quantum Graph Neural Network model trained to determine charged particle trajectories from hits in a LHC inner tracker detector
- one of the hard challenges with the HL-LHC upgrade, when the increase in the instantaneous rate of particle collisions will yield many more detector hits, and thus measurements will pose a combinatorial challenge to track reconstruction algorithms

Data:

- TrackML dataset from CERN/Kaggle Tracking Machine Learning challenge
- only barrel region considered due to constraints on the available quantum hw resources





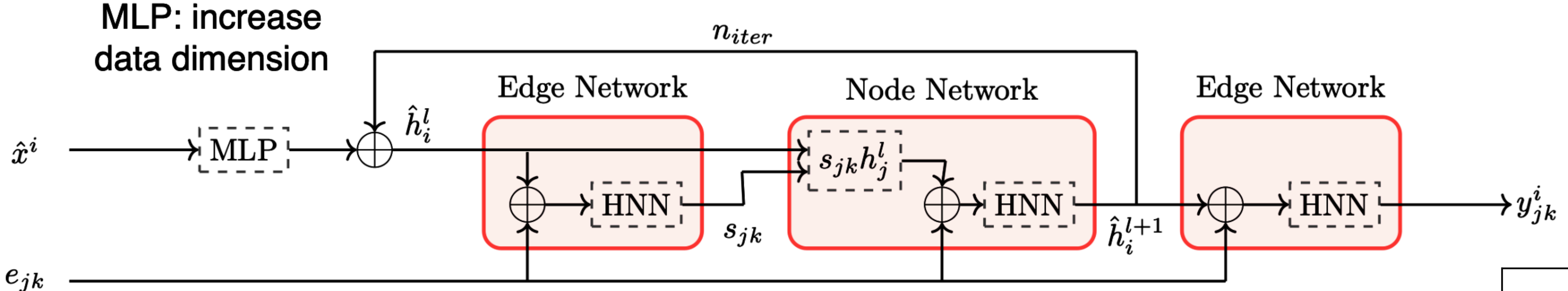
- QGNN input: pre-processed subgraphs
  - hits are nodes
  - tracks that connects hits are edges
  - ground truth informations about each edge

Cenk Tüysüz et al, arXiv:2012.01379

QML IN HEP: TRACKING RECONSTRUCTION WITH QGNN

- Quantum-Classical hybrid architecture:

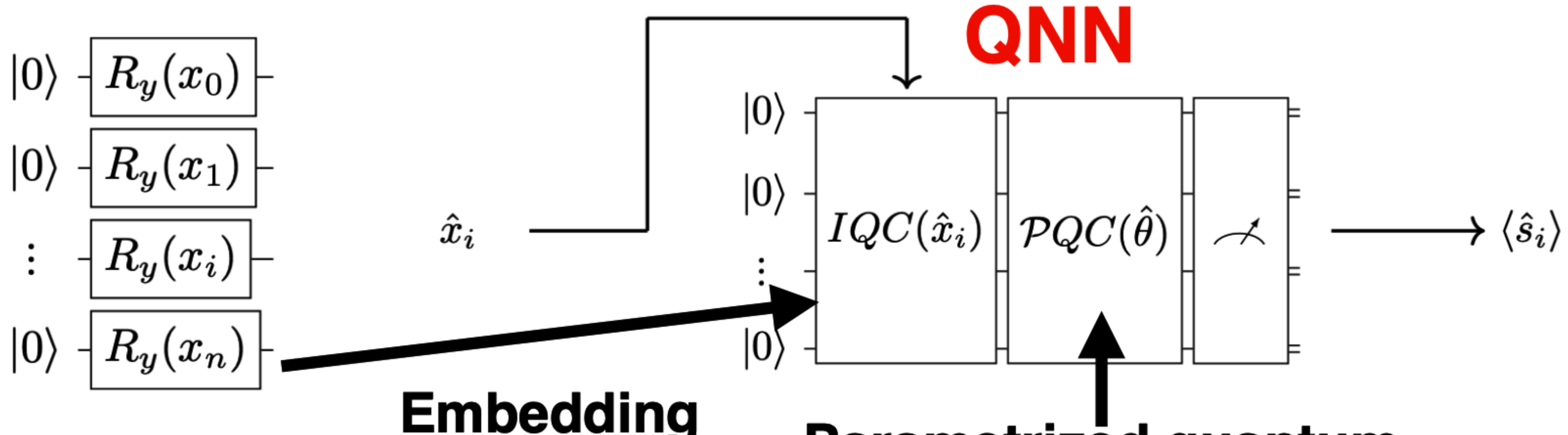
MLP: increase data dimension



Edge network: QNN with edges as inputs, and has as outputs probabilities for edges to be true (edge features)

Node network: Edges are weighted with edge features. Triplets of connected nodes are built, and fed to a QNN. QNN provides updated nodes as outputs.

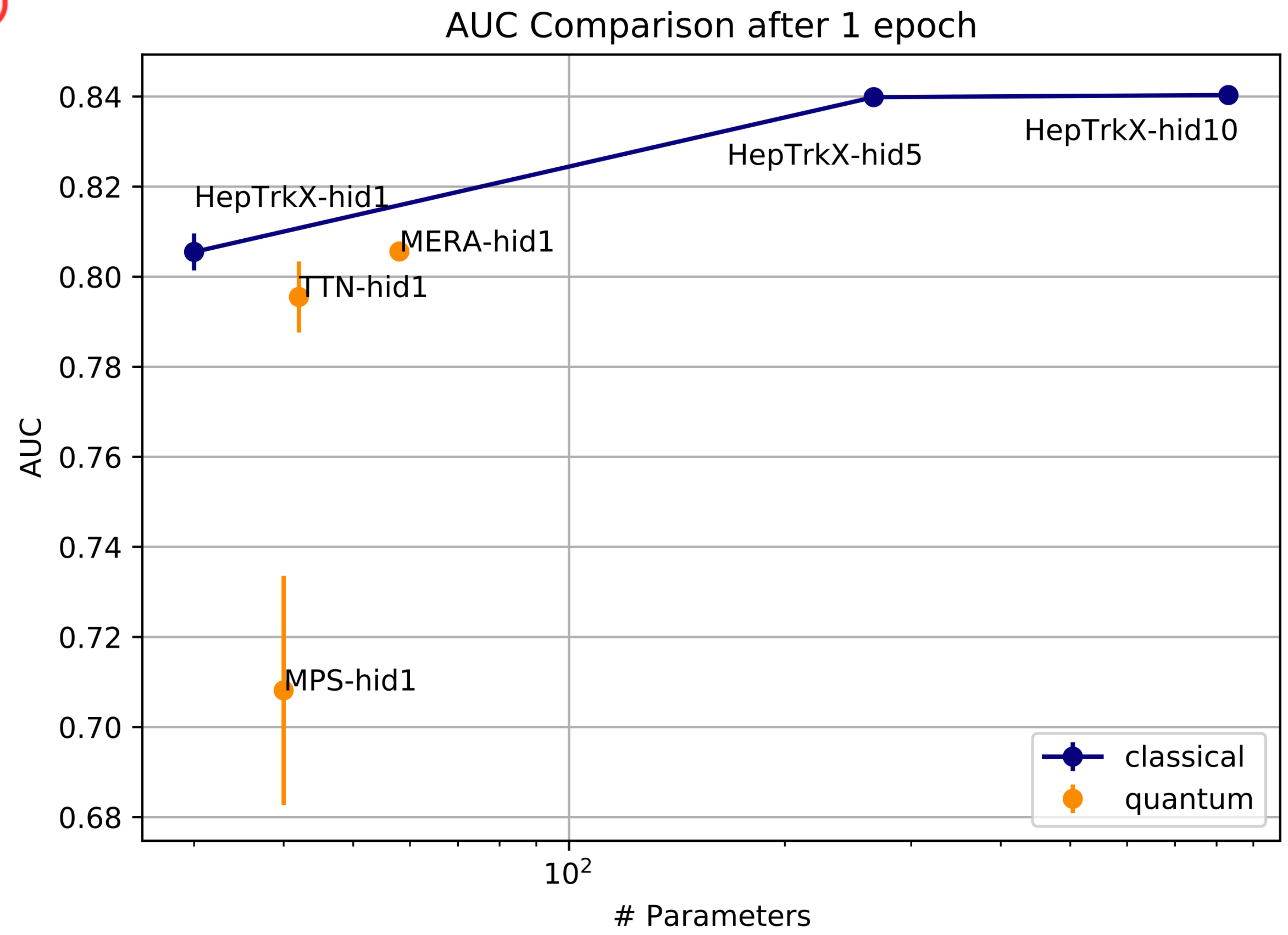
QNN



Embedding

Parametrized quantum circuit

Performance: AUC



Comparison with classical GNN after 1 epoch
QGNN trained on CPU/GPU (long training time)

Cenk Tüysüz et al, arXiv:2012.01379

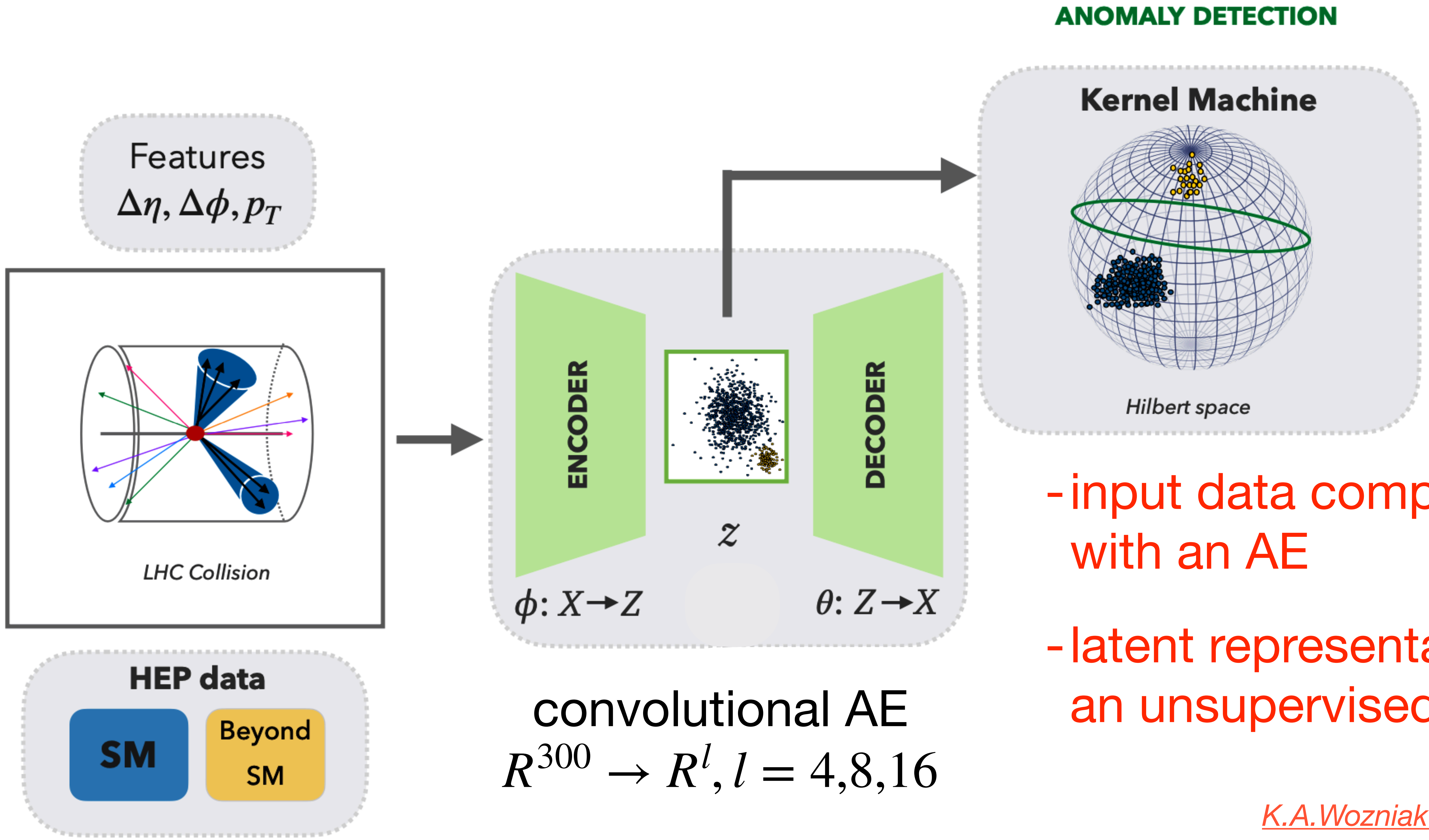
QML IN HEP: ANOMALY DETECTION FOR QCD JETS

- Anomaly Detection describes a class of algorithms that aims at the identification of rare items, events or observations, which deviate significantly from the majority of the data and do not conform to a well-defined notion of normal behavior

- Gained increasing interest recently in experiments at the LHC, as a viable ML approach to implement signal model-independent searches for NP effects

Use case:

- QCD multijets at the LHC
- delphes simulation
- build jets from 100 highest pt particles
- apply realistic event selection



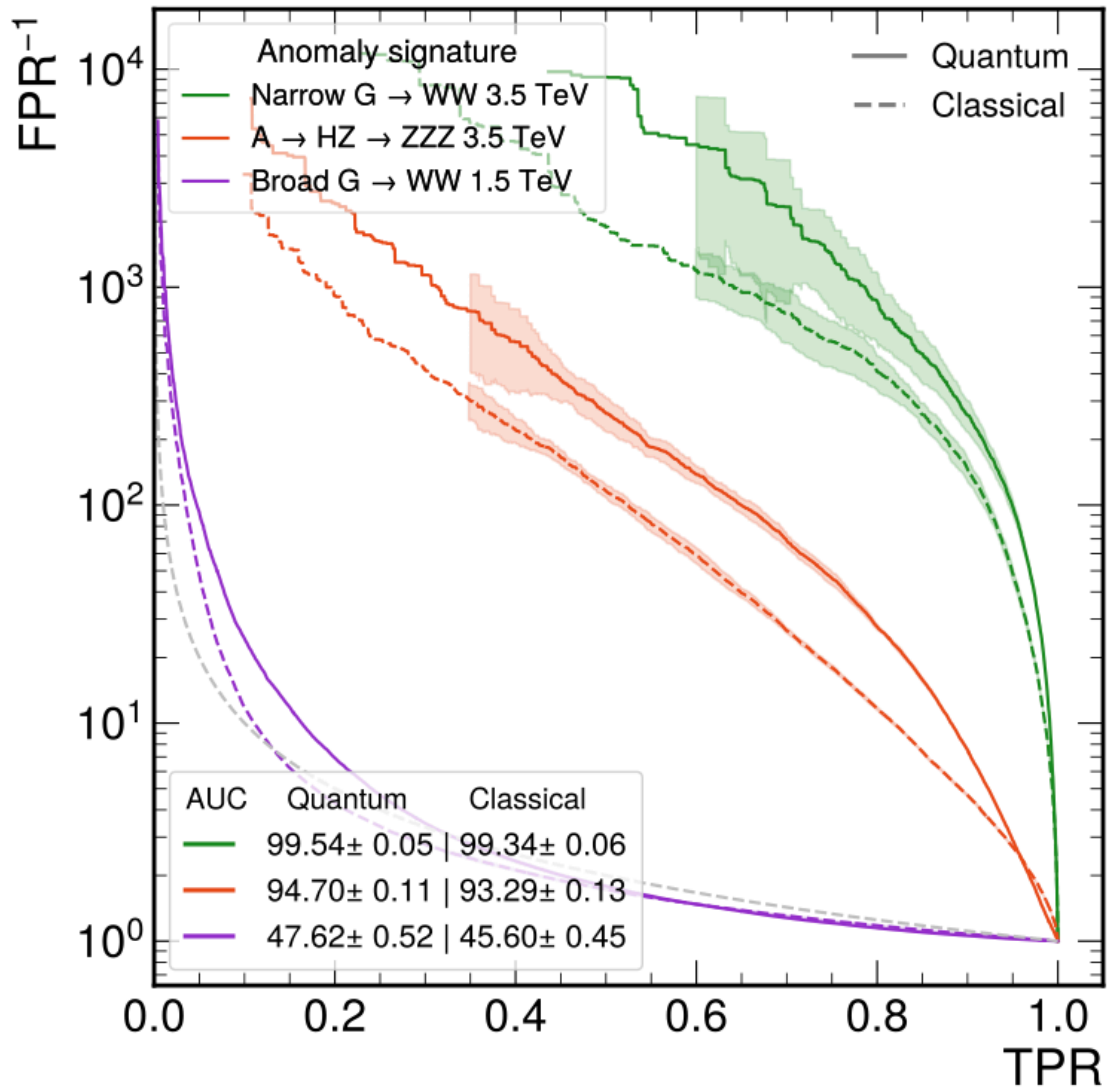
- input data compressed classically with an AE
- latent representation analysed by an unsupervised quantum kernel

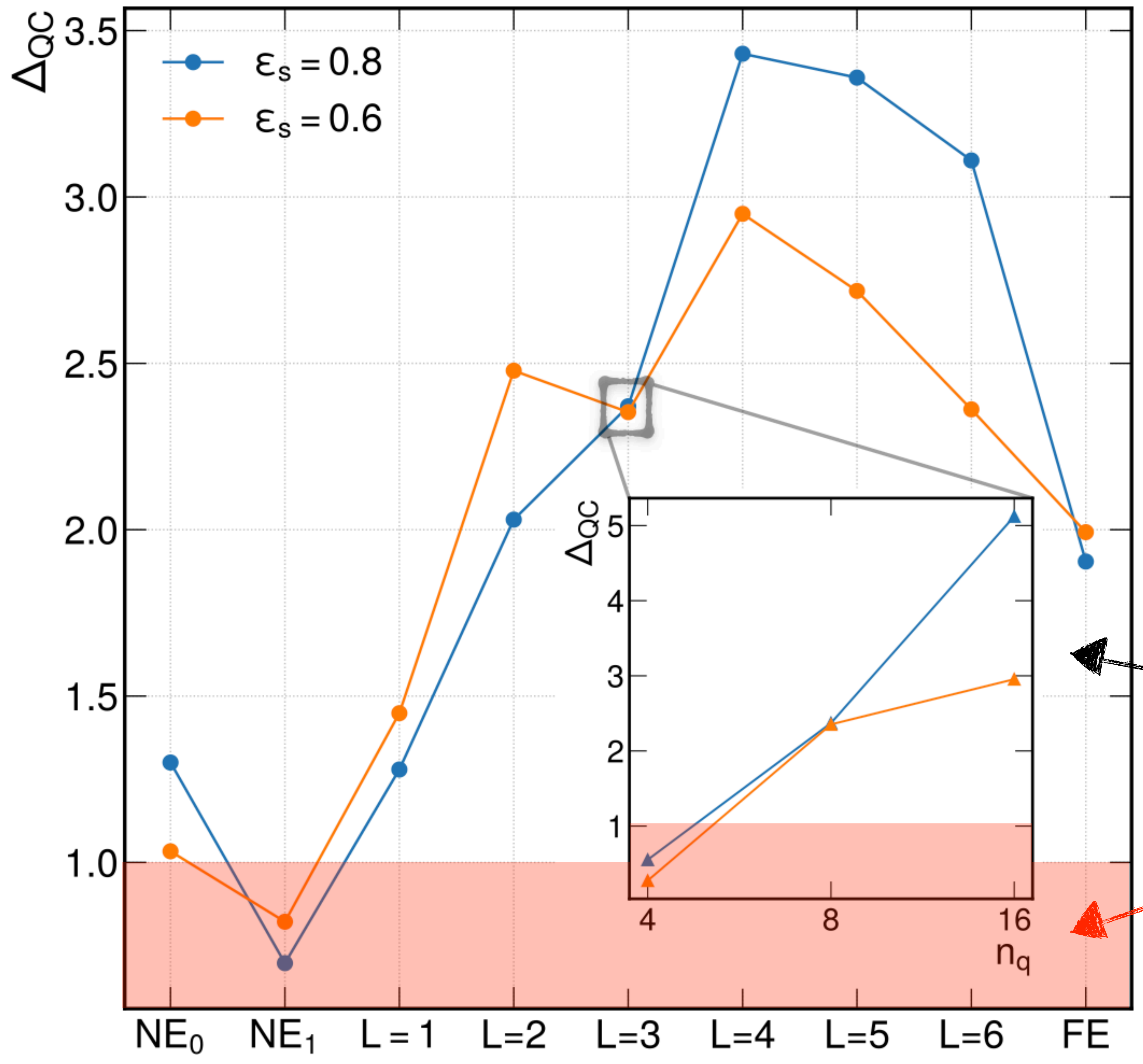
K.A.Wozniak et al, arXiv:2301.10780

QML IN HEP: ANOMALY DETECTION FOR QCD JETS

$$\Delta_{QC}(\epsilon_s) = \frac{\epsilon_b^{-1}(\epsilon_s; Q)}{\epsilon_b^{-1}(\epsilon_s; C)}$$

background rejection (FPR^{-1}) at a working point ϵ_s (TPR) given a specific quantum (Q) or classical (C) anomaly detection model





quantum is better

classical is better

entanglement and expressivity increase

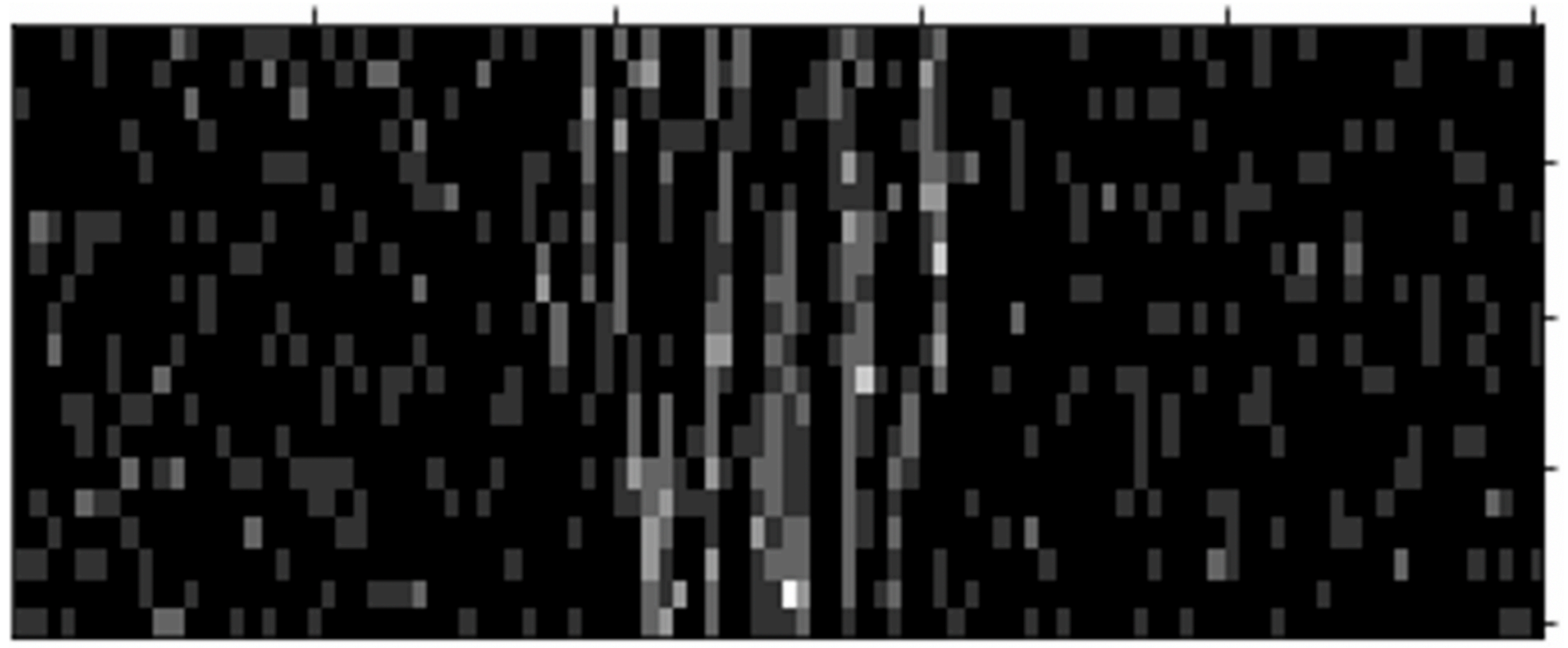
[K.A.Wozniak et al, arXiv:2301.10780](arXiv:2301.10780)

QML IN HEP: ANOMALY DETECTION FOR LONG LIVED PARTICLES

- Design and train a Quantum-AE able to identify highly displaced decays using the ATLAS muon spectrometer information

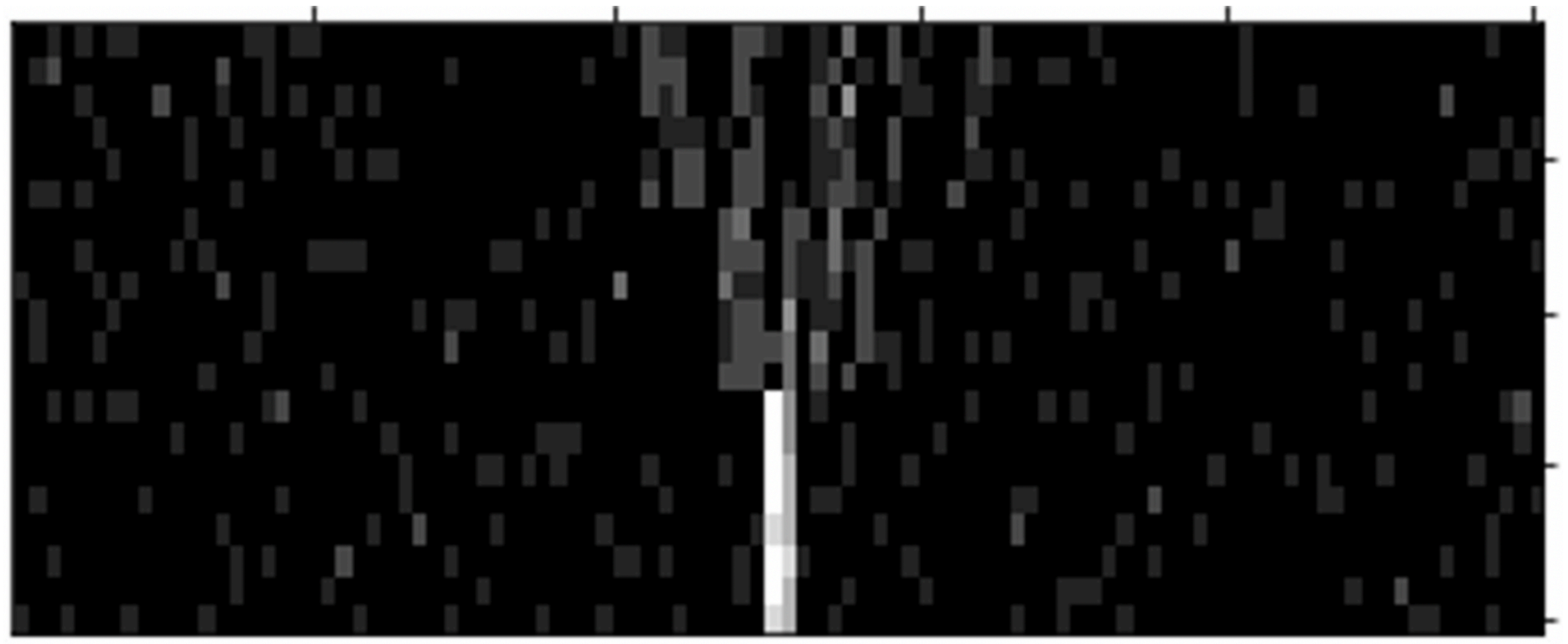
NORMAL event

“image” representation of a prompt decay in multi-muons

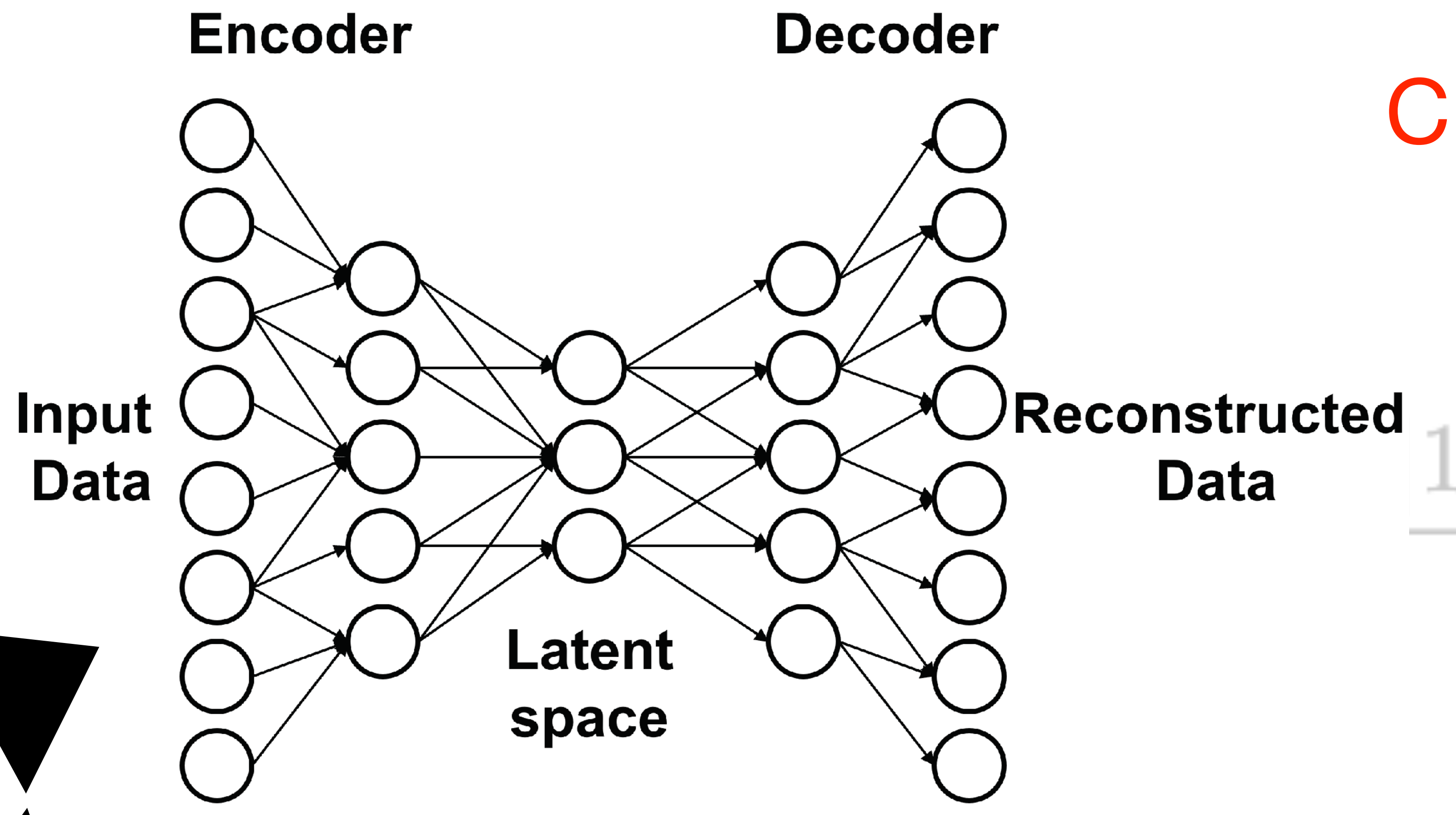


ANOMALOUS event

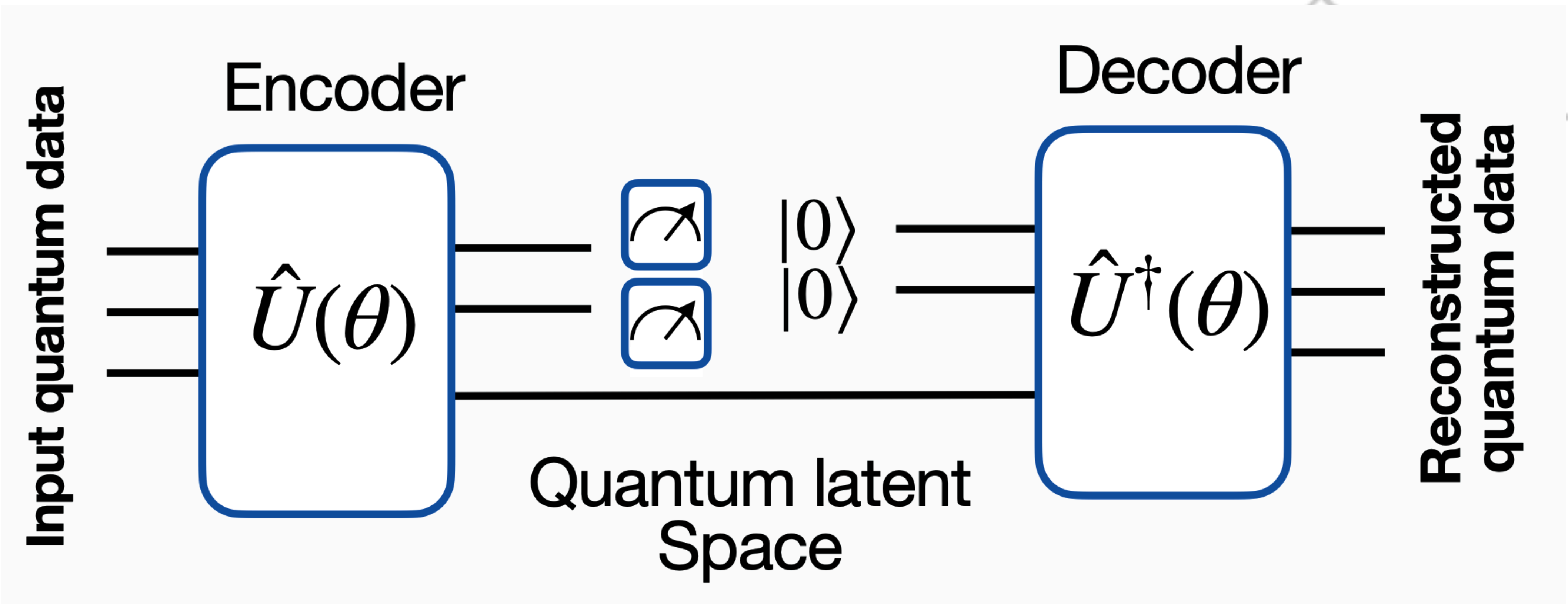
“image” representation of a highly displaced decay in multi-muons



Classical AE



Quantum-AE



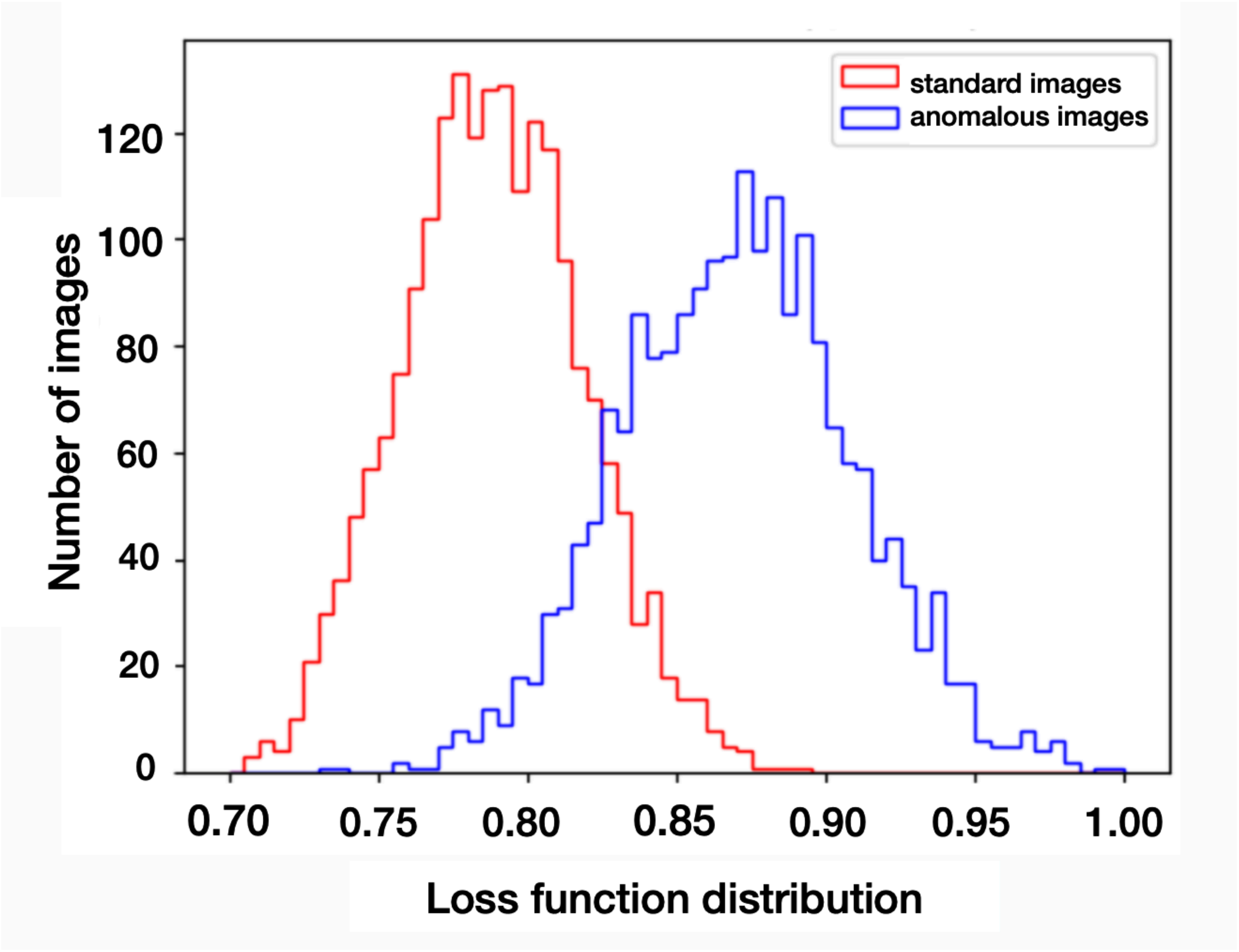
QML IN HEP: ANOMALY DETECTION FOR LONG LIVED PARTICLES

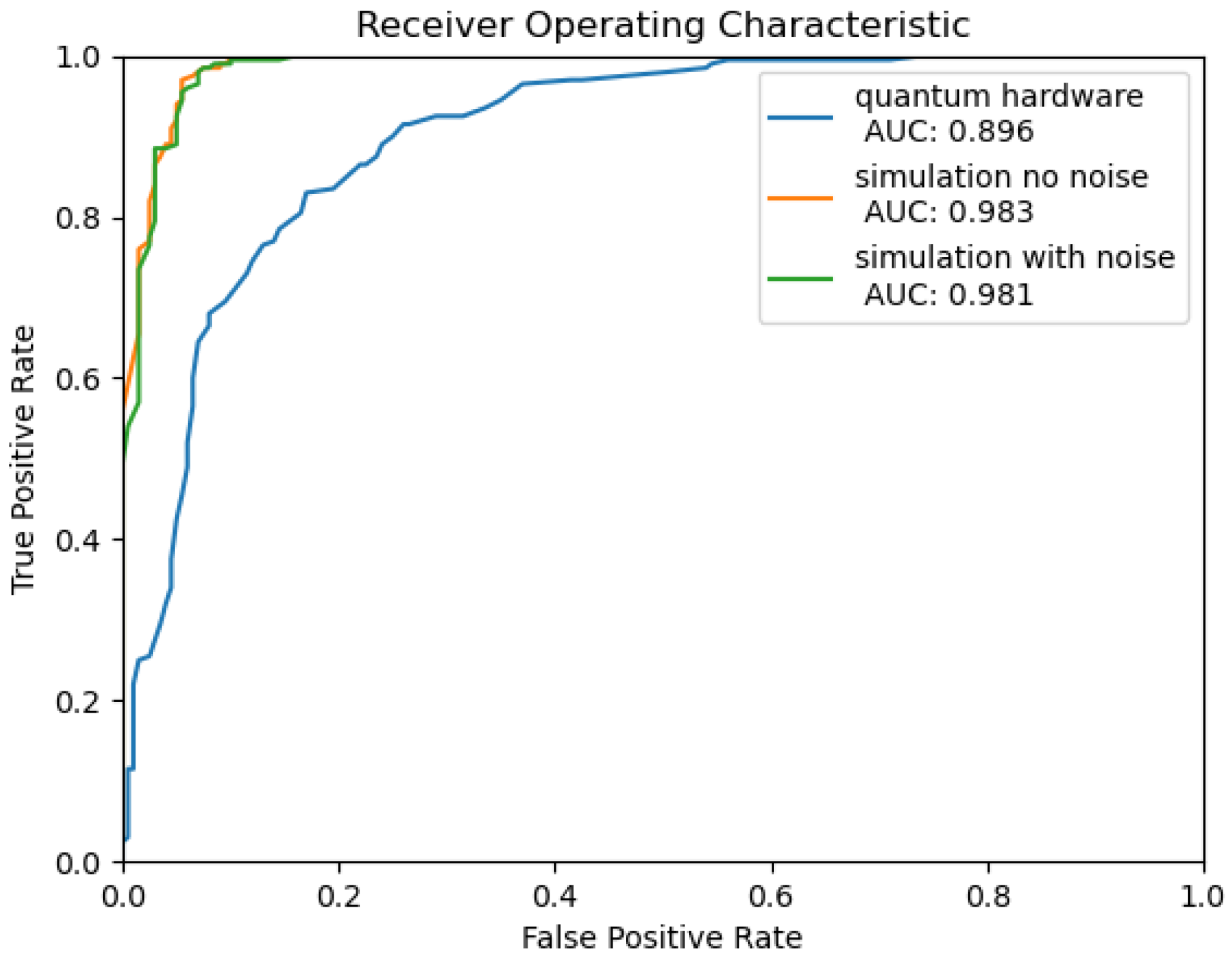
$U(\theta)$

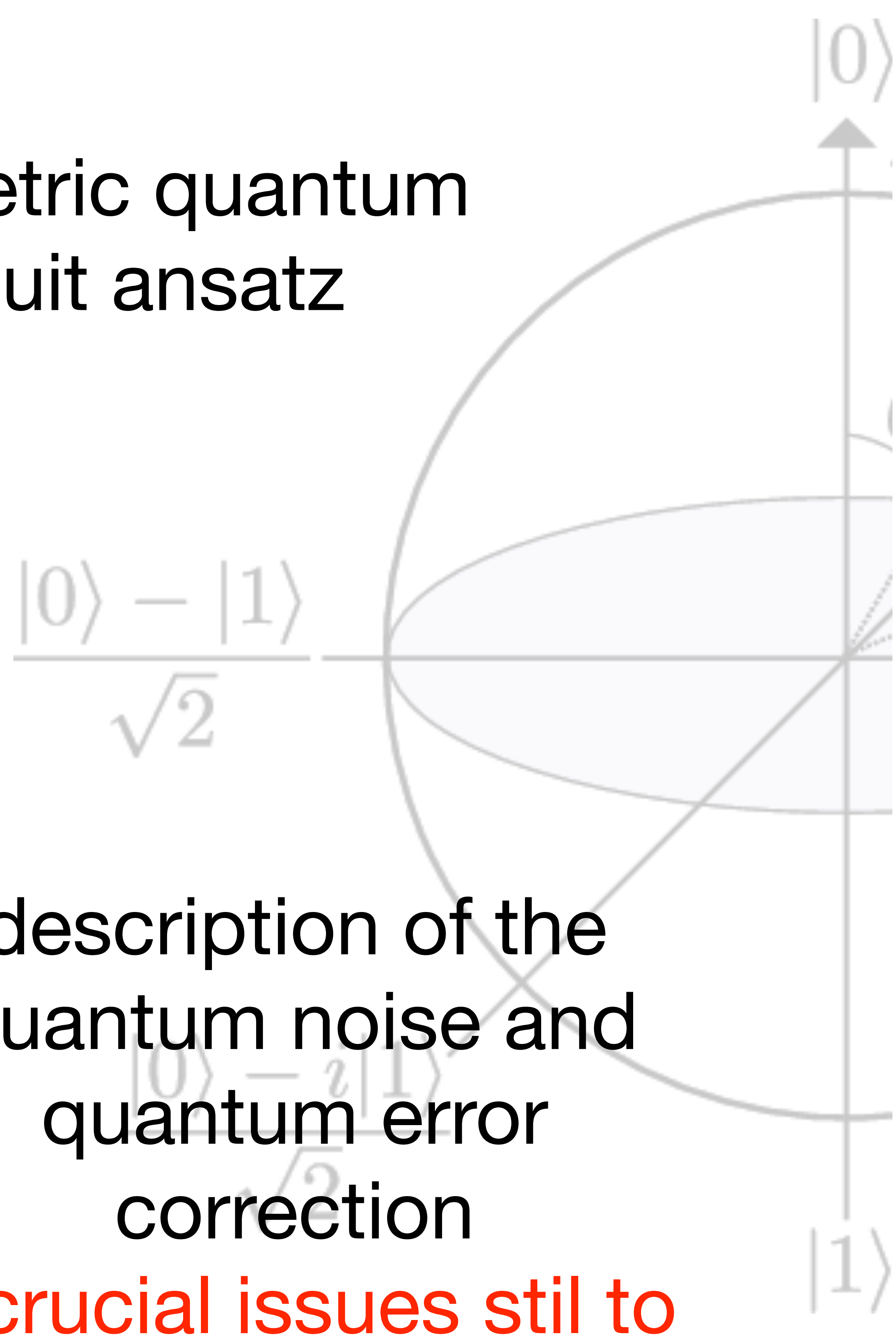
```
q0:     —RX—RY—RZ—o————————X—RX—RY—RZ—o————————X—RX—RY—RZ—o————————X—RX—RY—  ...
q1:     —RX—RY—RZ—X—o——————|—RX—RY—RZ—X—o——————|—RX—RY—RZ—X—o——————|—RX—RY—  ...
q2:     —RX—RY—RZ———X—o————|—RX—RY—RZ———X—o————|—RX—RY—RZ———X—o————|—RX—RY—  ...
q3:     —RX—RY—RZ—————X—o——|—RX—RY—RZ—————X—o——|—RX—RY—RZ—————X—o——|—RX—RY—  ...
q4:     —RX—RY—RZ———————X—o—|—RX—RY—RZ———————X—o—|—RX—RY—RZ———————X—o—|—RX—RY—  ...
q5:     —RX—RY—RZ—————————X—o—RX—RY—RZ—————————X—o—RX—RY—RZ—————————X—o—RX—RY—  ...

q0: ... RZ—o————————X—RX—RY—RZ—o————————X—RX—RY—RZ—o————————X—RX—RY—RZ—
q1: ... RZ—X—o——————|—RX—RY—RZ—X—o——————|—RX—RY—RZ—X—o——————|—RX—RY—RZ—
q2: ... RZ———X—o————|—RX—RY—RZ———X—o————|—RX—RY—RZ———X—o————|—RX—RY—RZ—
q3: ... RZ—————X—o——|—RX—RY—RZ—————X—o——|—RX—RY—RZ—————X—o——|————————————
q4: ... RZ———————X—o—|—RX—RY—RZ———————X—o—|—RX—RY—RZ———————X—o—|————————————
q5: ... RZ—————————X—o—RX—RY—RZ—————————X—o—RX—RY—RZ—————————X—o————————————
```

parametric quantum circuit ansatz





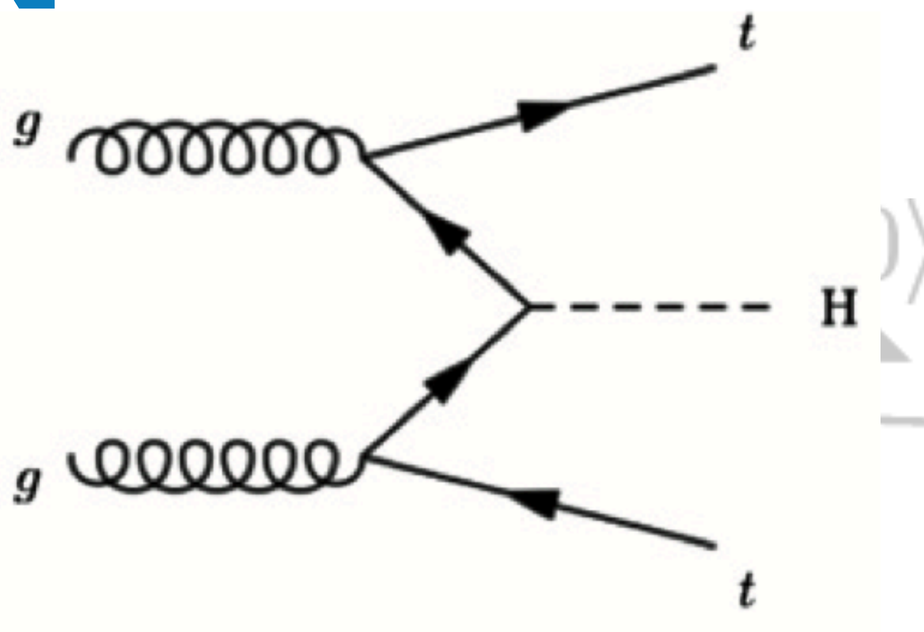


description of the quantum noise and quantum error correction

a crucial issues stil to be solved …

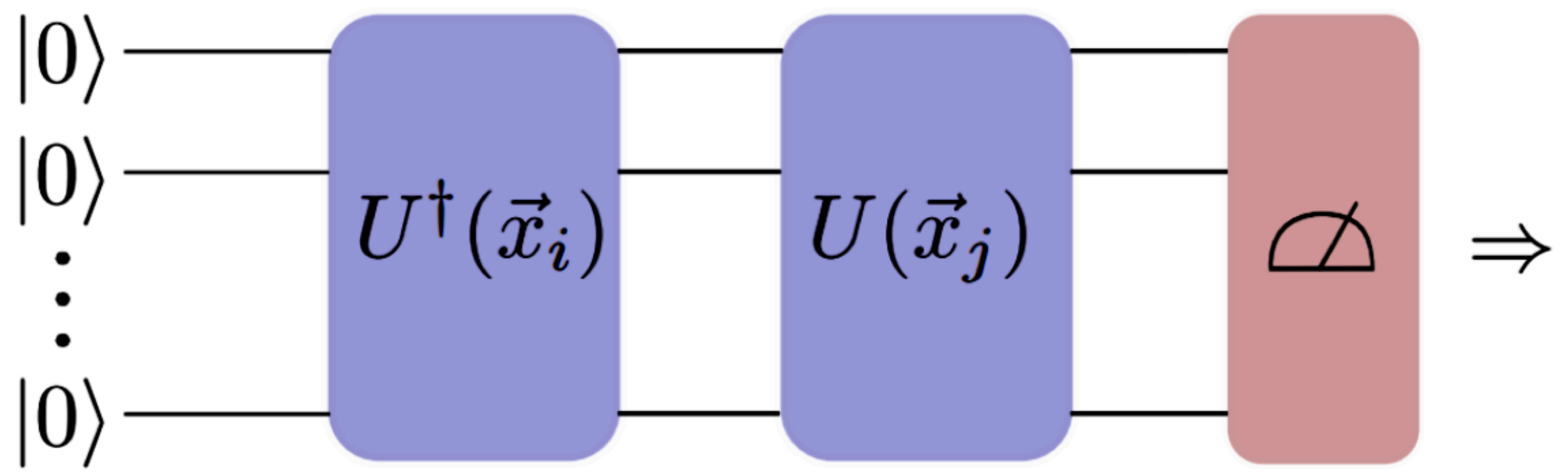
S.Bordoni et al, Particles 2023, 1, 1–15

QML IN HEP: HIGGS CLASSIFICATION



- Classical Support Vector Machine with Quantum Kernels acceleration employed in probing of the Higgs boson coupling to the top quark with the $t\bar{t}H(\rightarrow \gamma\gamma)$ channel

QSVM

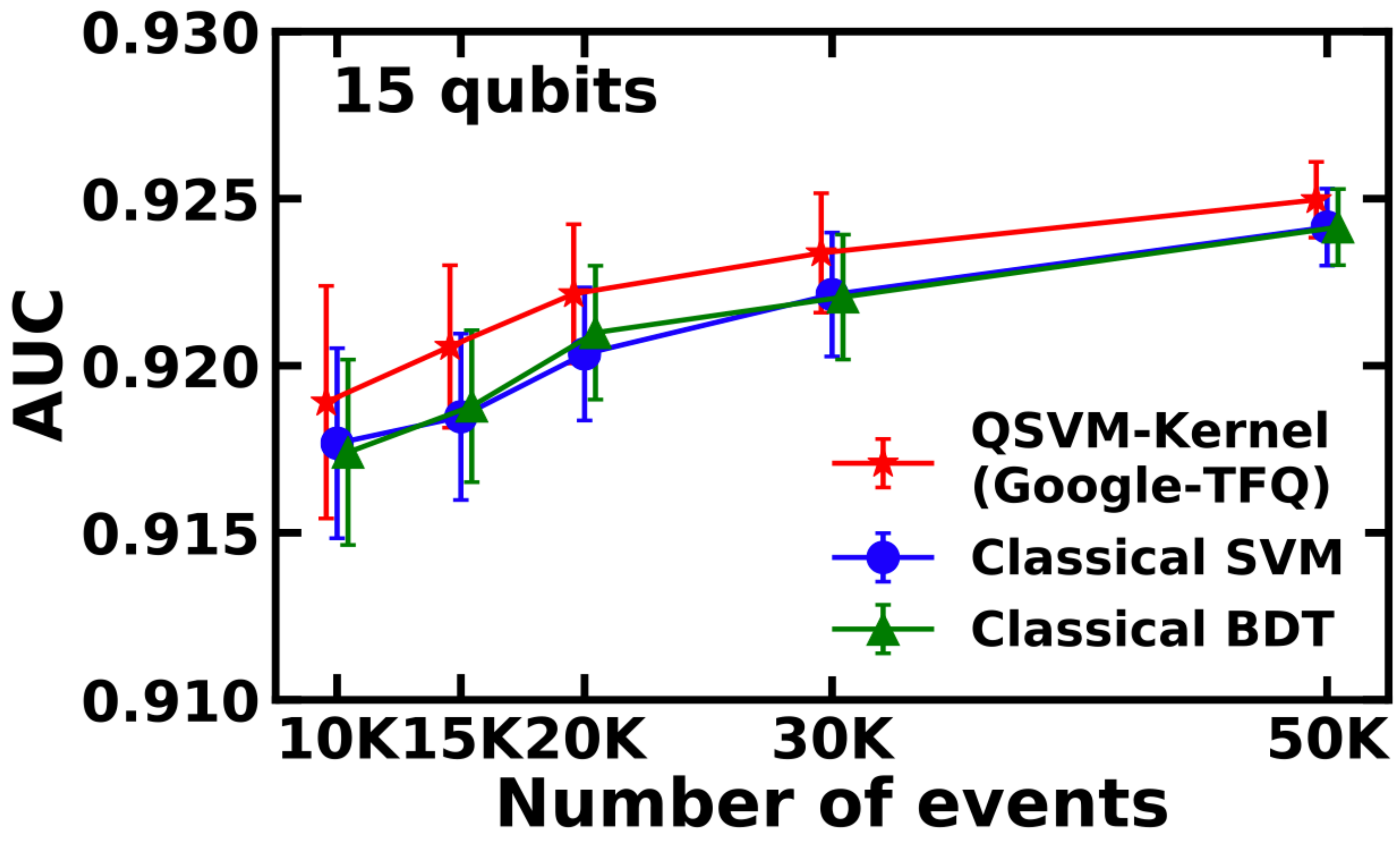


$$y' = sgn(\sum_{i=1}^{t} \alpha_i y_i k(\vec{x}_i, \vec{x}') + b)$$ SVM output

$$\Rightarrow \quad k(\vec{x_i}, \vec{x_j}) = |\langle \Phi(\vec{x_i}) | \Phi(\vec{x_j}) \rangle|^2 = |\langle 0^{\otimes N} | \mathcal{U}^\dagger_{\Phi(\vec{x_i})} \mathcal{U}_{\Phi(\vec{x_j})} | 0^{\otimes N} \rangle|^2$$

Dataset:

- signal and dominant backgrounds considered, simulated with Delphes
- input features: 23 object-based kinematic variables from the ATLAS analysis



Sau Lan Wu et al, arxiv:2104.05059

QML IN HEP: HIGGS CLASSIFICATION

- an alternative approach: using a programmable quantum annealer …
- task: classification of $H \to \gamma\gamma$ versus di-photon background

Quantum Annealing:

- define an ensamble of week classifiers $C_i(x) = \pm 1/N_c$
- maps the solution of the problem to the ground state of an Ising Hamiltonian

$$H = \sum_{i,j} J_{ij} s_i s_j + \sum_i h_i s_i$$

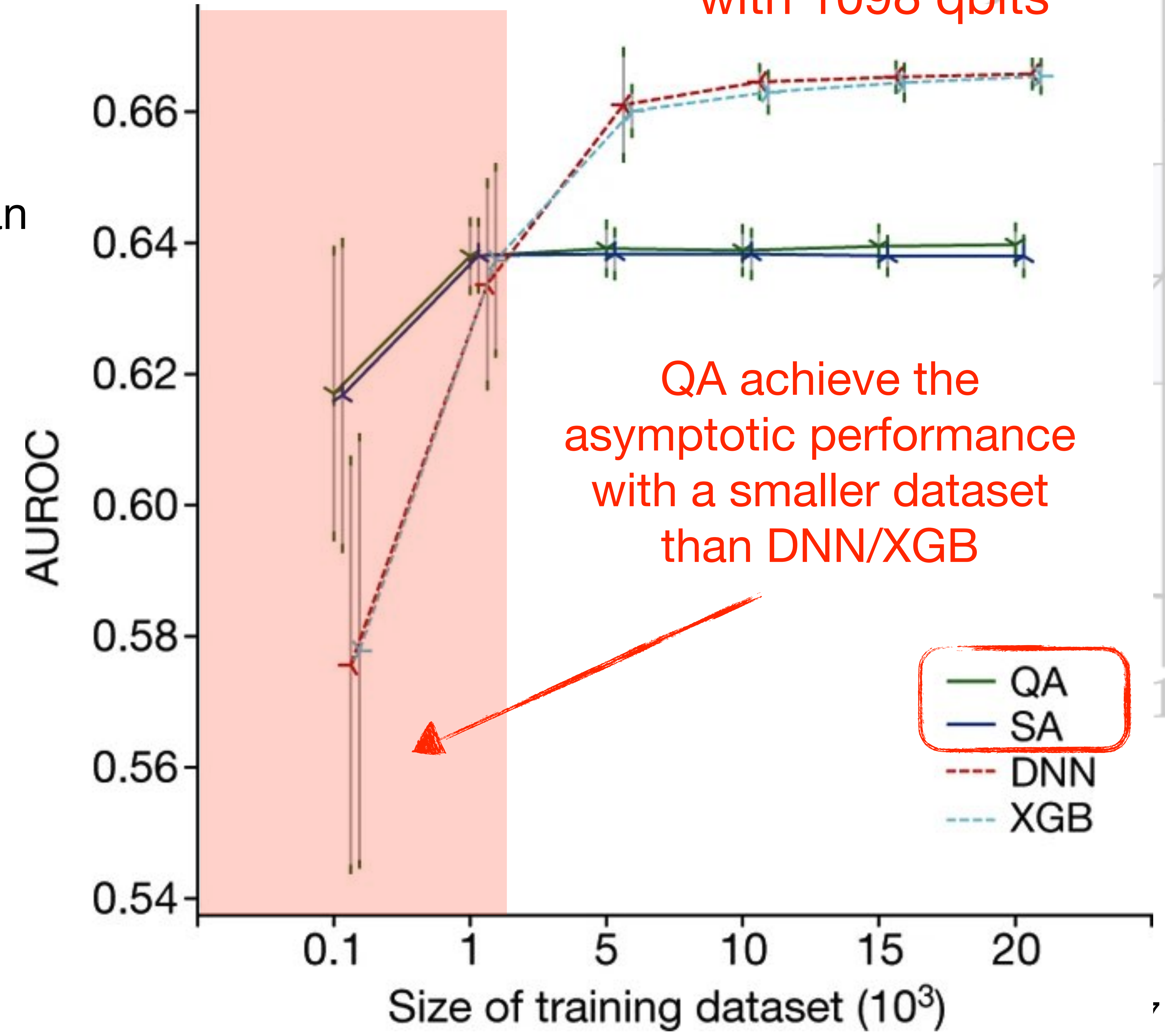
$$C_i = \sum_t C_i(x_t) y_t$$

$$C_{ij} = \frac{1}{4} \sum_t C_i(x_t) C_j(x_t) \qquad h_i = \lambda - C_i + \frac{1}{2} \sum_j C_{ij}$$

- minimize H and return the ground state, building a strong classifier as:

$$R(x) = \sum_i s_i^* c_i(x) \in [-1,1]$$

D-wave hardware with 1098 qbits

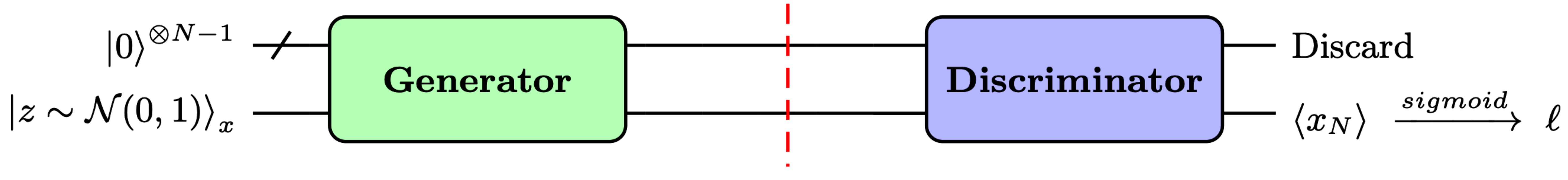


QA achieve the asymptotic performance with a smaller dataset than DNN/XGB

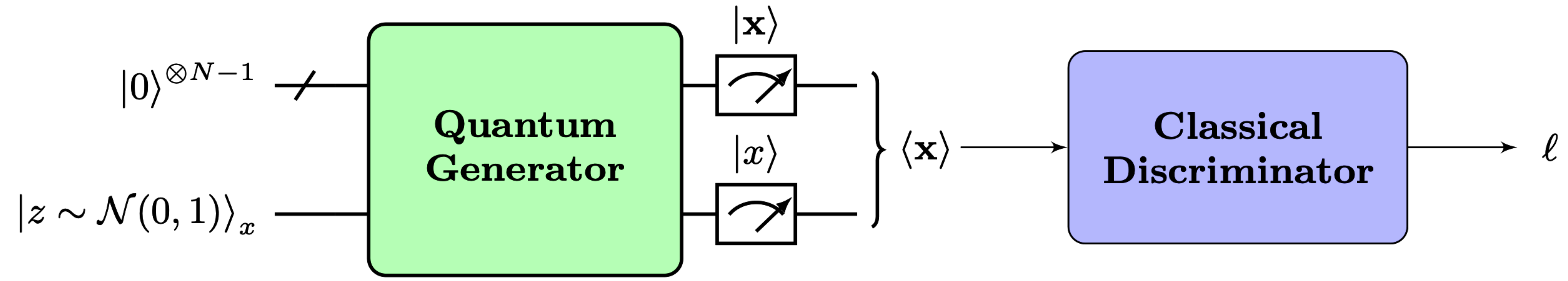
A. Mott et al, Nature volume 550, pages 375–379 (2017)

GENERATIVE QML APPLICATION: QUANTUM-GAN

- Quantum Generative Adversarial Networks: a quantum generator is trained against a discriminator (classical or quantum)
- In general, GAN could replace time-consuming and cpu-intensive simulations as Geant4
- with qGAN, N qubits can be used to simulate 2N features
- main issue (common to GANe qGAN): stability and convergence: to mitigate it it is useful to increase the latent space dimension, e.g. adding ancillary qubits

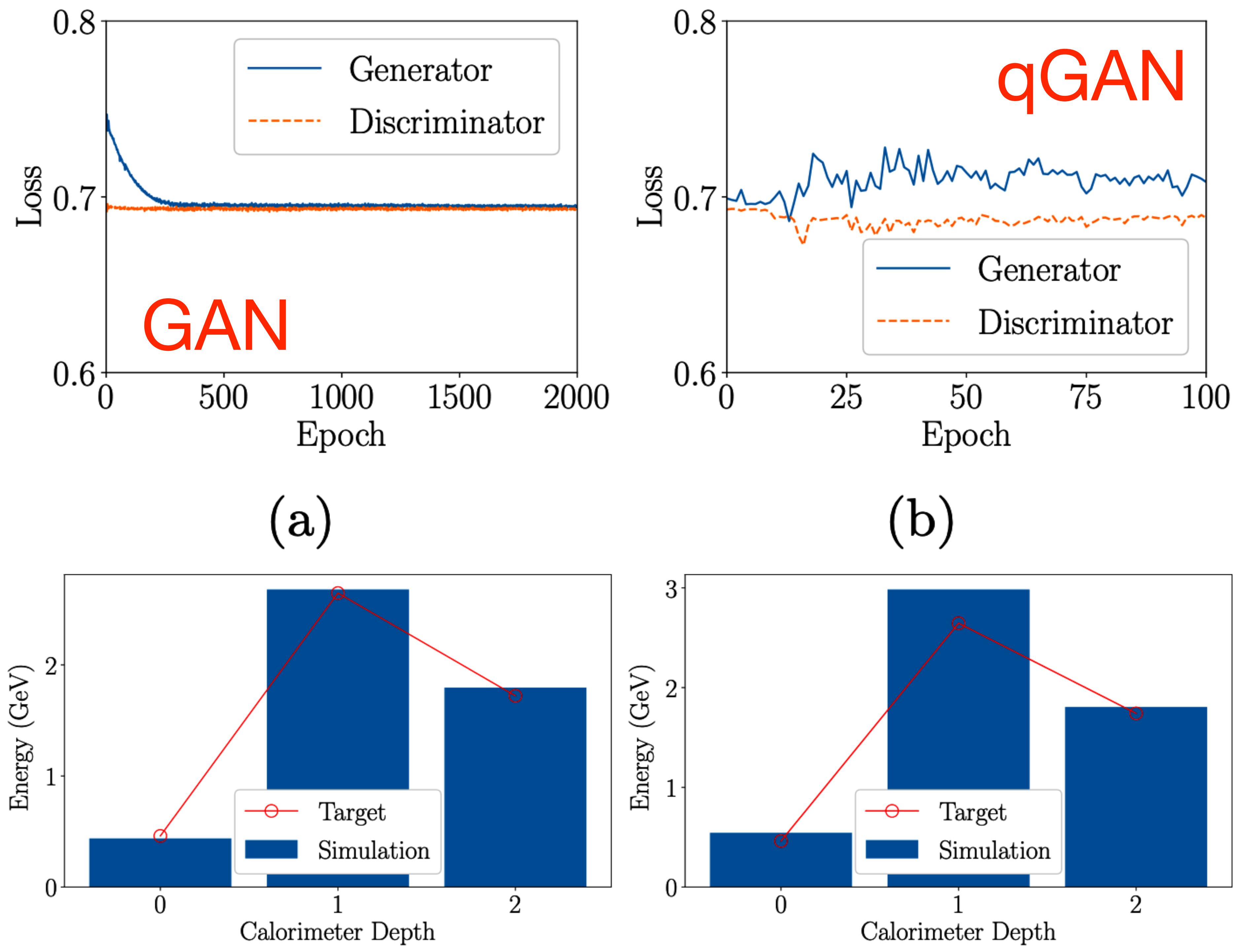


(a) *Fully quantum model.*



(b) *Hybrid model.*

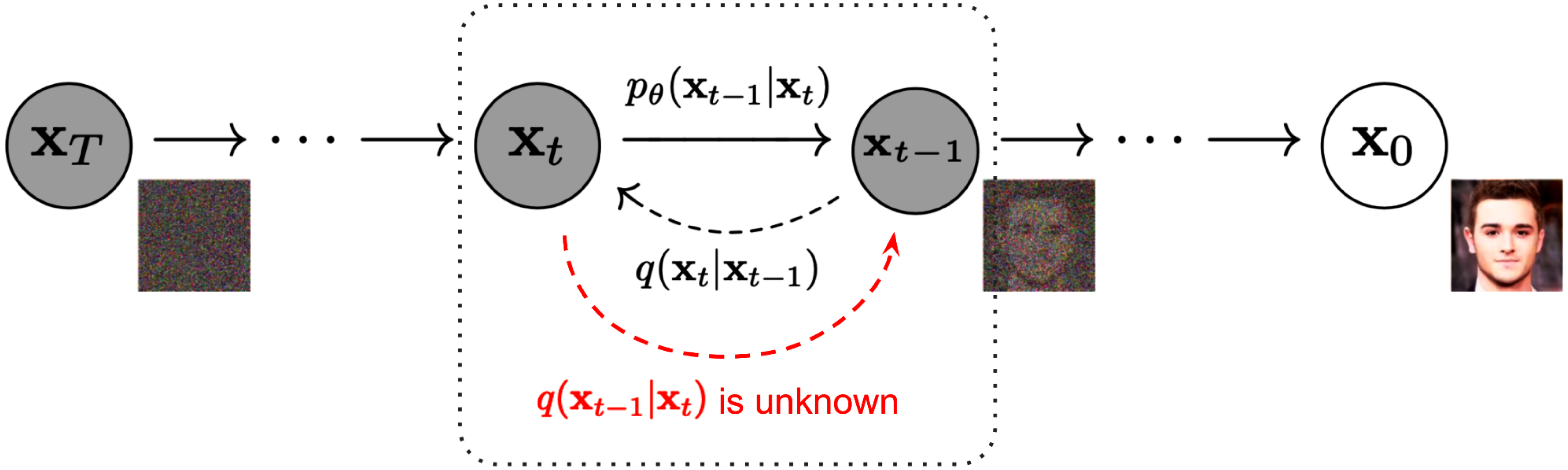
Calorimeter simulation: energy as a function of the depth (3 bins)



S.Y. Chang et al, arXiv:2101.11132

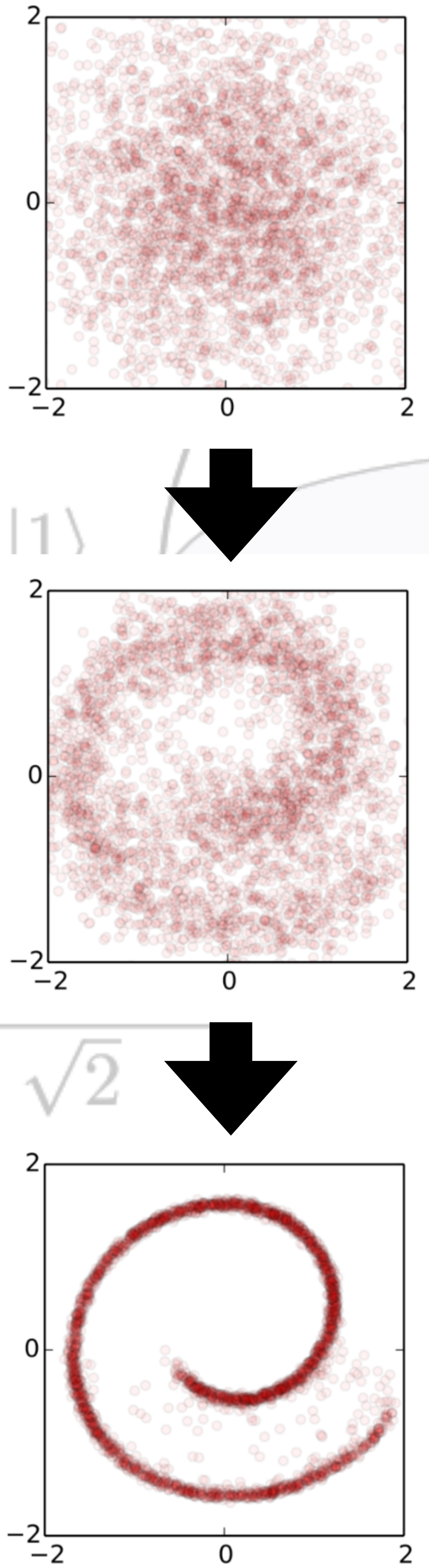
GENERATIVE QML APPLICATION: QUANTUM DIFFUSION MODEL

- classical deep diffusion models are generative models that leverage neural networks to implement a Markov chain of diffusion steps to slowly add random noise to data and then learn to reverse the diffusion process to construct desired data samples from the noise



$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

predicted by a NN

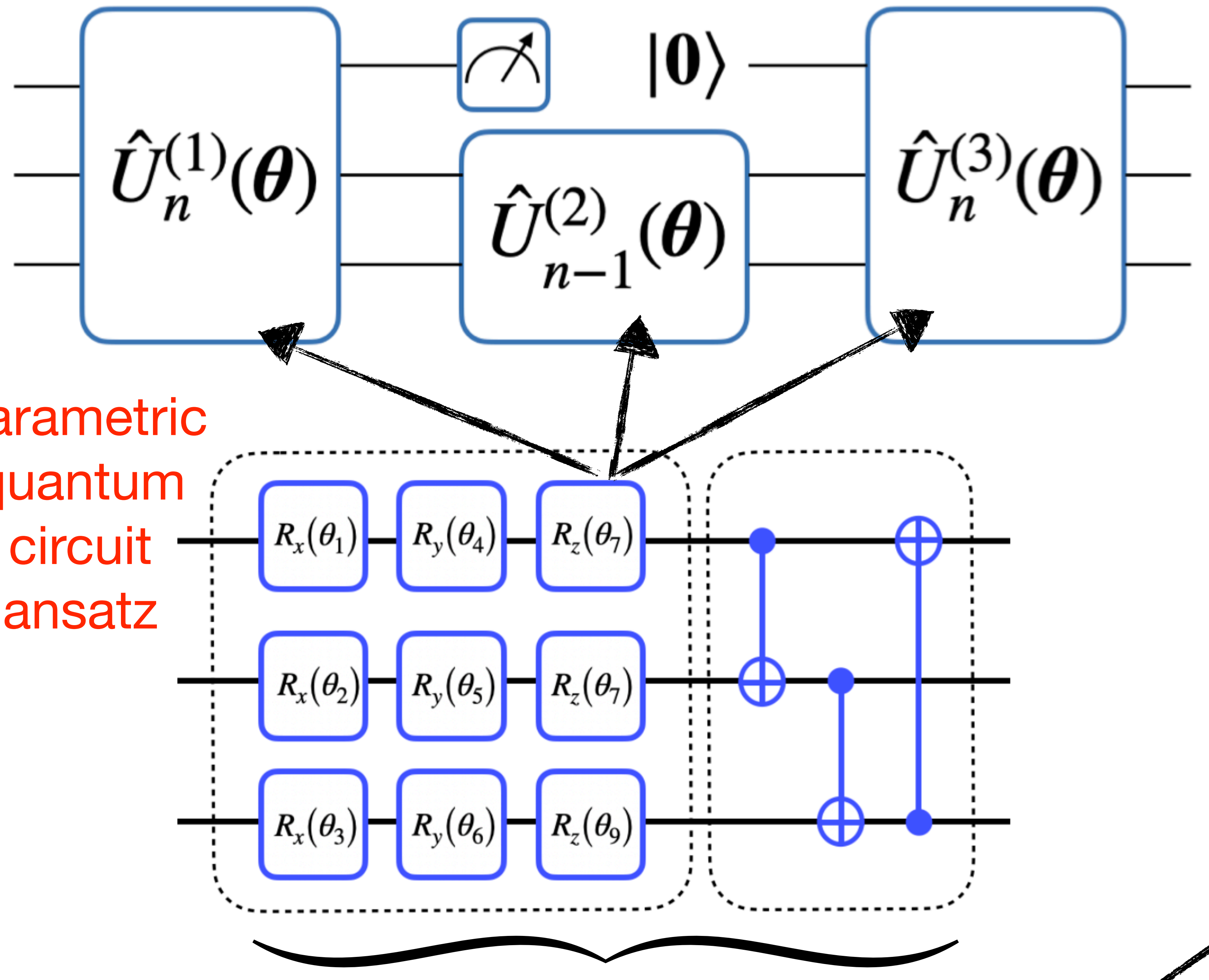


- today used in several tasks: image denoising, inpainting, super-resolution, image generation (ex. text-conditional image generators like DALL-E, Stable Diffusion, …)

GENERATIVE QML APPLICATION: QUANTUM DIFFUSION MODEL

- Quantum Diffusion Models: data points encoded into quantum states. Markov chain implemented by a quantum circuit acting as a denoiser
- can be used in a full quantum model or a hybrid model, where the quantum circuit is trained in the latent space of a classical AE
- conditioning achieved by adding ancillary qubits to encode labels

Quantum Denoiser

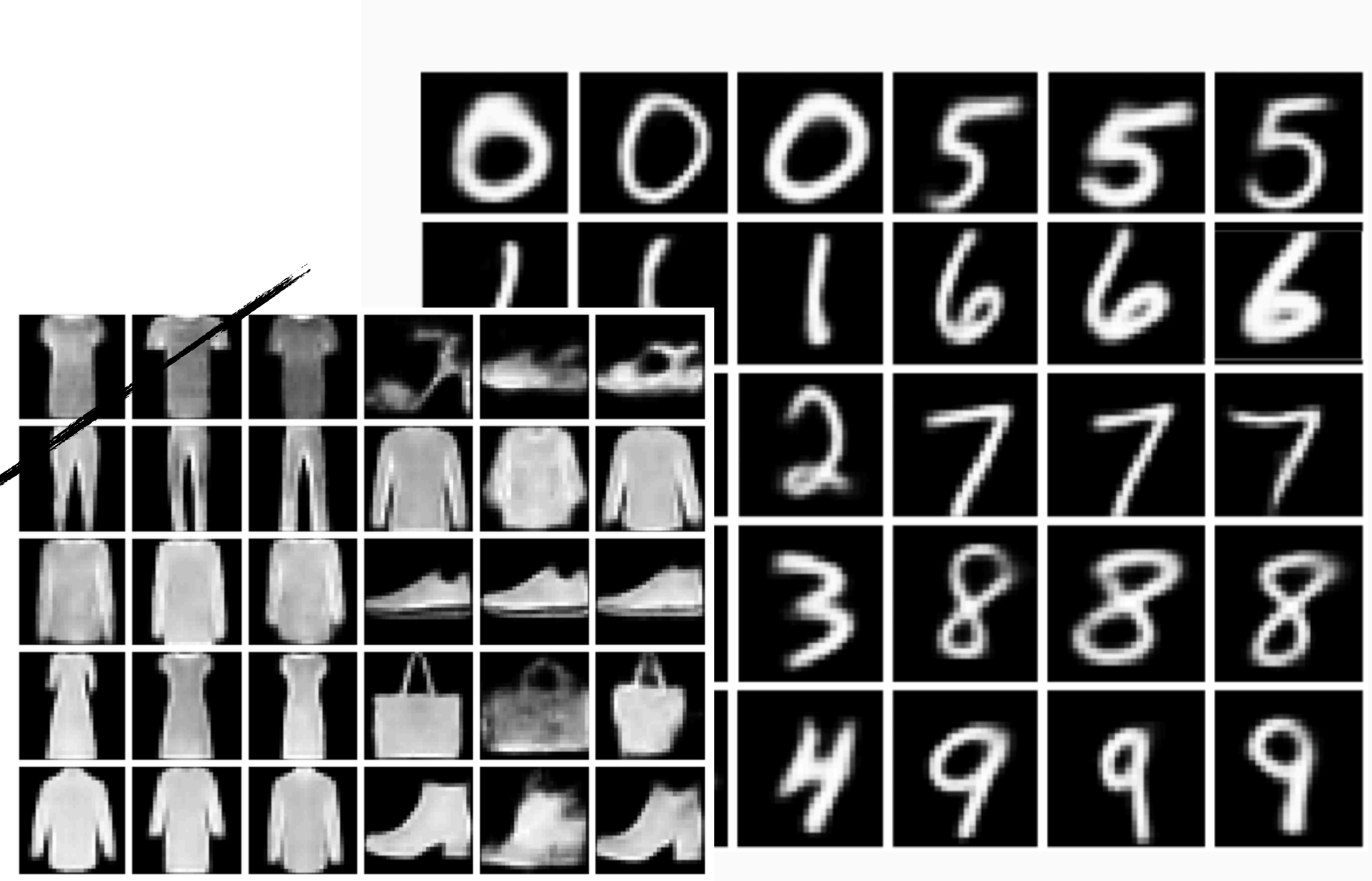


$$P(\theta, t)\,|\mathbf{x}_t\rangle = |\mathbf{x}_{t-1}\rangle \Rightarrow \quad P(\theta,1)\cdots P(\theta,T)\,|\mathbf{x}_T\rangle = |\mathbf{x}_0\rangle$$

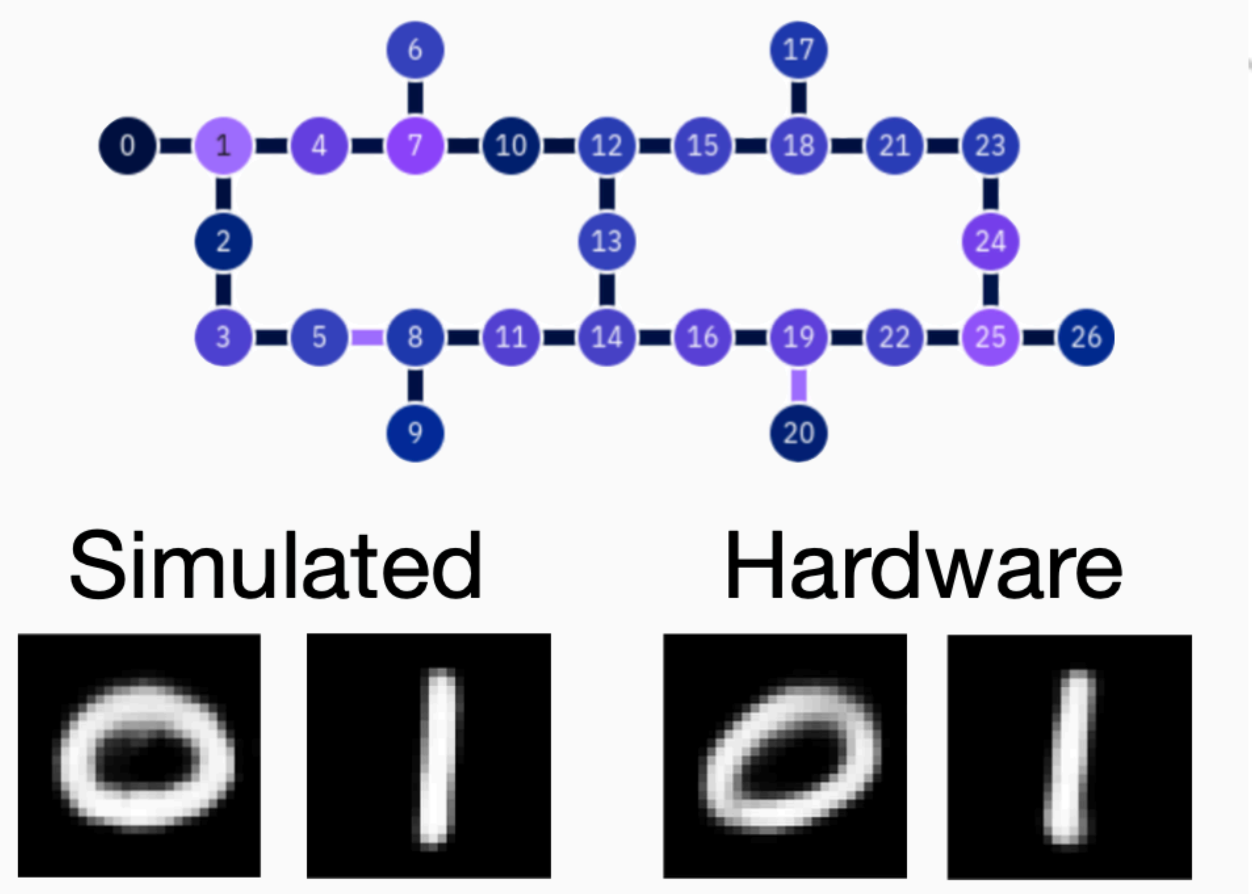
$$Loss = 1 - \mathbb{E}[F]$$ quantum in-fidelity

Digit	0	1	2	3	4	5	6	7	8	9
AUC	0.951	0.977	0.983	**0.989**	**0.857**	0.899	0.975	0.928	0.908	0.933

Conditioned hybrid (simulation)



Conditioned hybrid (quantum hw)



A. Cacioppo et al. arXiv:2311.15444 [quant-ph]

THE ROAD AHEAD (CONCLUSION)

- Quantum computing offers great opportunities in High Energy Physics:
  - exciting field supported in the public and private sectors
  - a lot of space for original ideas and new algorithms yet to be discovered

- Many questions need to be answered:
  - what are the really promising applications in our field?
  - how we benchmark performances?
  - how to cope with classical data encoding/reduction?
  - QML trainability?
  - …

- quantum advantage in real-word applications will require a new generation of quantum computers in terms of size, fault tolerance, connectivity and quantum gates implementation …

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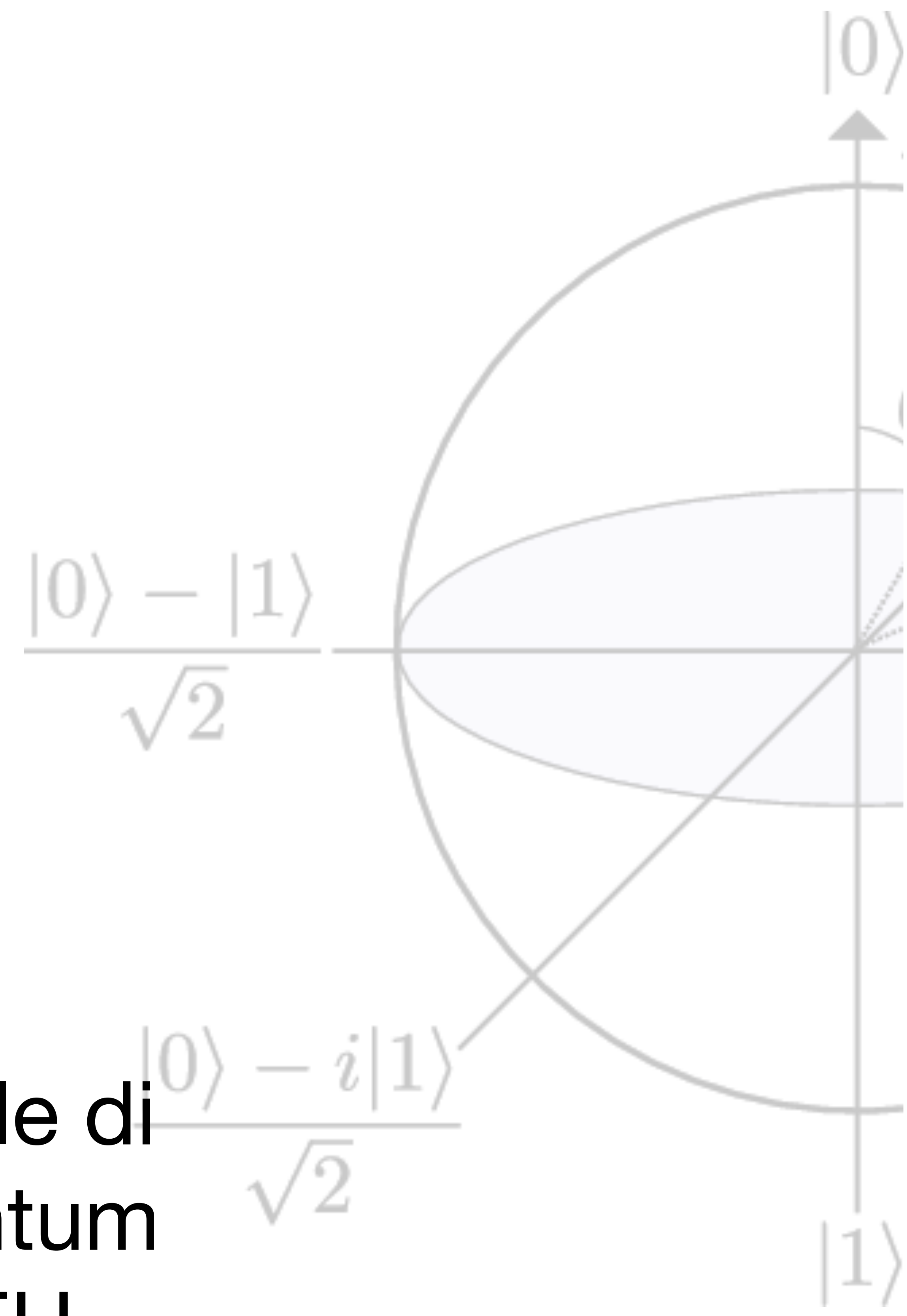

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