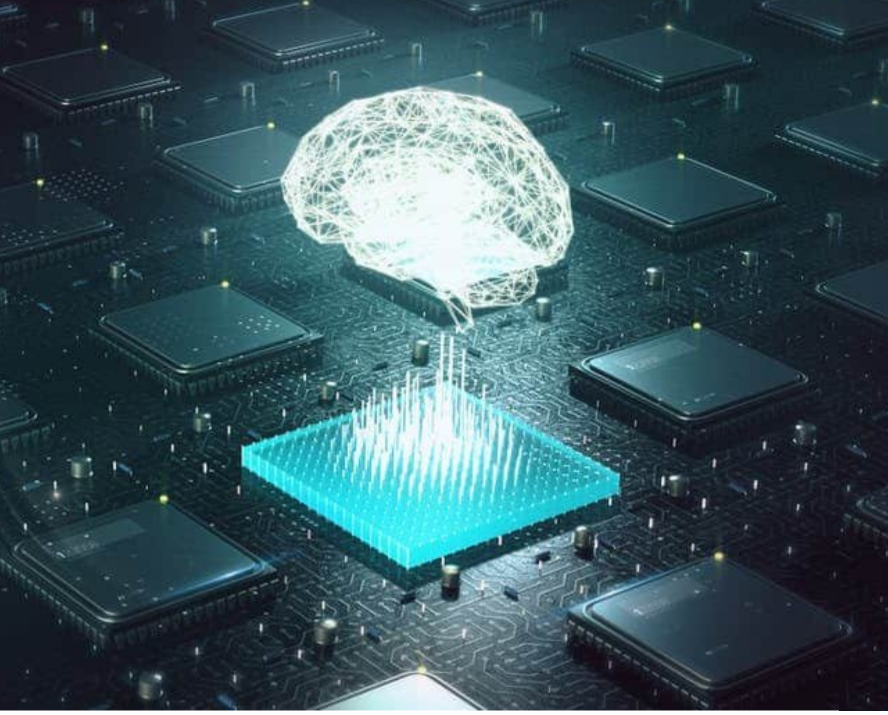
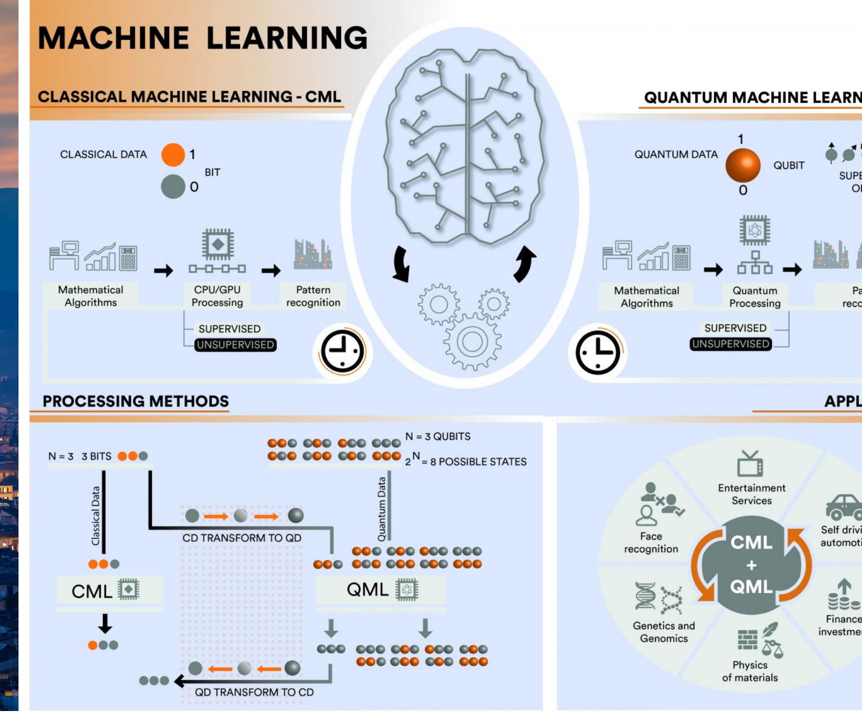


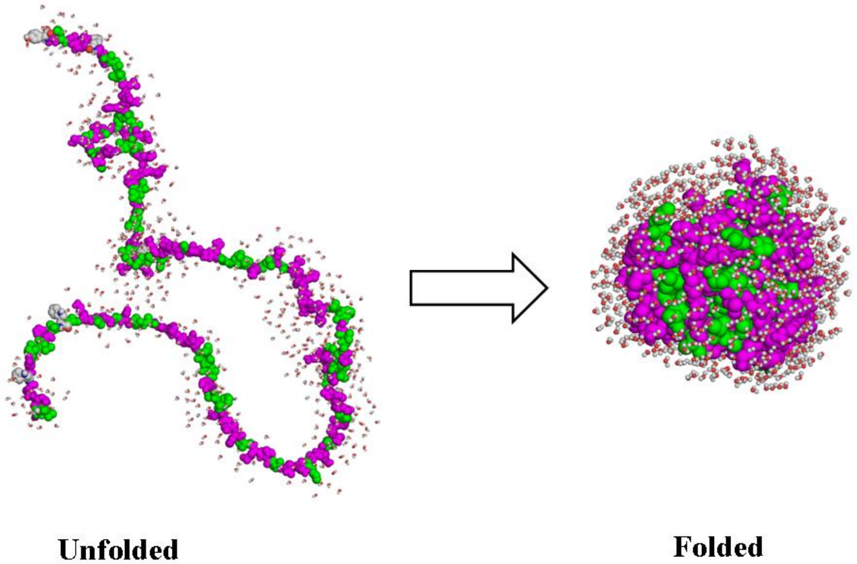


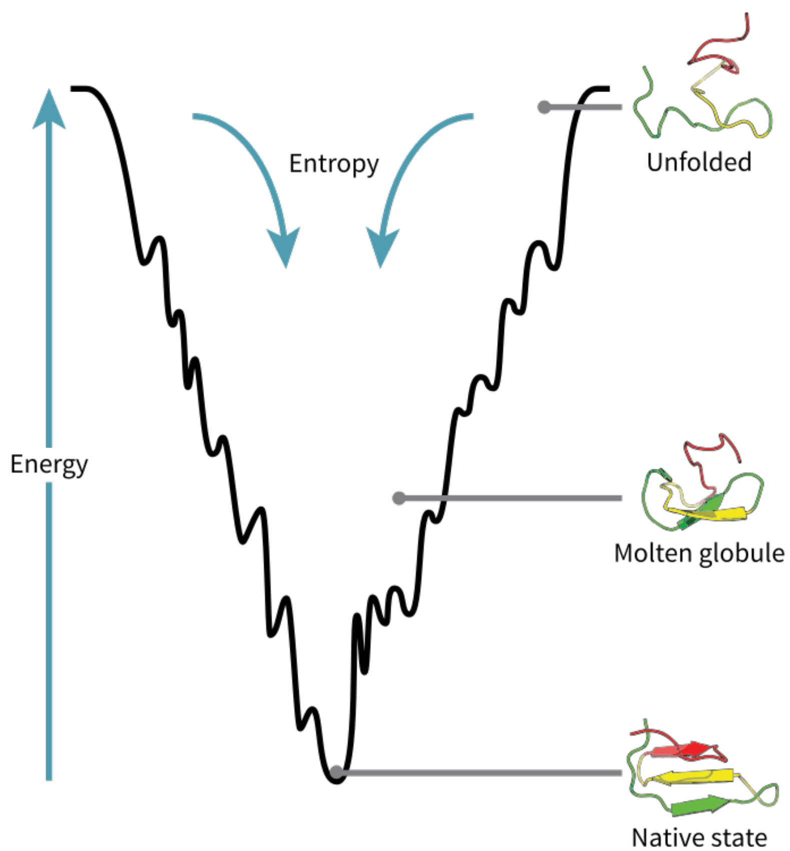
Quantum Computing for High-Energy Physics

Michael Spannowsky

IPPP, Durham University

Protein-folding and Levinthal's Paradox





- Elongated proteins fold to same state within microseconds
- Some proteins have 3^{300} conformations
- <u>Levinthal's Paradox (1969)</u>:
  Sequential sampling of states would take longer than lifetime of Universe (even if only nanoseconds per state spent)
- Solution: No sequential sampling, but rapid descend into the potential minimum.

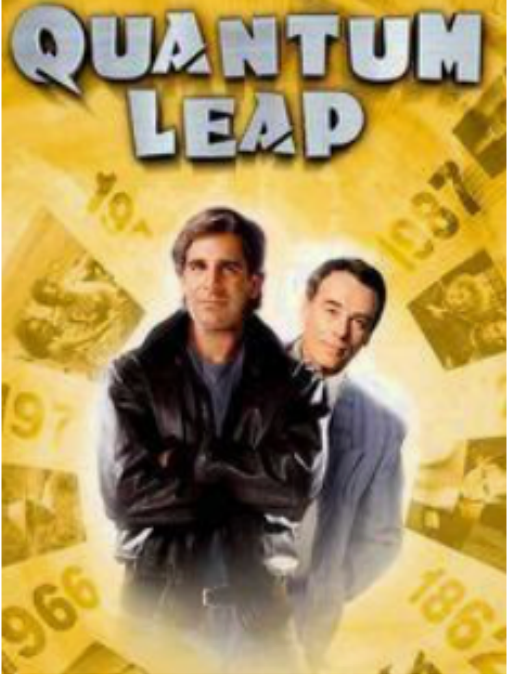
→ **Optimisation = Life**

→ Solution of mathematical problem can be found quickly if encoded in ground state of complex system

"Nature is quantum [...] so if you want to simulate it, you need a quantum computer"
– Richard Feynman (1982)

Easily said … so how do we do that?

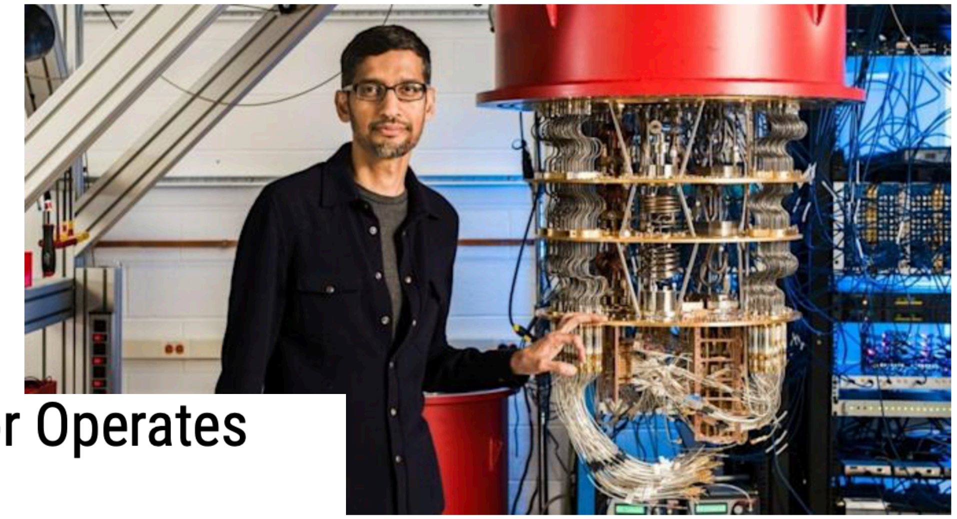
Beginning of a scientific journey that accelerated in recent years tremendously….



The Morning After: Google claims 'quantum supremacy'

And a controversial 'Ghost in the Shell' trailer.

R. Lawler
@Rjcc
October 24th, 2019



Master in Elektrotechnik, Informatik, Robotik, Maschinenwesen o. ä. (w/m/d)
German Aerospace Center (DLR) · Oberpfaffenhofen, Bavaria, Germany (On-site)
4 company alumni

Professor Cyber Security im Online Fernstudium (m/w/d)
IU International University of Applied Sciences · Germany (Remote)
Actively recruiting

Expertin für Post-Quanten-Kryptographie (w/m/d)
Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)
Actively recruiting

Master Thesis: Design of digitally enhanced power management circuits for Future Quantum Computers
Forschungszentrum Jülich · Jülich, North Rhine-Westphalia, Germany (On-site)
1 company alum

Expertin für Quantenkommunikation (w/m/d)
Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)
Actively recruiting

First Quantum Computer Simulator Operates The Speed Of Light

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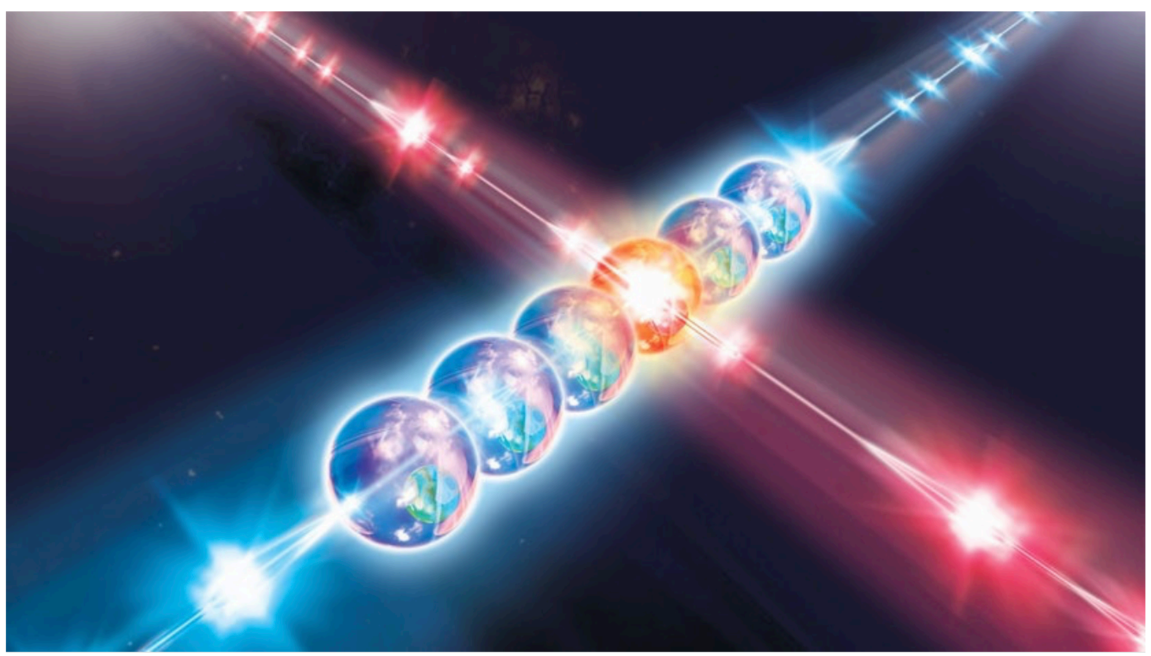
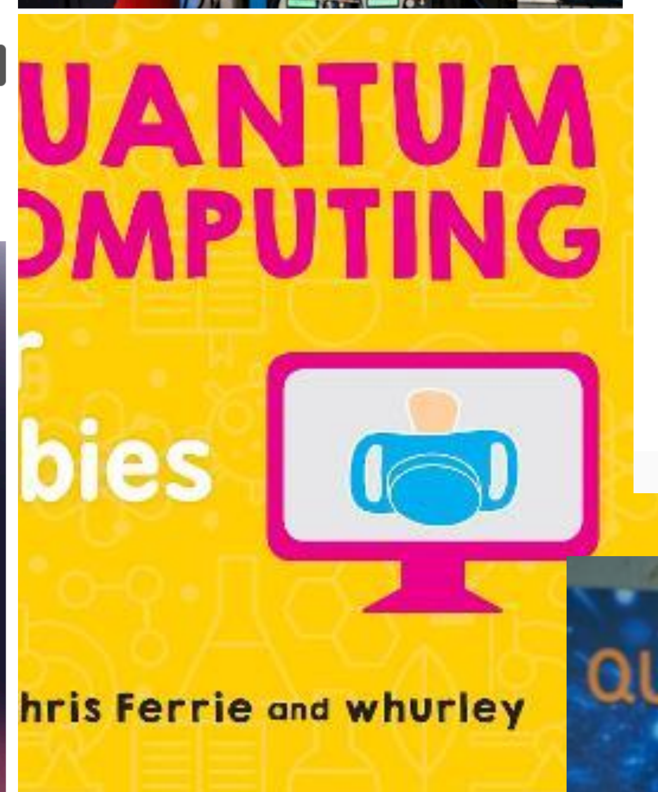
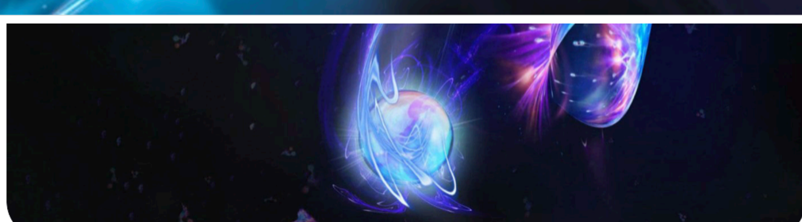
Kristen Philipkoski
Published 10 years ago: September 2, 2011 at 7:02 am - Filed to: COMPUTING





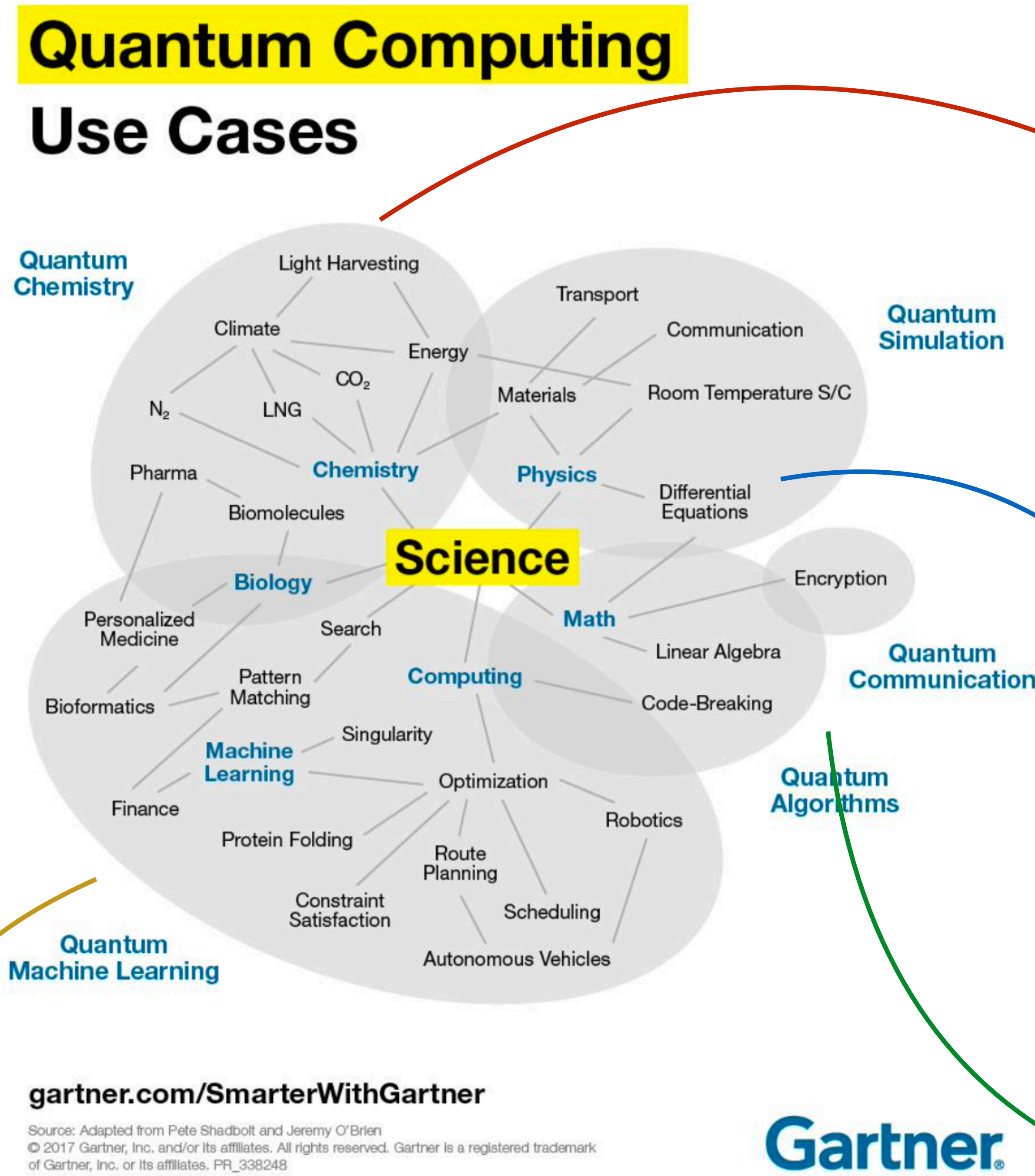


uantum Computers Will Be Incredibly Useful For

Computers don't exist in a vacuum. They serve to solve problems, and the type of problems they can solve are influenced by their hardware. Graphics processors are specialized for rendering images; artificial intelligence processors for AI; and quantum computers designed for... what? While the power of quantum computing is impressive, it does not mean that existing ...

Futuristic News
208 followers

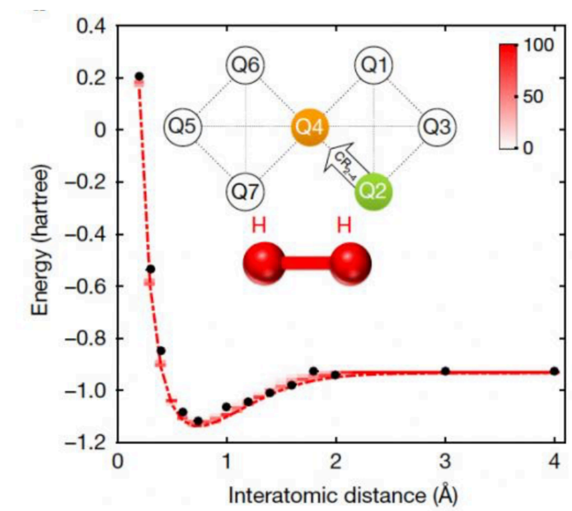
Private and Public Sector is placing big bets on Quantum Computing



Quantum Chemistry

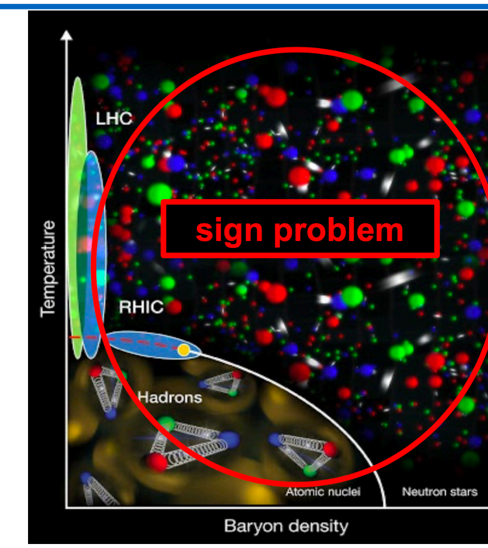
- Bound state
- Sampling
- Optimisation

Logistics problems



Fundamental Physics

- Cond Mat/PP/QOptic
- Hamiltonian simulation
- Non-perturbative
- Entanglement



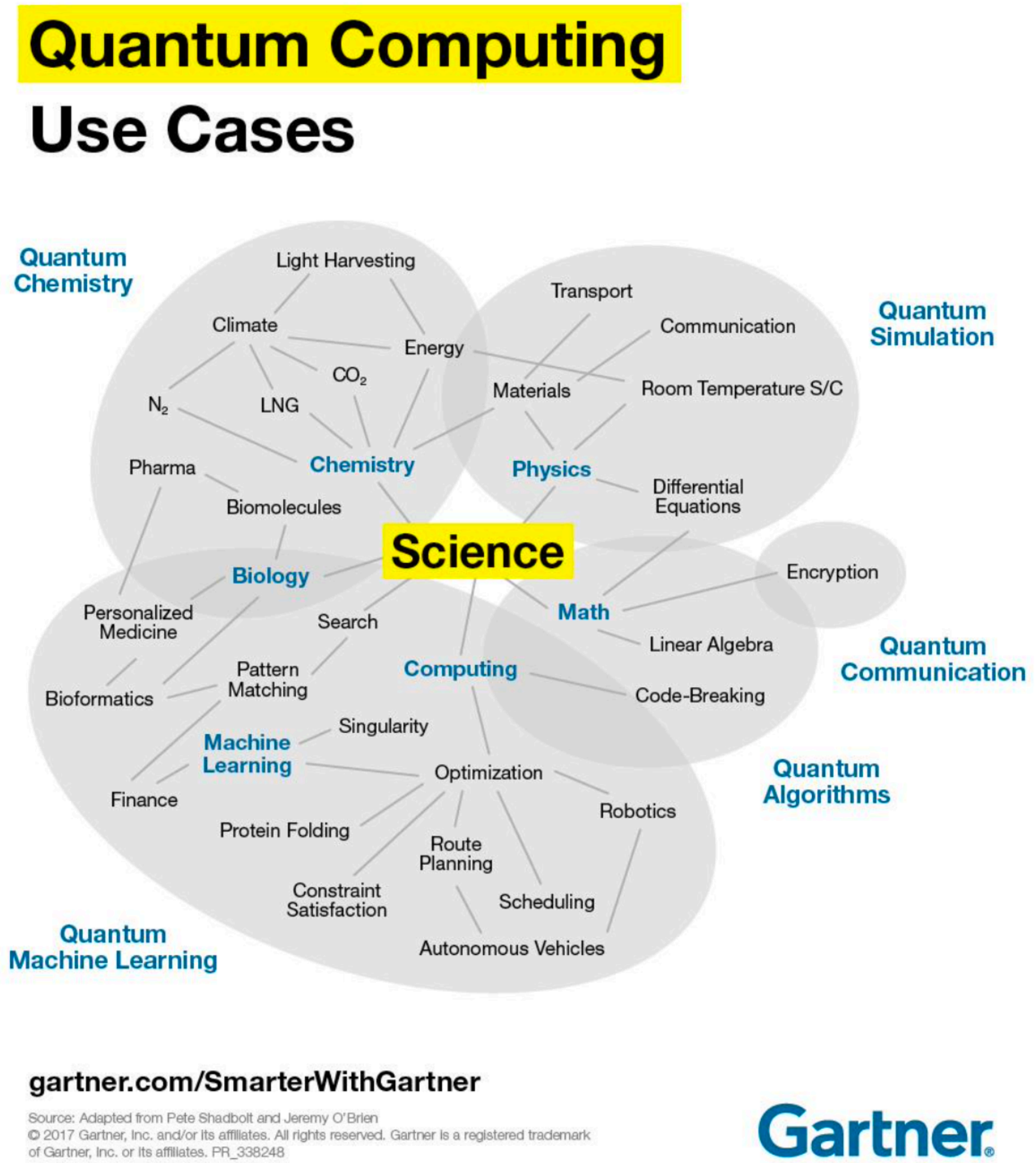
Quantum Information

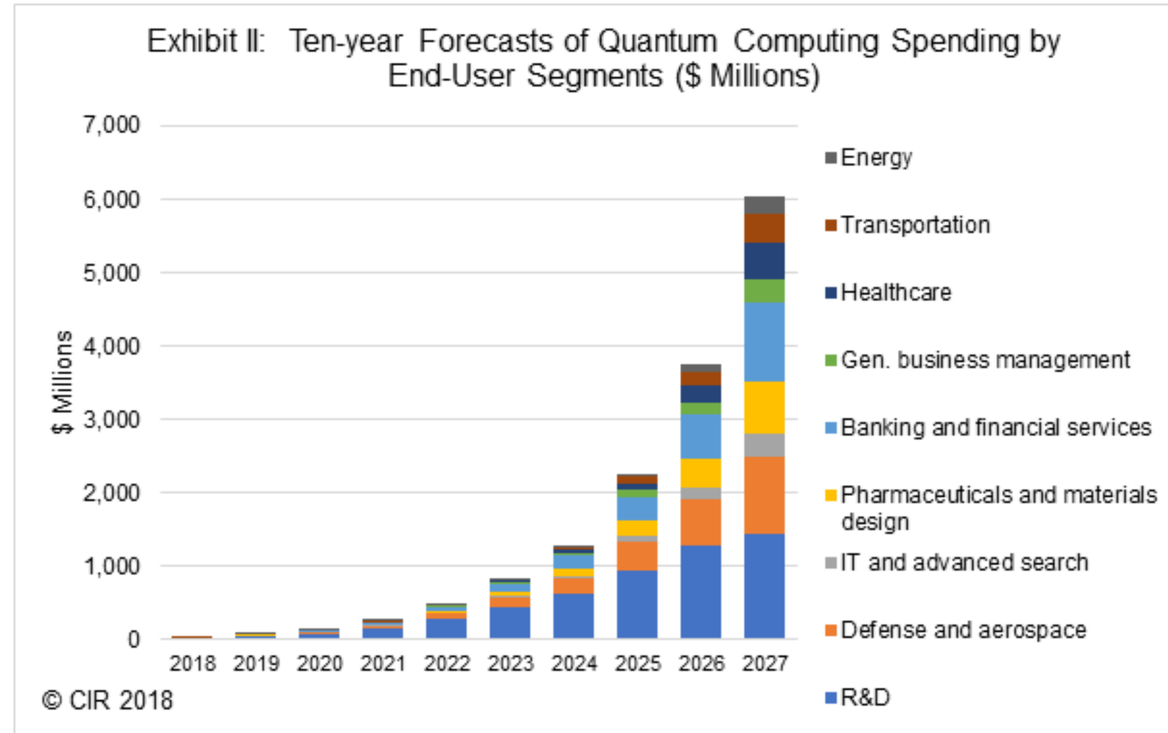
- Teleportation
- Quantum Internet
- Encryption
- Information access / storage

Machine Learning

- QNN
- Quantum reservoirs
- Quantum reservoirs

Private and Public Sector is placing big bets on Quantum Computing



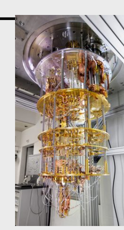
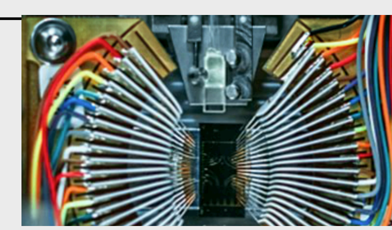
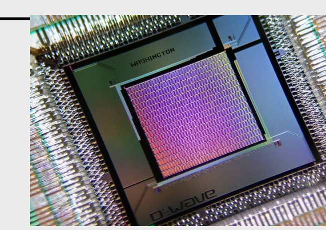
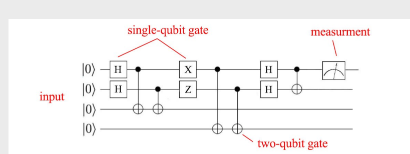
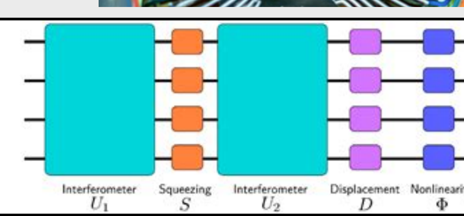
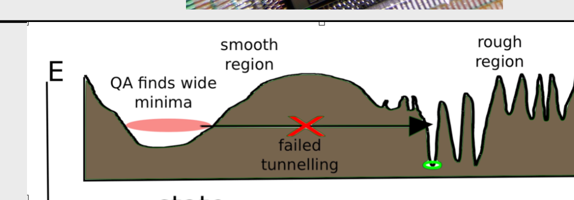


Significant financial investment expected across many sectors

In US, already now higher financial investment from private than public sector

→ All national and international labs have QC programmes (Fermilab, BNL, LBNL, CERN, Singapur, Abu Dhabi, …)

Popular Quantum Computing paradigms

Type	Discrete Gate (DG)	Continuous Variable (CV)	Quantum Annealer (QA)
Computing	Digital	Digital/Analog	Analog
Property	Universal (any quantum algorithm can be expressed)	Universal - GBS non-Universal	Not universal — certain quantum systems
Advantage	most algorithms and tech support	uncountable Hilbert (configuration) space	continuous time quantum process
How?	IBM - Qiskit ~500 Qubits	Xanadu	DWave - LEAP ~7000 Qubits
What?			
			

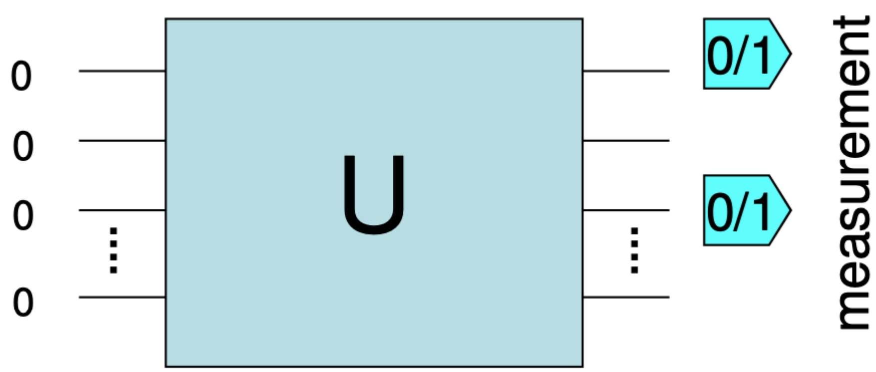
How most quantum algorithms work

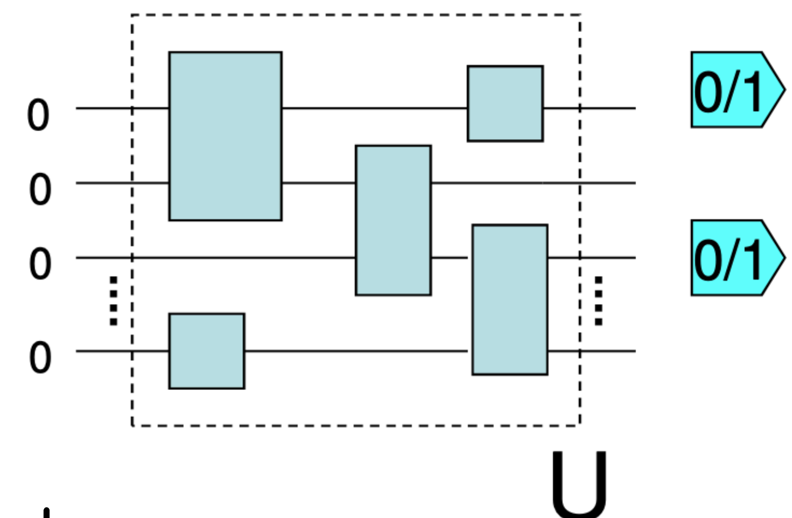
operator acts on Hilbert space states $U\,|x\rangle = |\Psi_1\rangle$

measurement of observable $\hat{U}$ corresponds to exp. value of operator U $\left\langle \hat{U} \right\rangle_\Psi = \frac{\langle\Psi|U|\Psi\rangle}{\langle\Psi|\Psi\rangle}$

statistical statement need to evaluate often

Need to encode Hilbert space and operator suitable for quantum system



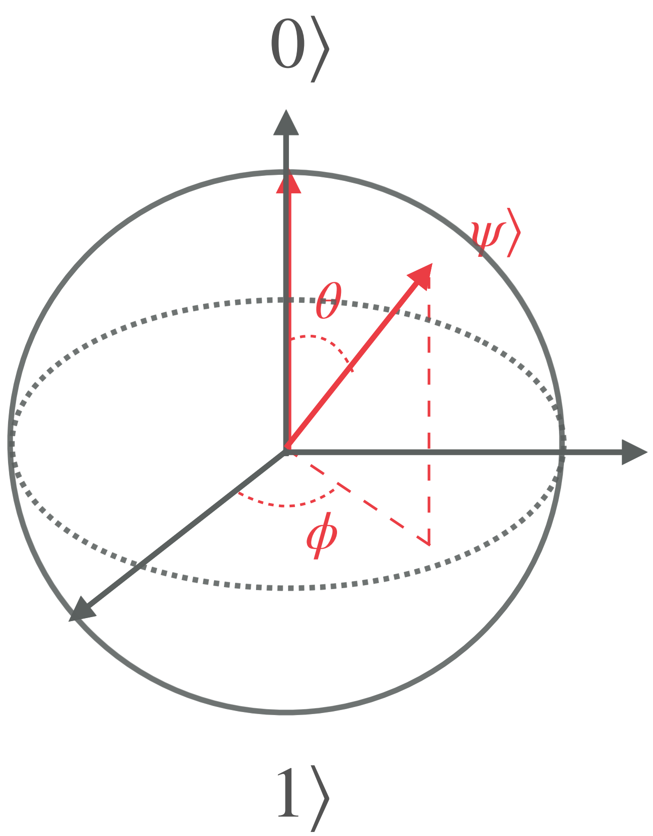


- Operator expressed in terms of individual gates
- Often 'Trotterization' (Suzuki-Trotter decomposition) needed:

For $H = \sum_{j=1}^{m} H_j \longrightarrow e^{iHt} = \left(\prod_{j=1}^{m} e^{-iH_j t/r} \right)^r + \mathcal{O}(m^2 t^2 / r)$

Rotation about the Bloch Sphere and state parametrisation

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



Measure

$0\rangle$

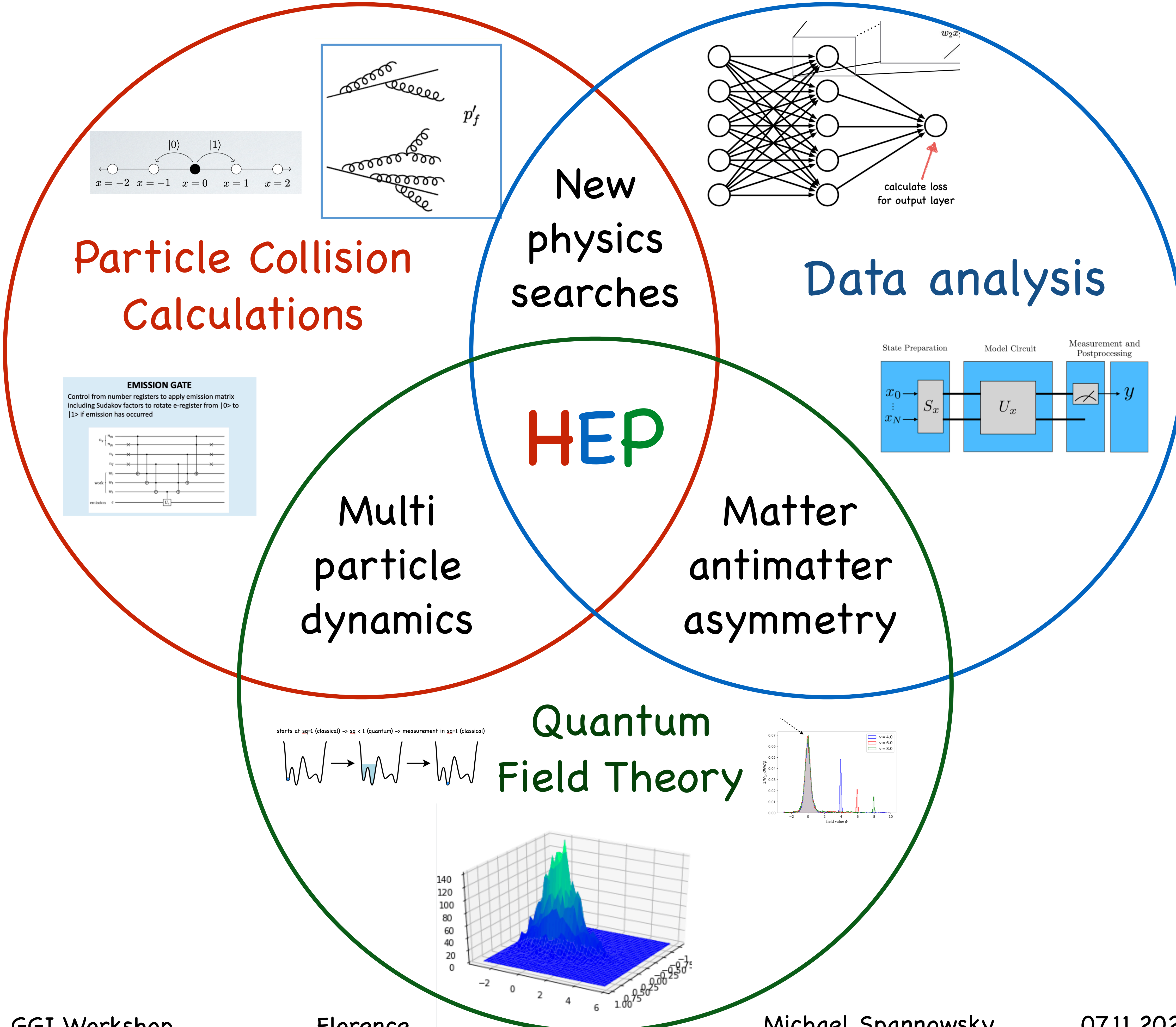
$1\rangle$ $\text{Prob}\left(\ 1\rangle\right) = \left(e^{i\phi}\sin\frac{\theta}{2}\right)^2$

$0\rangle$ $\text{Prob}\left(\ 0\rangle\right) = \left(\cos\frac{\theta}{2}\right)^2$

$1\rangle$

Apply Unitary rotation $U_3\ \ 0\rangle$: $U_3(\theta,\phi,\lambda) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}\sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}\sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}$

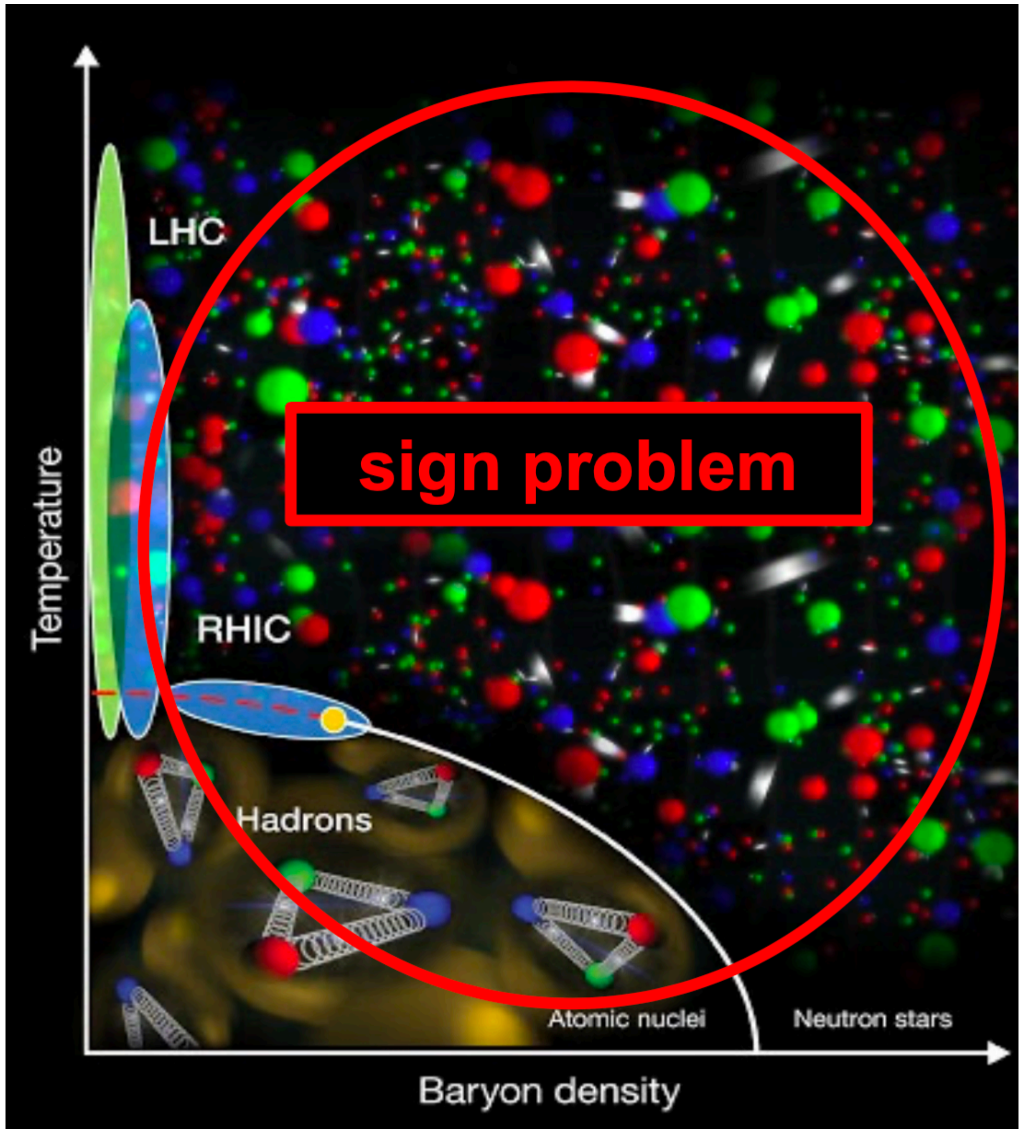
Extending this to a system of N qubits forms a 2^N-dimensional Hilbert Space


Particle Collision Calculations
New physics searches
Data analysis
HEP
Multi particle dynamics
Matter antimatter asymmetry
Quantum Field Theory
EMISSION GATE
Control from number registers to apply emission matrix including Sudakov factors to rotate e-register from |0> to |1> if emission has occurred
calculate loss for output layer
State Preparation
Model Circuit
Measurement and Postprocessing
starts at sq=1 (classical) -> sq < 1 (quantum) -> measurement in sq=1 (classical)

HEP application focused quantum simulations

- Sign problem - profound challenge for simulation of field theories

  - Can arise in presence of chemical potential, topological terms, multi-particle dynamics, …



- Example chemical potential $\mu\bar{\psi}\gamma^0\psi$

$$Z = \int \mathscr{D}\bar{\psi}\mathscr{D}\psi\mathscr{D}A\ e^{-S[\bar{\psi},\psi,A]} \quad \text{(partition function)}$$

$$S = \int_0^{1/T} d\tau \int d^3x \left[\bar{\psi}(\gamma^\mu D_\mu + m)\psi + \frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \mu\bar{\psi}\gamma^0\psi\right]$$

and integration over fermion fields and wick rotation

$$Z = \int \mathscr{D}A e^{-S_{\text{gauge}}[A]} \cdot \det(i\gamma^\mu D_\mu - m + i\mu\gamma^4) \longrightarrow$$ For $\mu \neq 0$ complex phases don't cancel

HEP application focused quantum simulations

- Importance sampling

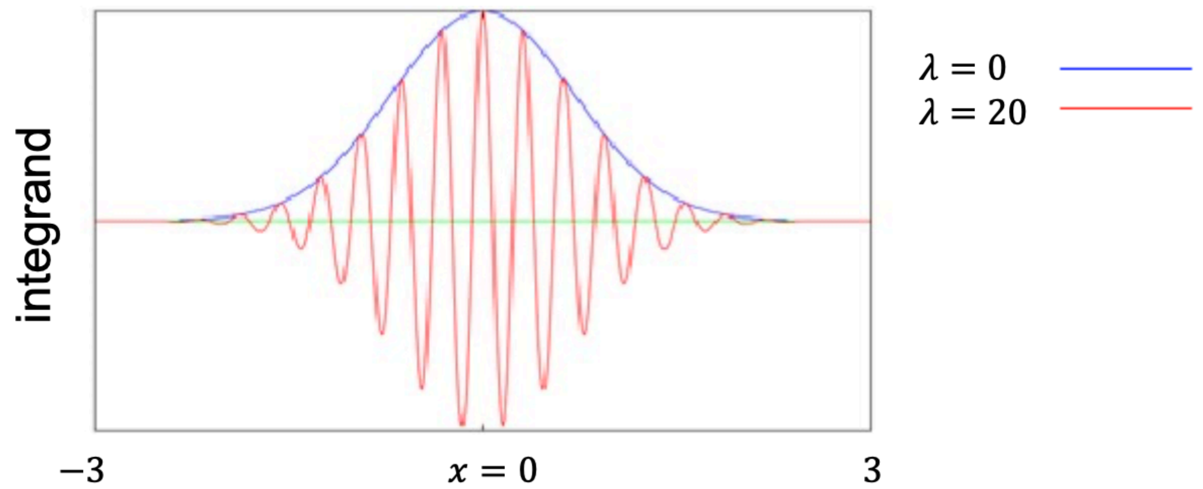
  Interpretation of $e^{-S_{\text{gauge}}} \det(M)$

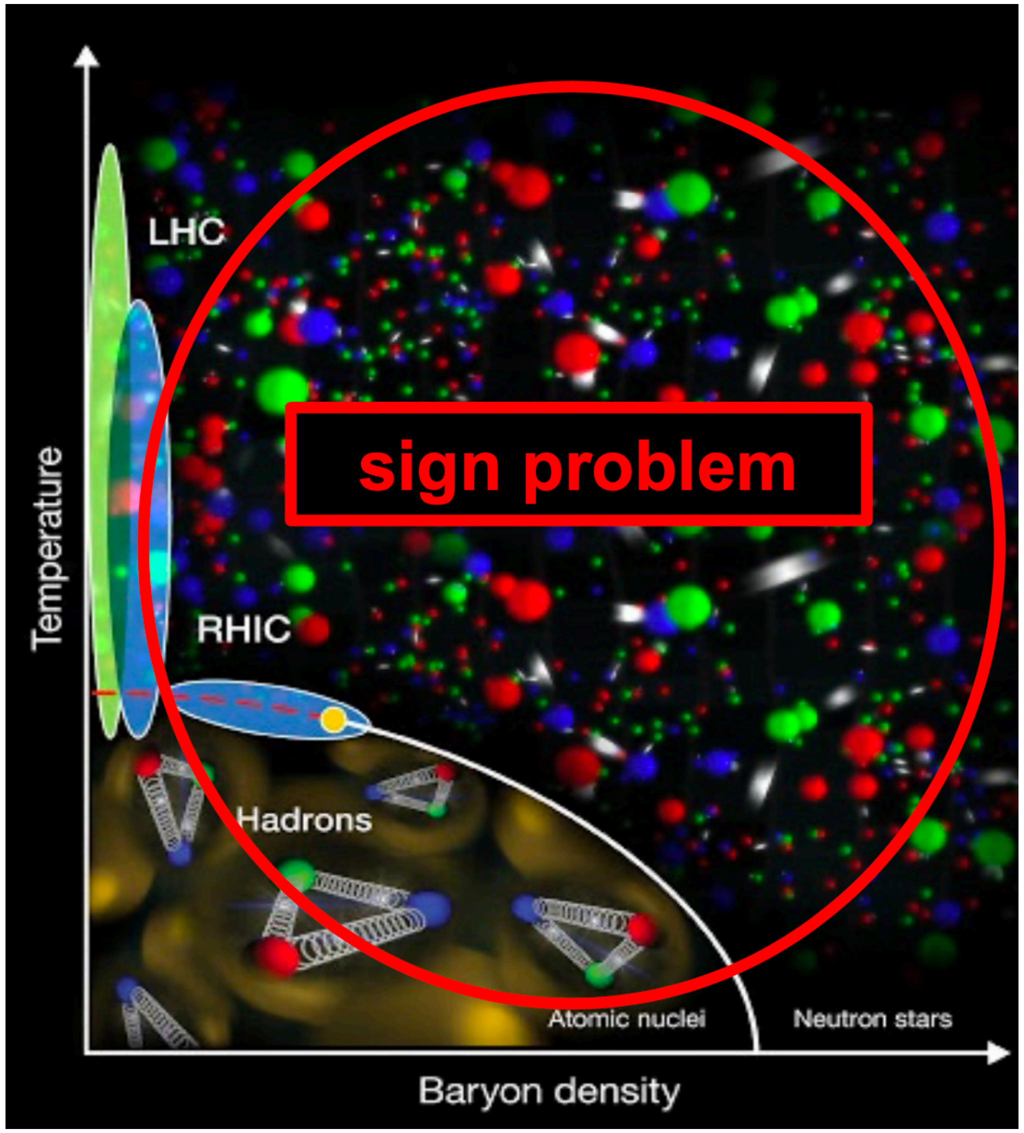
  as probability weight

- Highly oscillatory integrands

$$\langle O \rangle = \frac{\int \mathscr{D}A e^{-S_{\text{gauge}}} O \det(M) \ e^{i\phi}}{\int \mathscr{D}A e^{-S_{\text{gauge}}} \det(M) \ e^{i\phi}}$$

near cancellation of pos and neg contribs

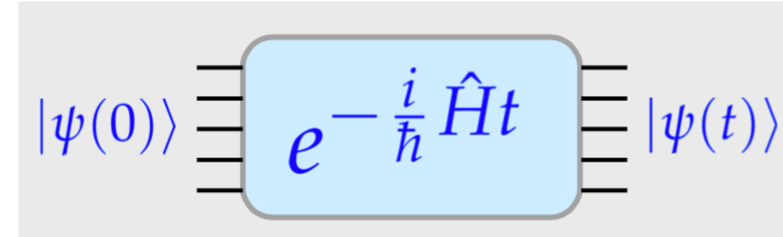




$$\int dx \exp(-x^2 + i\lambda x) \rightarrow \int dx \exp(-x^2)\cos(\lambda x)$$

HEP application focused quantum simulations

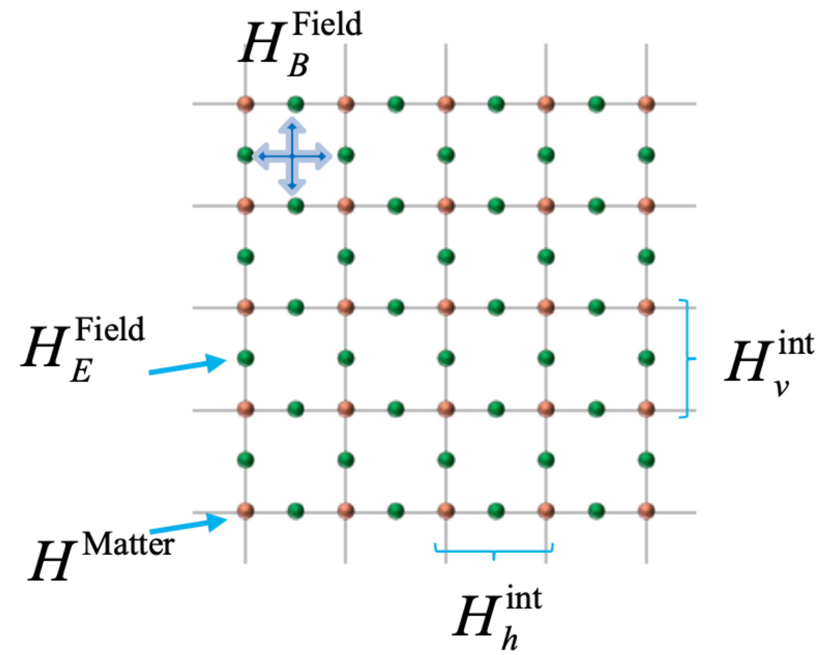
- Real-time evolution on quantum computer can avoid sign problem [Kogut, Susskind '74]



Kogut-Susskind formulation

$$H = H^{\text{Matter}} + H^{\text{Field}} + H^{\text{int}}$$

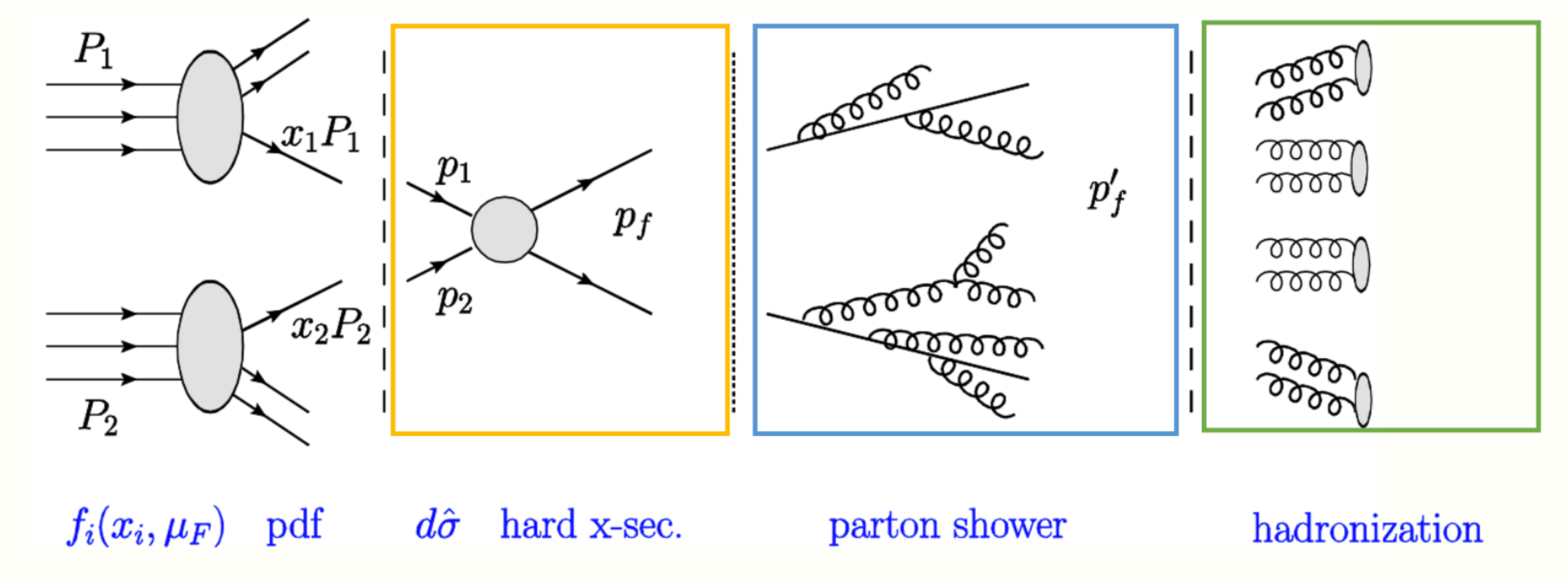
Gauge group G $\quad u_g^p H u_g^{p\dagger} = H$



Some recent examples:

- Sigma model with topological term [Araz, Schenk, MS '22]
- U(1) lattice gauge theory - real-time propagation and collisions in 2d [Lewis, Woloshyn '19]
- SU(2) non-Abelian gauge field (1d) - calculation of plaquette operator [Klco, Stryker, Savage '19]
- Simulate Lattice Gauge Theories with continuous gauge groups in Hamiltonian formulation [Haase, Dellantonio, Celi, Paulson, Kan, Jansen, Muschik '20]
- Z2 Lattice Gauge Theory at finite temperature [Fromm, Philipsen, MS, Winterowd '23]

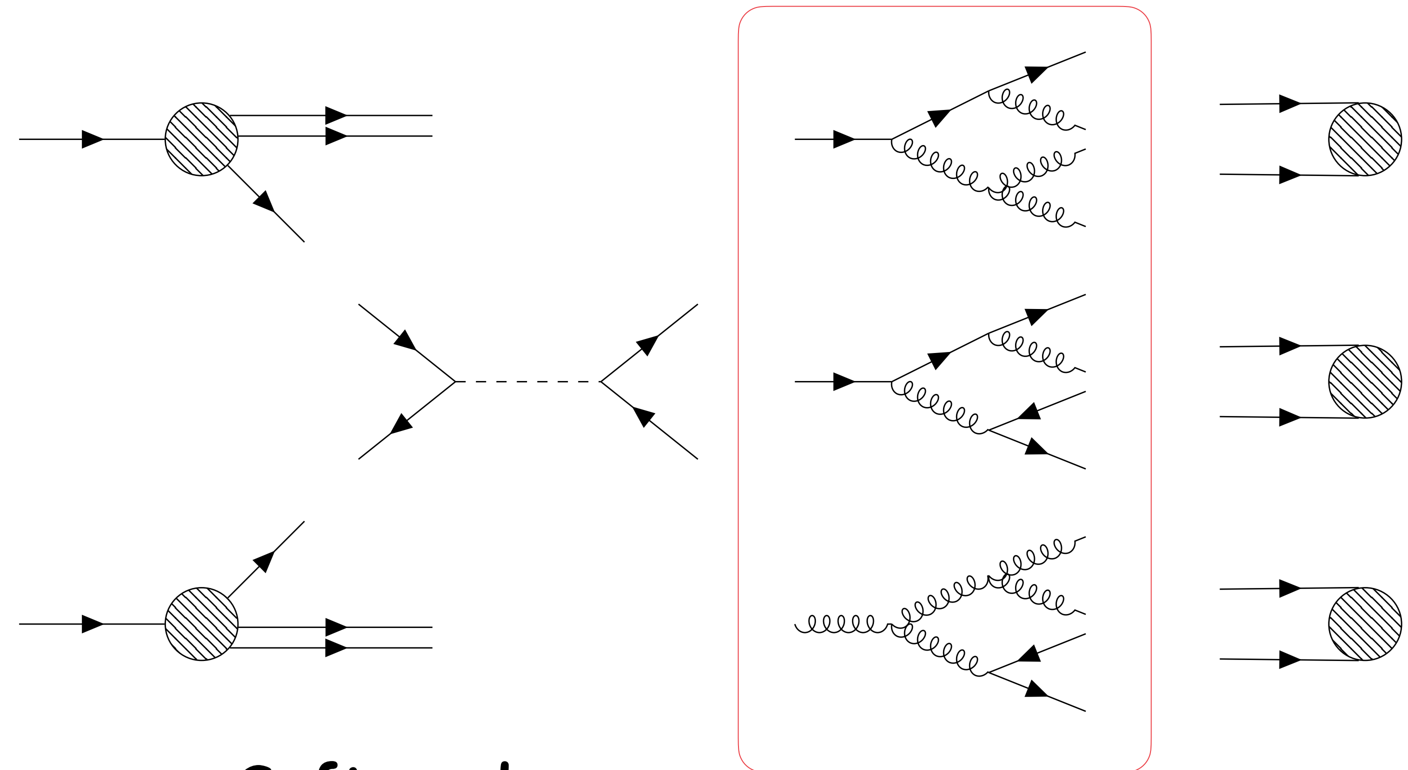
Calculation of particle collisions



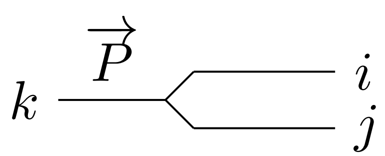
- hard process and parton shower most time consuming parts of event simulation - though carries most information!
- hard process calculated using modern helicity amplitude techniques and parton showers using perturbative QCD resummation techniques.

⟶ Event generators: Pythia, MadEvent, Herwig, Sherpa, ...

Parton shower



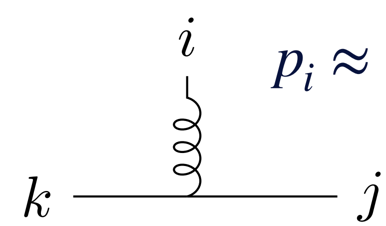
Collinear mode:



$p_i = zP, \quad p_j = (1-z)P$

Successive decay steps factorise into independent quasi-classical steps

Soft mode:



$p_i \approx 0$

Interference effects only allow for partial factorisation

Leading contributions to the decay rate in the collinear limit are included in the soft limit

Splitting functions:

$$P_{q\to qg}(z) = C_F \frac{1+(1-z)^2}{z},$$

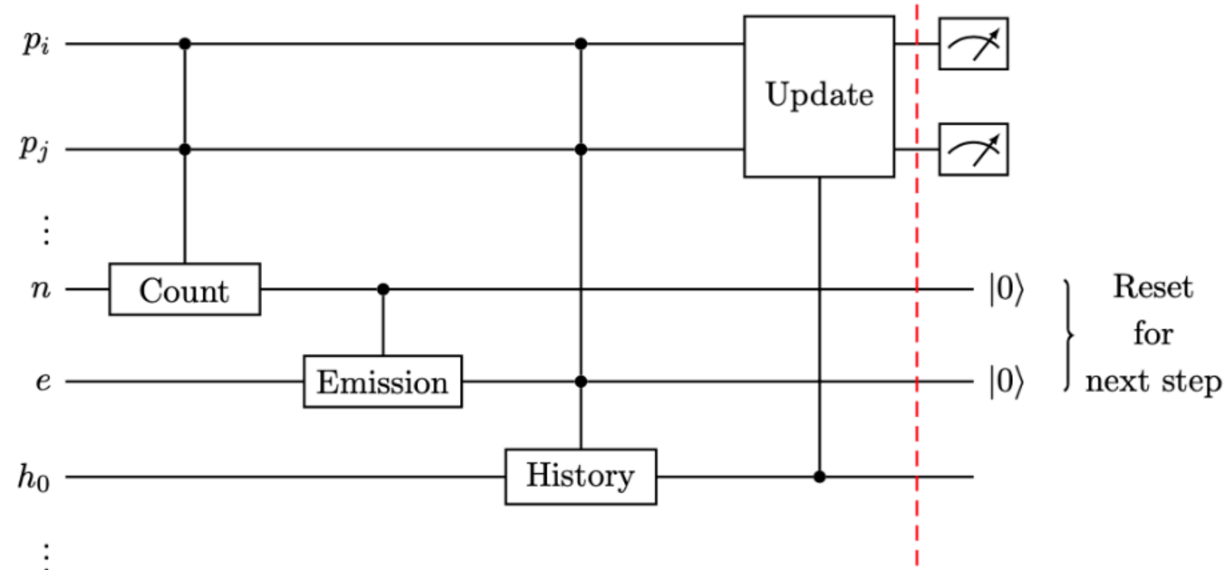
$$P_{g\to q\bar{q}}(z) = n_f T_R (z^2 + (1-z)^2), \qquad P_{g\to gg}(z) = C_A\left[2\frac{1-z}{z} + z(1-z)\right],$$

Sudakov factors for non-emission probability $\Delta_{i,k}(z_1, z_2) = \exp\left[-\alpha_s^2 \int_{z_1}^{z_2} P_k(z')dz'\right]$

QC parton shower algorithm

- Interference effects in parton shower-picture for Yukawa model [Bauer, de Jong, Nachman, Provasoli '19]
- For QCD and efficient implementation [Bepari, Malik, MS, Williams '20]

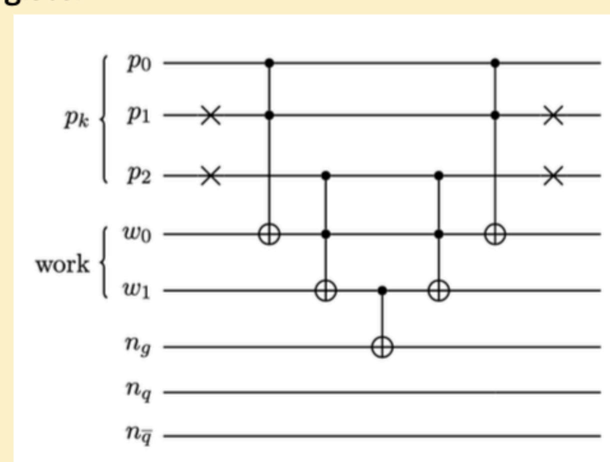
	gluon	quark	antiquark
p0	1	0	0
p1	0	0	1
p2	0	1	1



Update Gate - Controls from history register to update the final particles in the particle register

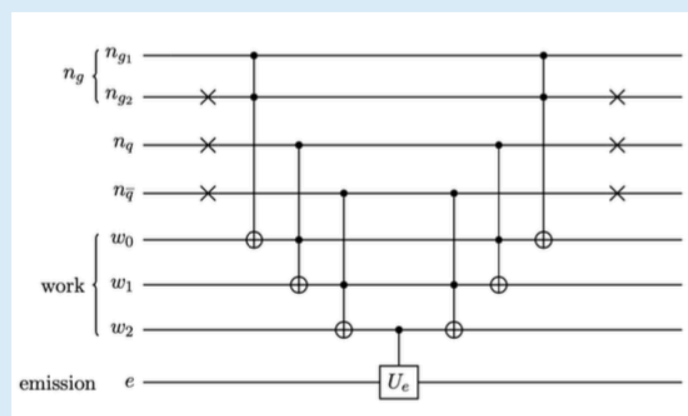
COUNT GATE

Use NOT, CNOT, CCNOT gates to read particle register and flip corresponding number register



EMISSION GATE

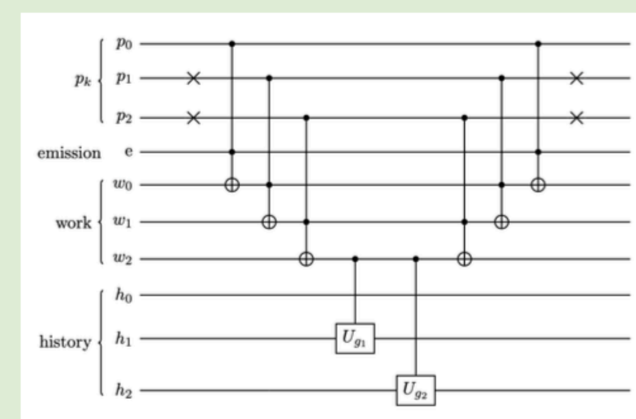
Control from number registers to apply emission matrix including Sudakov factors to rotate e-register from |0> to |1> if emission has occurred



$$U_e = \begin{pmatrix} \sqrt{\Delta_{\text{tot}}(z_1, z_2)} & -\sqrt{1 - \Delta_{\text{tot}}(z_1, z_2)} \\ \sqrt{1 - \Delta_{\text{tot}}(z_1, z_2)} & \sqrt{\Delta_{\text{tot}}(z_1, z_2)} \end{pmatrix}$$

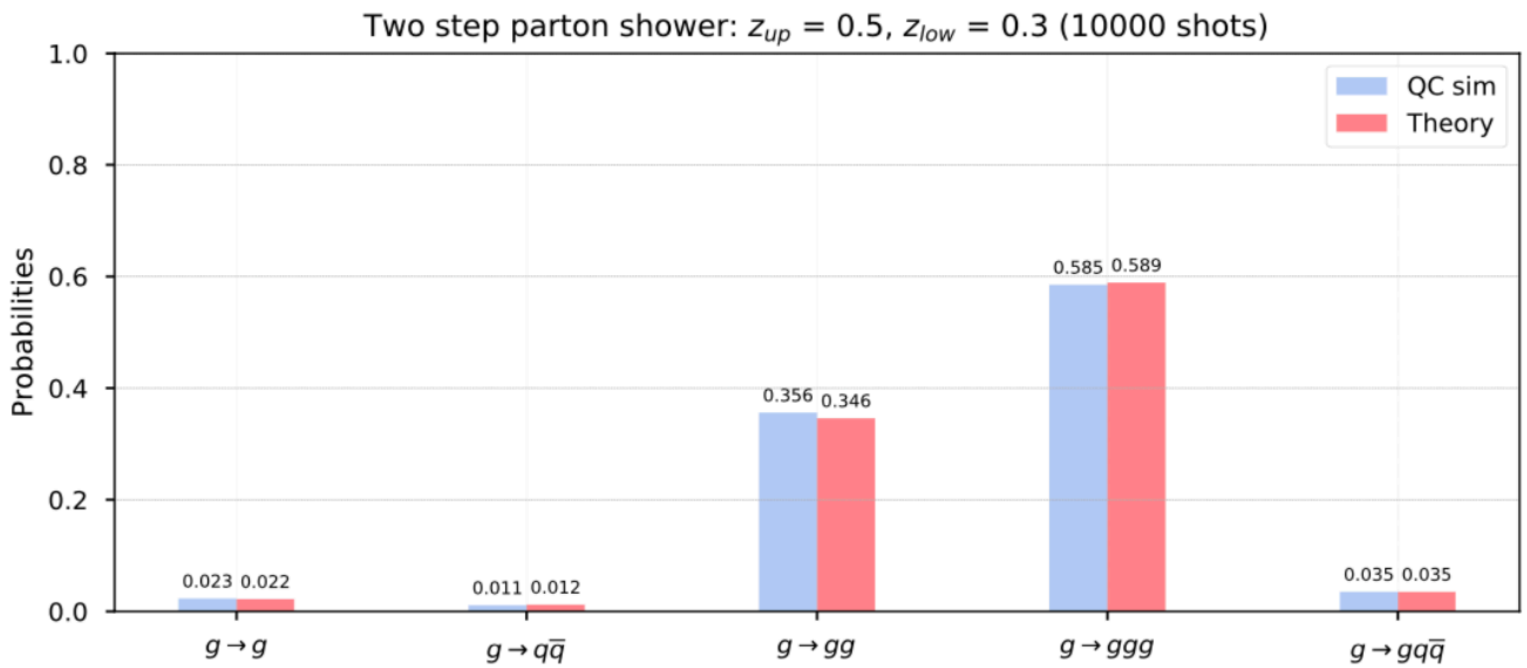
HISTORY GATE

Control from particle and emission registers to apply specific rotations to history registers

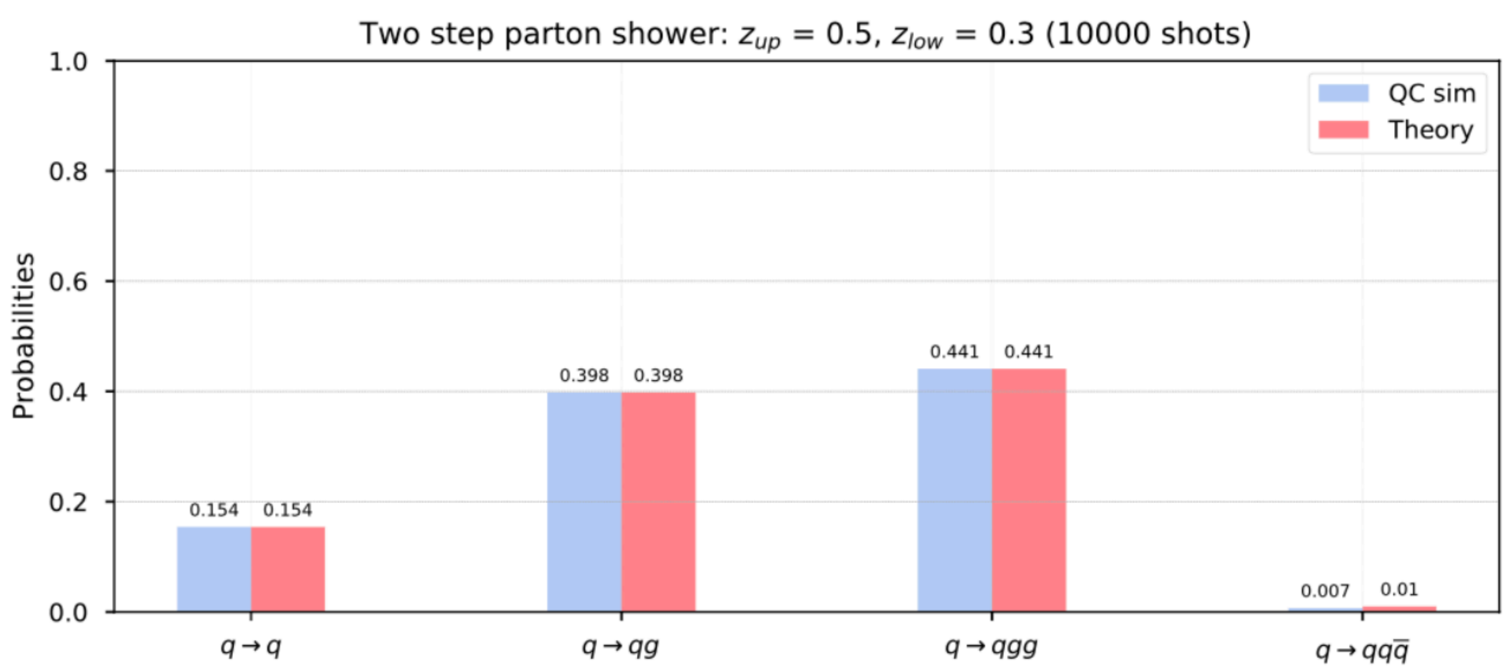


$$U_h = \begin{pmatrix} \sqrt{1 - \frac{P_{k\to ij}(z)}{P_{\text{tot}}(z)}} & -\sqrt{\frac{P_{k\to ij}(z)}{P_{\text{tot}}(z)}} \\ \sqrt{\frac{P_{k\to ij}(z)}{P_{\text{tot}}(z)}} & \sqrt{1 - \frac{P_{k\to ij}(z)}{P_{\text{tot}}(z)}} \end{pmatrix}$$

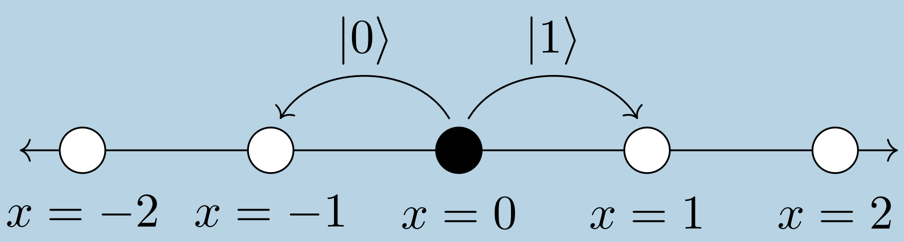
- **Initial gluon:**
  - step 1
  - $g \to g$
    - Step 2:
    - Same final states as step 1
  - $g \to q\bar{q}$
    - Step 2:
    - $\to gq\bar{q}$
  - $g \to gg$
    - Step 2:
    - $\to ggg$
    - $\to gq\bar{q}$



- **Initial quark:**
  - step 1
  - $q \to q$
    - Step 2:
    - Same final states as step 1
  - $q \to qg$
    - Step 2:
    - $\to qgg$
    - $\to qq\bar{q}$



The Quantum Walk



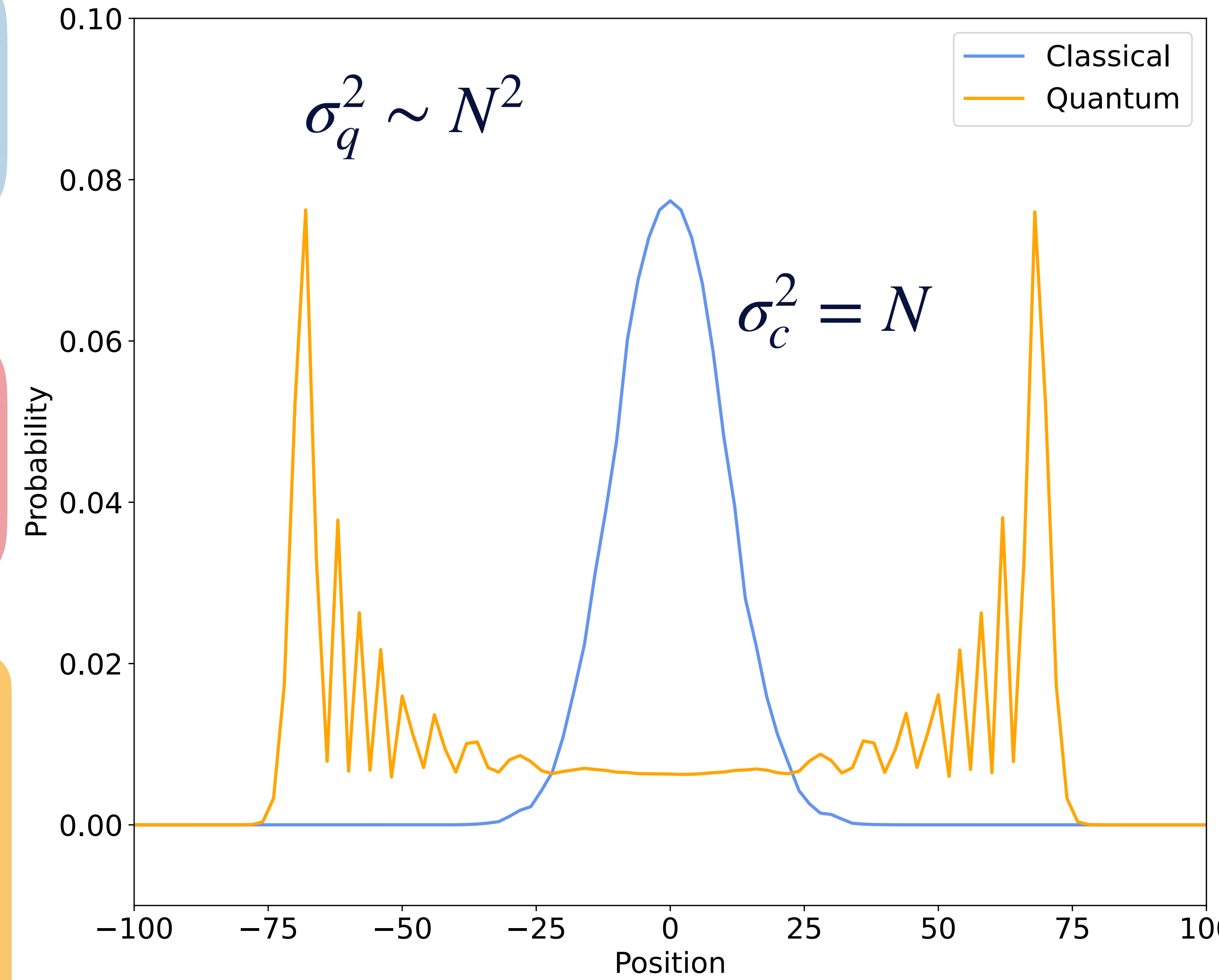
$$\left.\begin{array}{l}\mathscr{H}_P = \{\; i\rangle : i \in \mathbb{Z}\} \\ \mathscr{H}_C = \{\; 0\rangle,\;\; 1\rangle\}\end{array}\right\} \mathscr{H} = \mathscr{H}_C \otimes \mathscr{H}_P$$

Unitary Transformation:

$$U = S \cdot (C \otimes I)$$

Coin Operation:

$$C\;\; 0\rangle = \frac{1}{\sqrt{2}}\Big(\;\; 0\rangle + \;\; 1\rangle\Big)$$



Quantum Walk Parton Shower

[Bepari, Malik, MS, Williams '21]

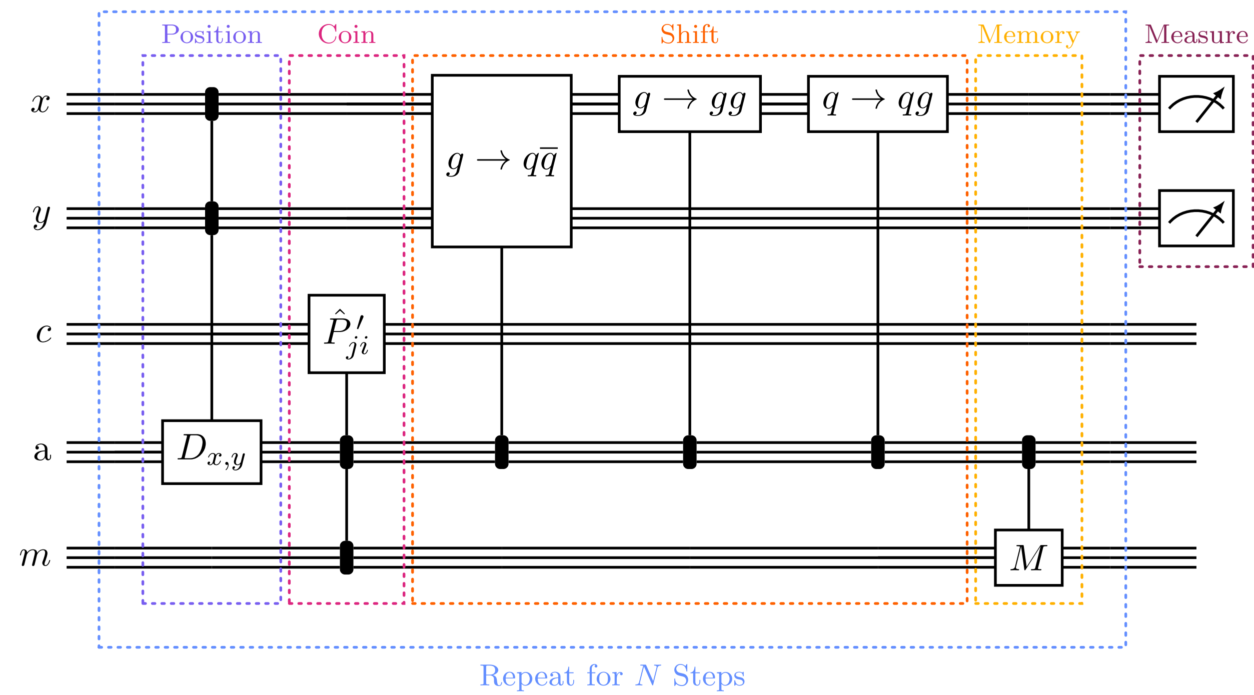
Identifying the probability for a specific emission as

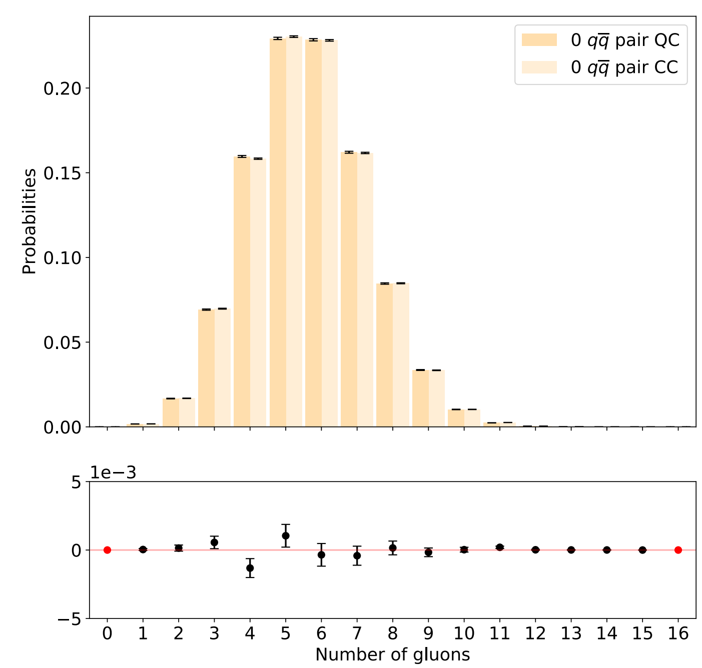
$$P'_{ij} = (1 - \Delta_i) \times P_{ij}$$

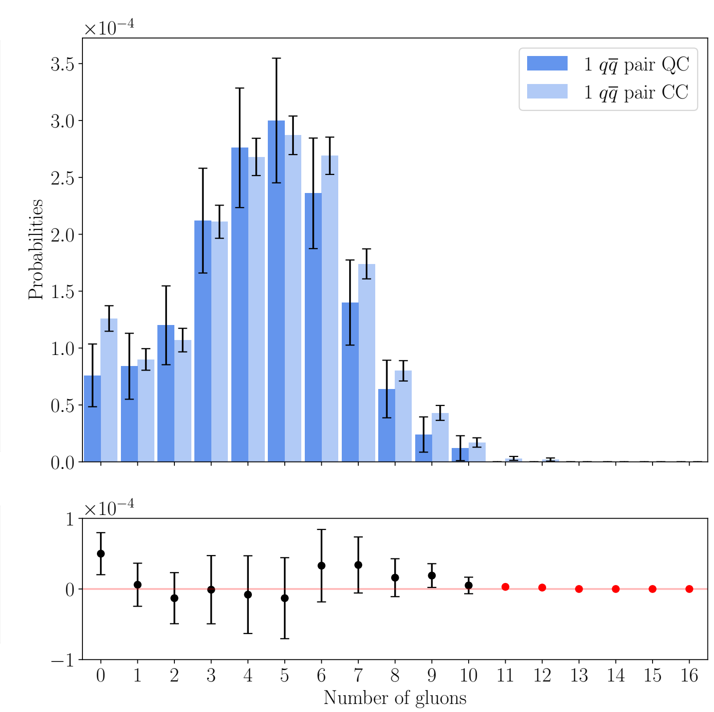
$\mathscr{H}_C$: increase the dimension of the coin space to accommodate collinear splittings

$\mathscr{H}_P$: increase the dimension of the position space to accommodate parton species

Coin and **Shift** operations now propagate the determine-identify-update routine.







Discrete QCD - Abstracting the Parton Shower Method

[Gustafson, Prestel, MS, Williams '22]

QW parton shower still no kinematics! ➡ Algorithm for QC with kinematics

Parameterise phase space in terms of gluon transverse momentum and rapidity:

$$k_\perp^2 = \frac{s_{ij}s_{jk}}{s_{\mathrm{IK}}} \quad \text{and} \quad y = \frac{1}{2}\ln\left(\frac{s_{ij}}{s_{jk}}\right) \quad \text{where} \quad \kappa = \ln\left(\frac{k_\perp^2}{\Lambda^2}\right)$$

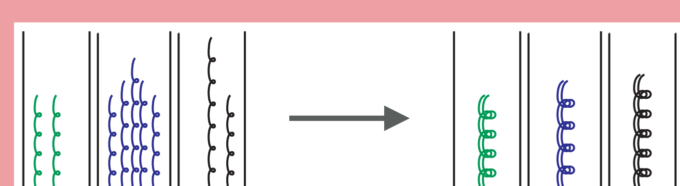
leads to inclusive probability: $d\mathcal{P}\left(q(p_\mathrm{I})\bar{q}(p_\mathrm{K}) \to q(p_i)g(p_j)\bar{q}(p_k)\right) \simeq= \frac{C\alpha_s}{\pi}d\kappa dy$

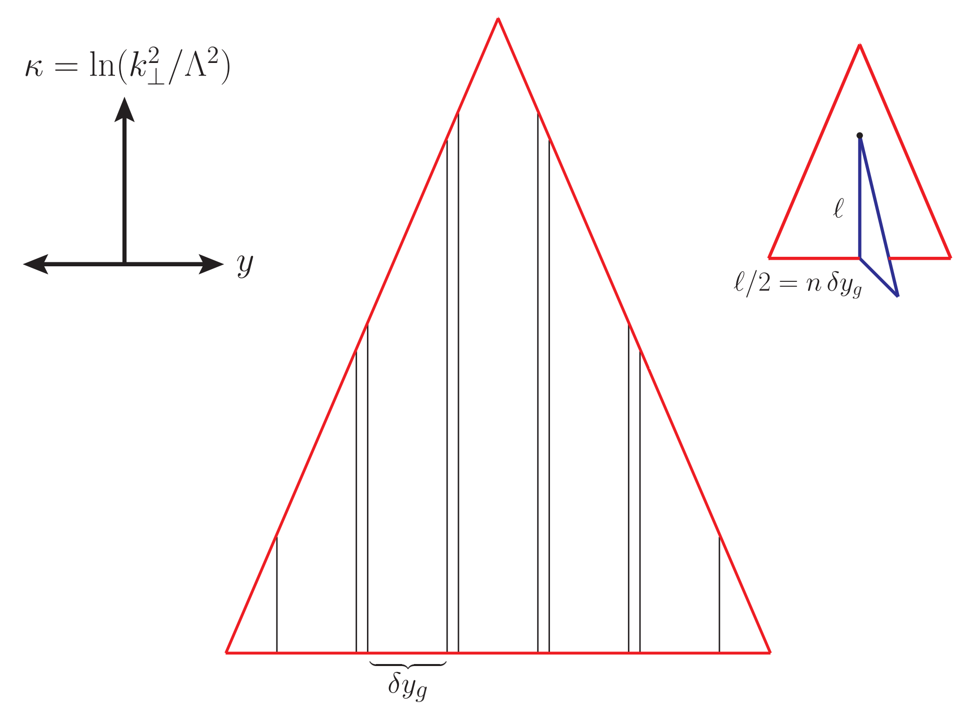
Now express with momentum-dependent running coupling

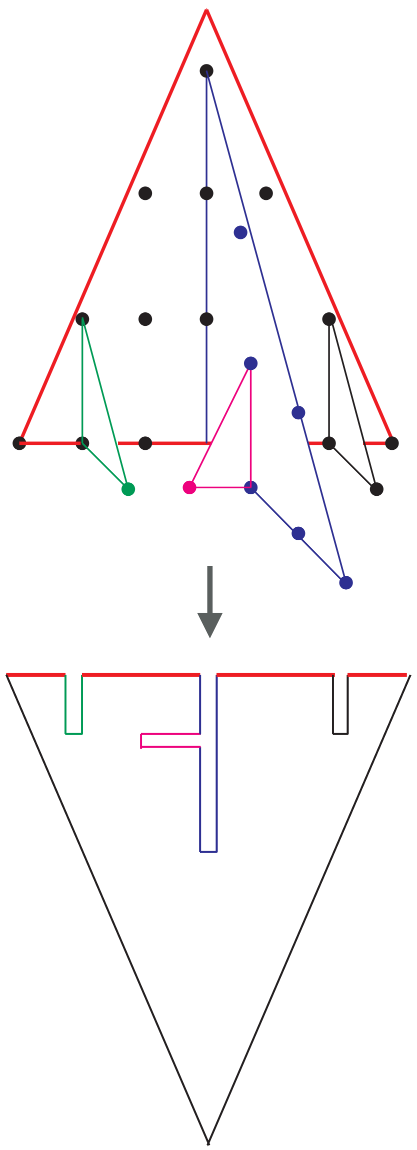
$$\alpha_s(k_\perp^2) = \frac{12\pi}{33-2n_f}\frac{1}{\ln(k_\perp^2/\Lambda_{\mathrm{QCD}}^2)} = \frac{\mathrm{const.}}{\kappa} \Rightarrow d\mathcal{P}\left(q(p_\mathrm{I})\bar{q}(p_\mathrm{K}) \to q(p_i)g(p_j)\bar{q}(p_k)\right) \simeq= \frac{d\kappa}{\kappa}\frac{dy}{\delta y_g} \text{ with } \delta y_g = \frac{11}{6}$$

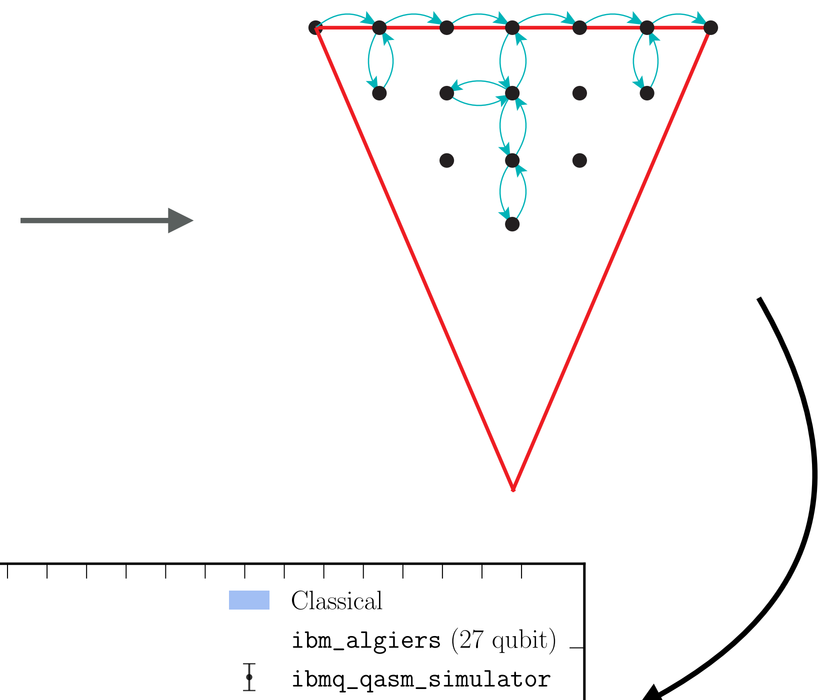
Interpreting the running coupling renormalisation group as a gain-loss equation:

Gluons within δy_g act coherently as one effective gluon



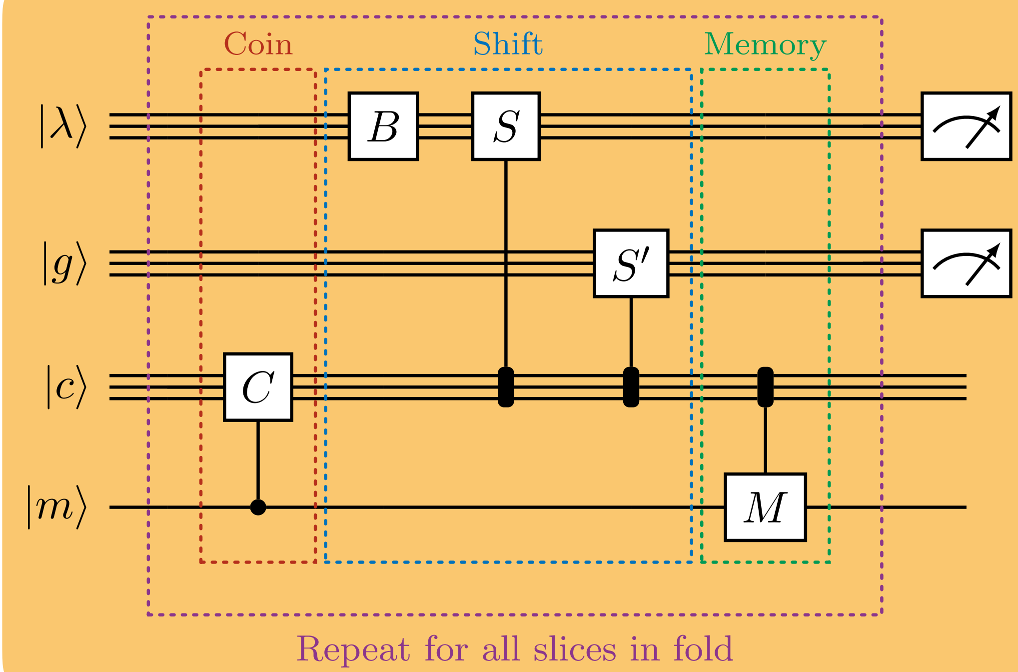


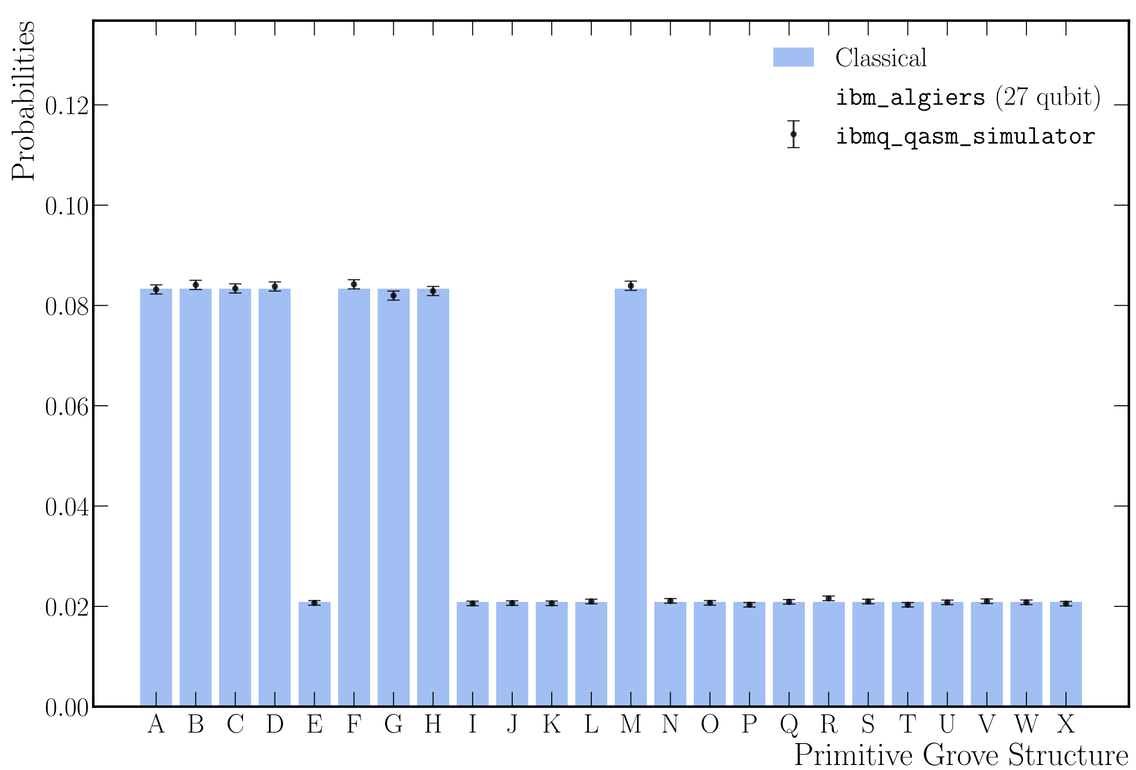




The **baseline** of the grove structure contains all kinematics information

The Discrete-QCD dipole cascade can therefore be implemented as a simple **Quantum Walk**

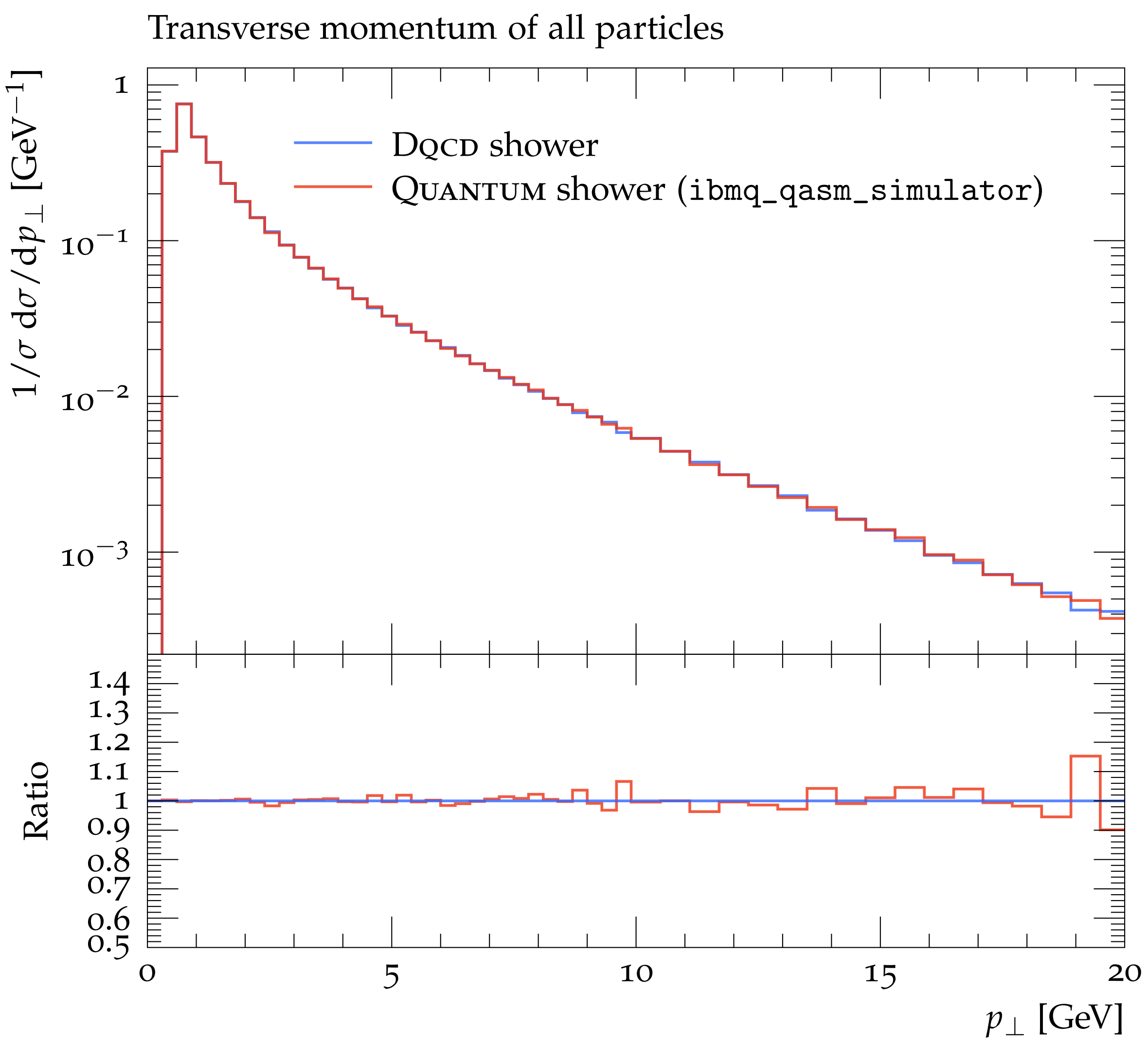


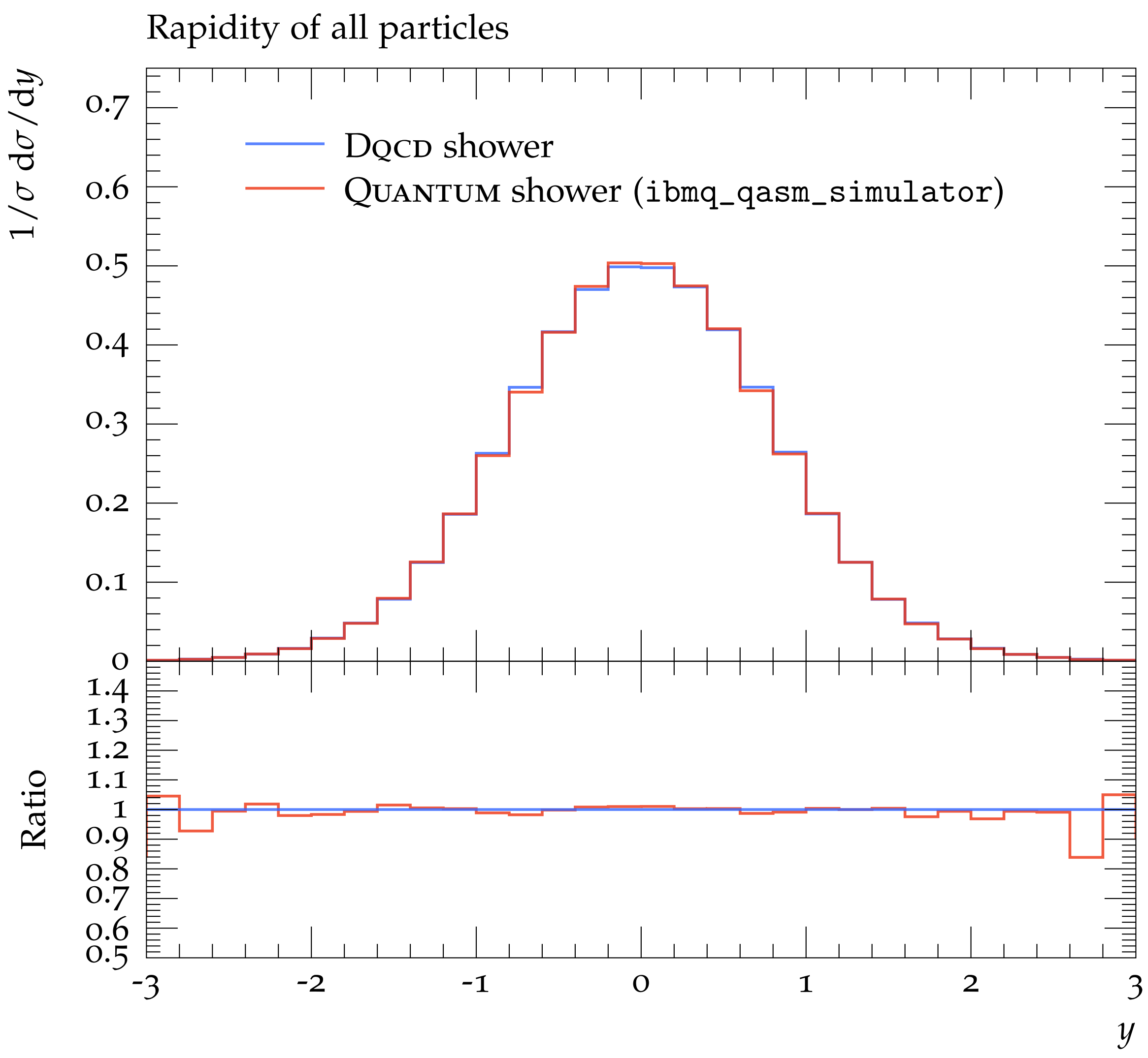


The algorithm has been run on the **IBM QASM 32-qubit simulator**

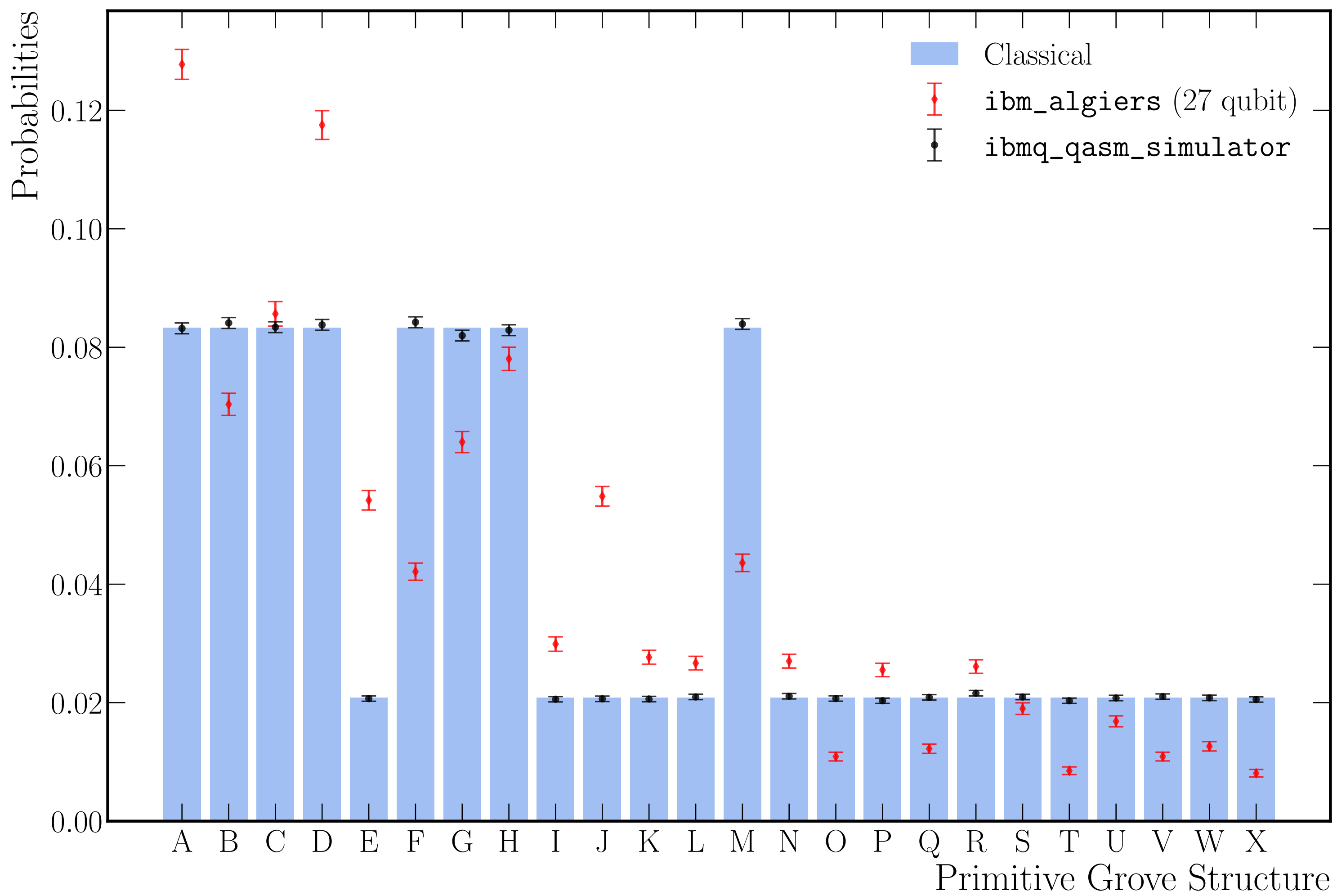
The device simulates a **fully fault tolerant** quantum computer without a noise model

Running on a Quantum Simulator





Discrete QCD as a Quantum Walk - IBM device



The algorithm has been run on the **IBM Falcon 5.11r chip**

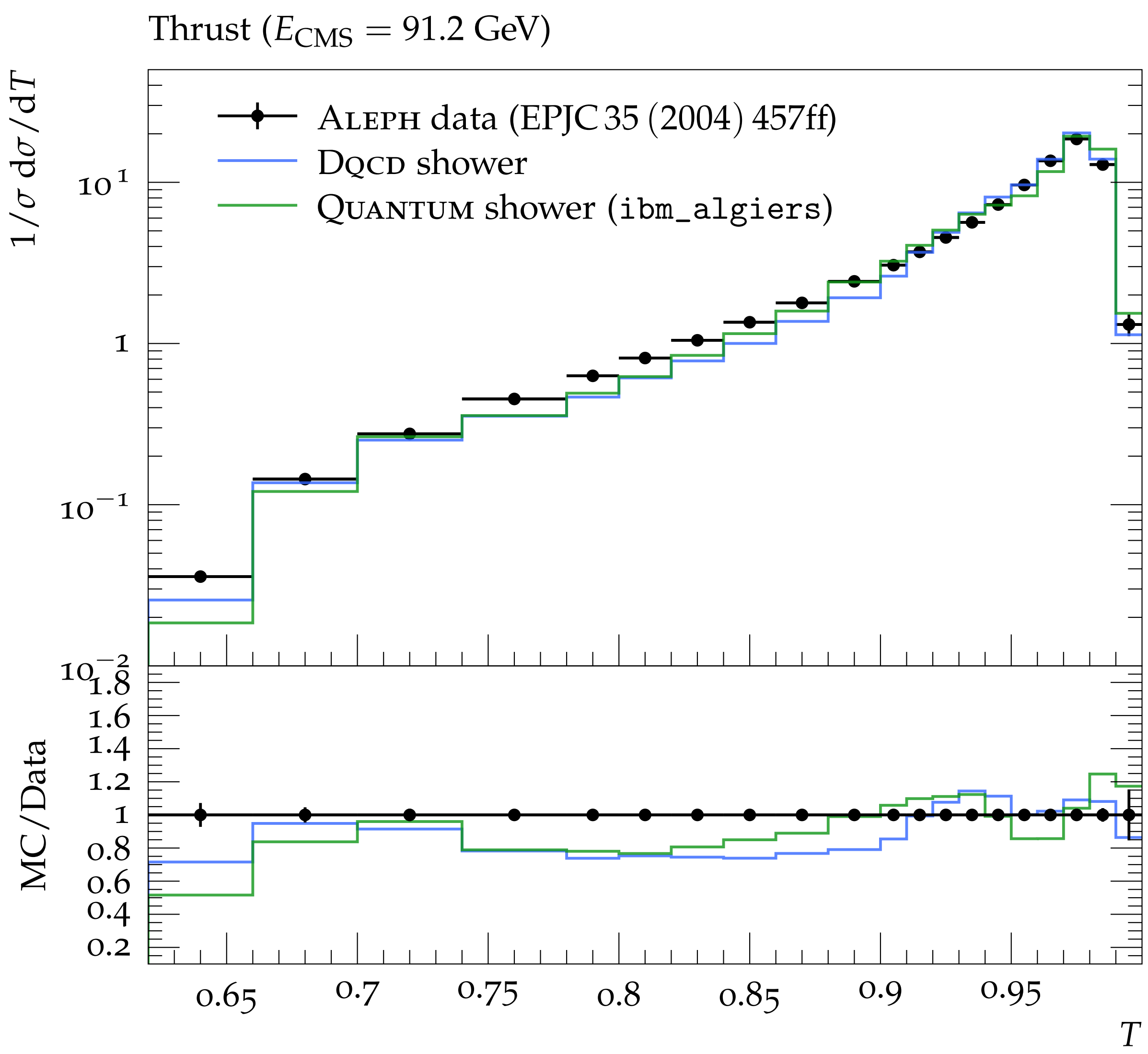
The figure shows the uncorrected performance of the **ibm_algiers** device compared to a simulator

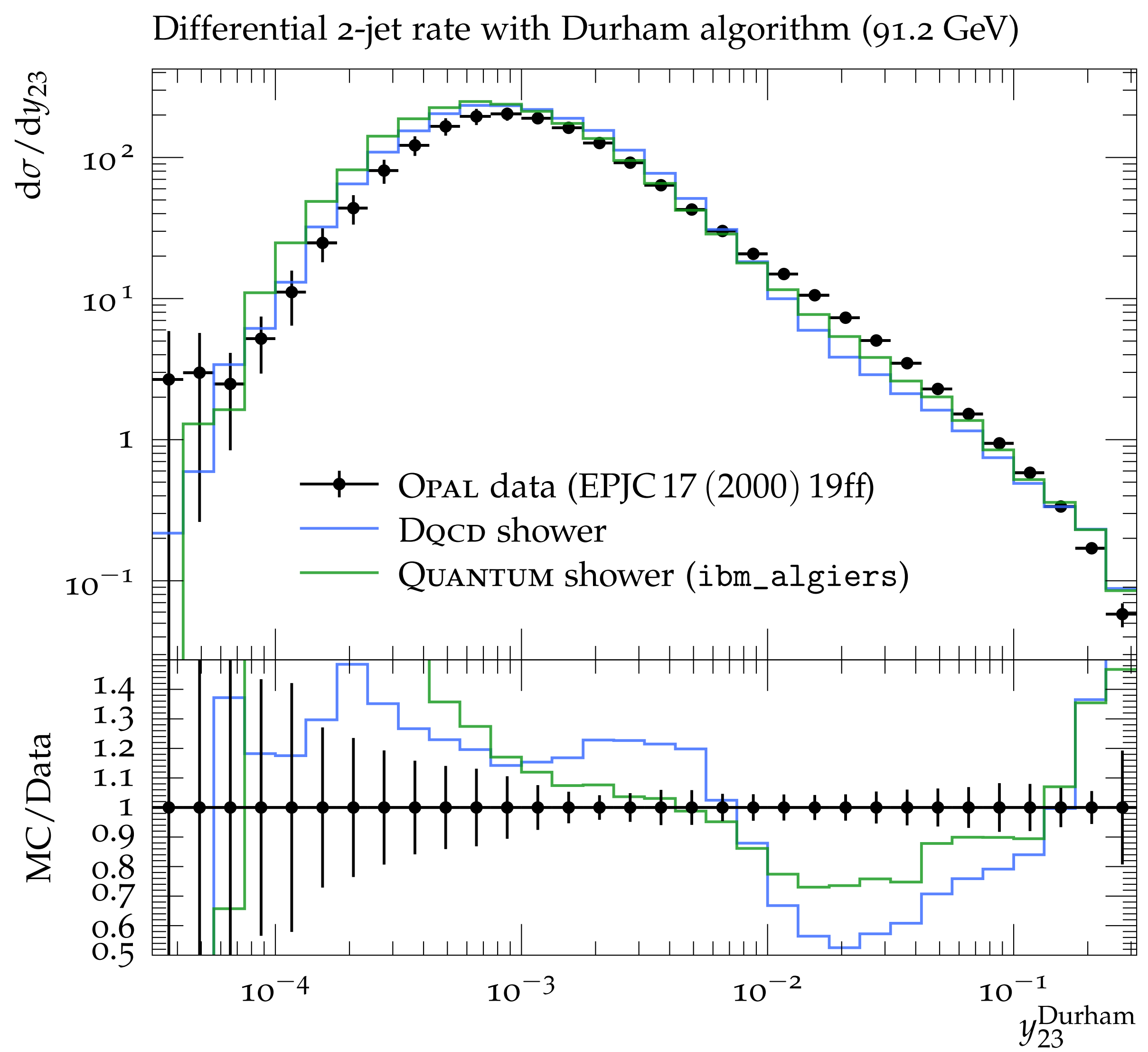
The 24 grove structures are generated for a $E_{CM} = 91.2$ GeV, corresponding to typical collisions at LEP.

Main source of error from CNOT errors from large amount of SWAPs

Collider Events on a Quantum Computer

Theory - LEP-data comparison



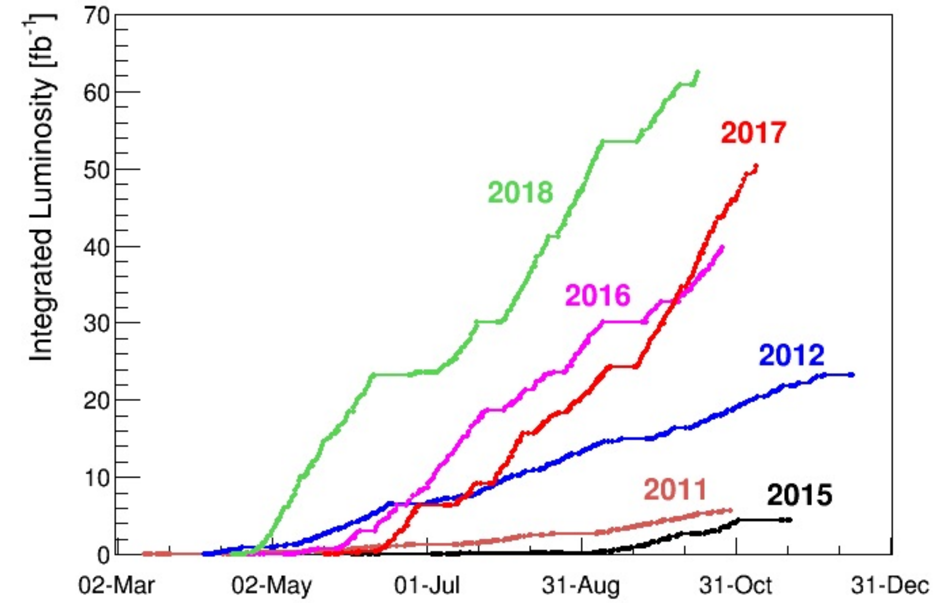


[Gustafson, Prestel, MS, Williams '22]

Big Data in HEP @ the LHC

→ ATLAS/CMS 200 events/s passing triggers

→ ATLAS/CMS 2 PB/year of data



High-Energy Physics
Tremendous amount of highly complex data However, theoretically very precise description of data

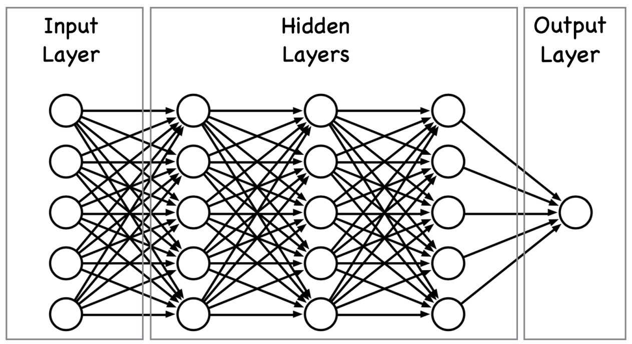
↔

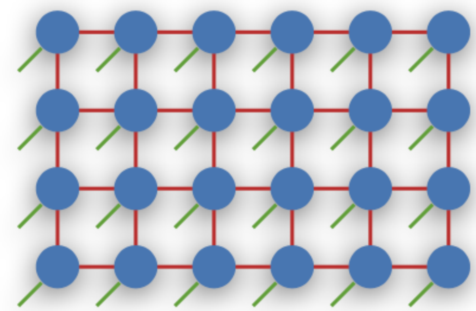
Ideal interplay

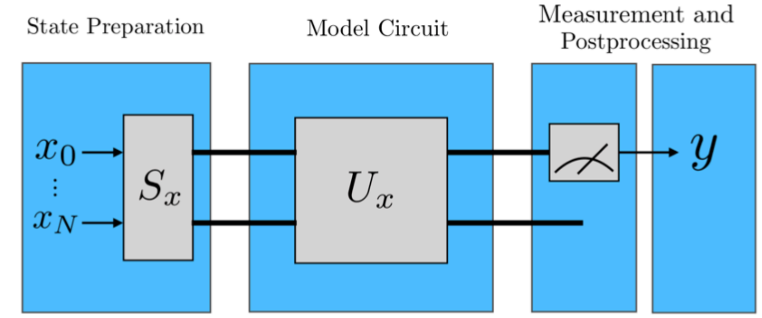
Machine Learning
Highly performant data analysis techniques Often used for classification in HEP: • Supervised learning • Anomaly detection

Classical ML Algorithms | Tensor Networks | Quantum Computing

1. an adaptable complex system that allows approximating a complicated function







2. the calculation of a loss function used to define the task the method

$$E(y, y') = \frac{1}{2}|y - y'|^2$$

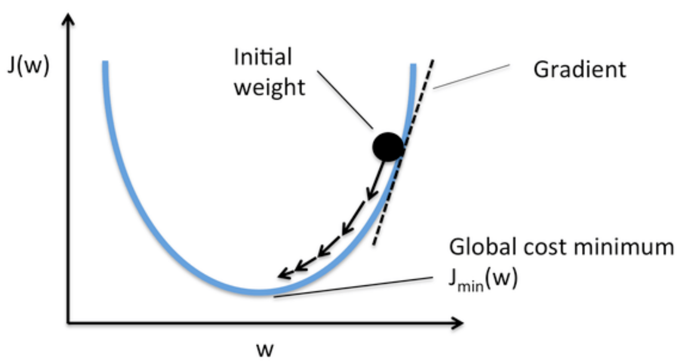
$$B^{s_2}{}_{p_1 p_2} \Gamma^{l p_1 p_2}{}_{s_2} = f^l(\mathbf{x}^{(\mathbf{n})})$$

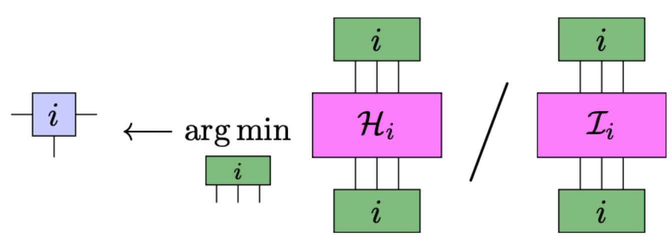
$$\mathcal{L} = L\left(p(l, \mathbf{x}),\ l^{truth}\right)$$

ground state

$$|\Gamma\rangle := \underset{|\psi\rangle \in \mathcal{D}}{\arg\min} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

3. a way to update 1. while minimising the loss function





quantum: annealing

hybrid: classical opti.

optimisation →
- Data Analysis (Classification, anomaly, regression, fitting, …)
- Simulation of field theories (Groundstate, tunnelling, Real-time…)
- Calculation of differential equations, etc etc

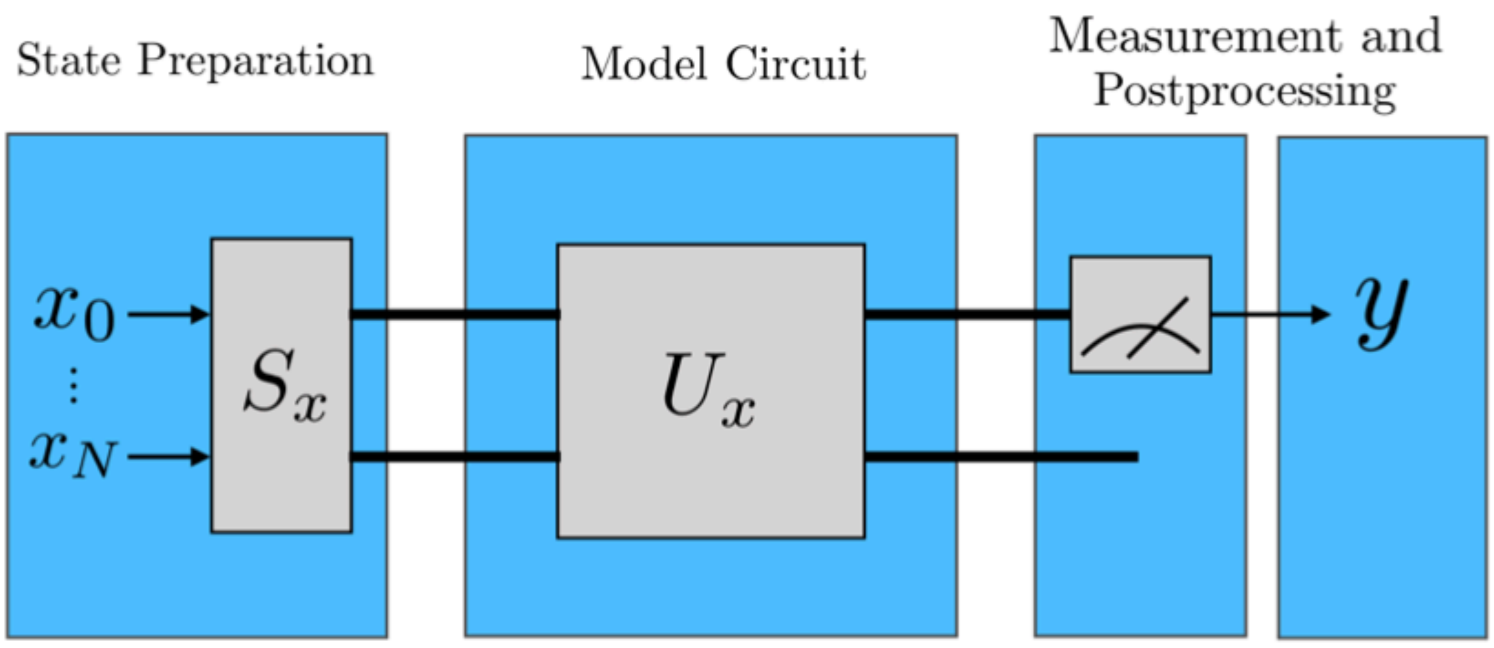
Quantum Machine Learning with a Variational Quantum Circuit

[McClean et al '16]

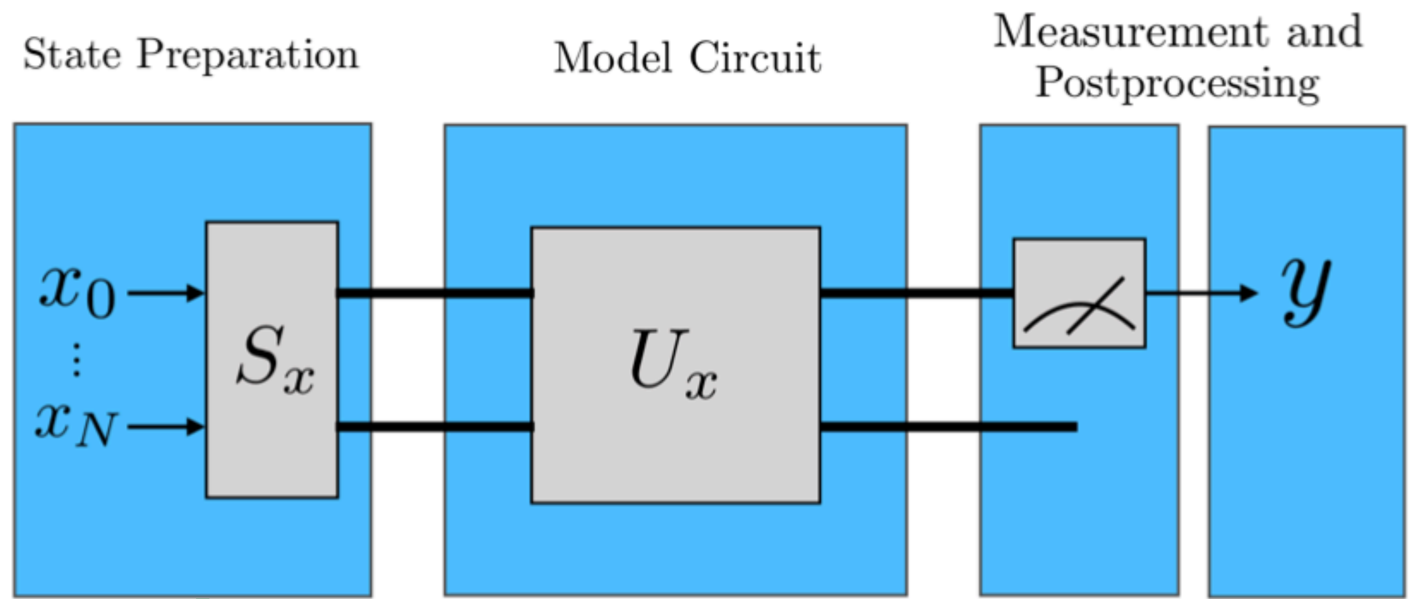
[Farhi, Neven '18]

[Schuld et al '20]

[Blance, MS '20]



Quantum Machine Learning
with a Variational Quantum Circuit



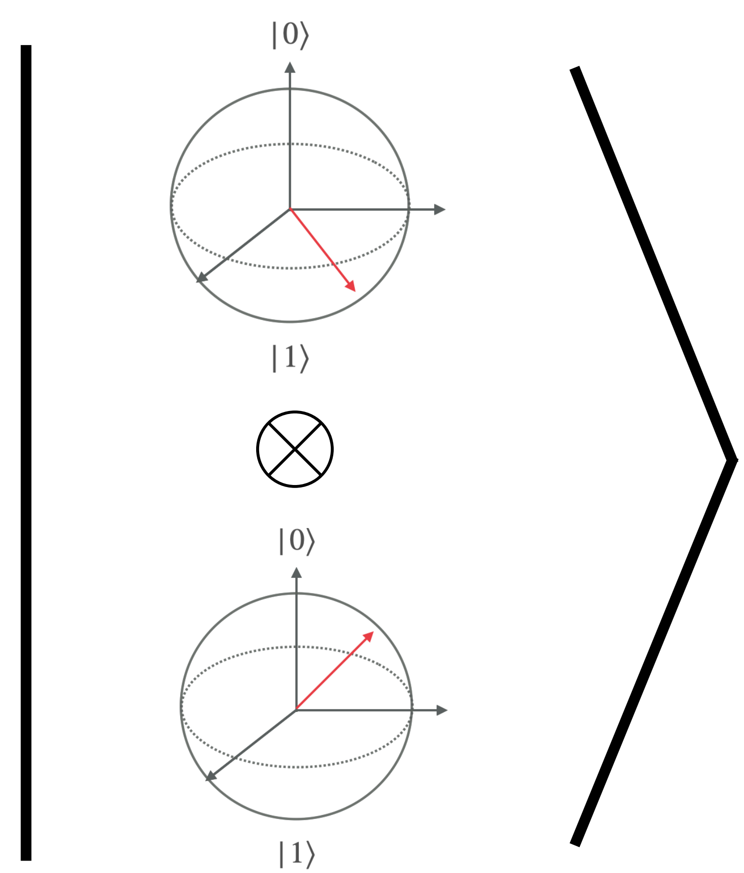
state preparation

n corresponds to # features

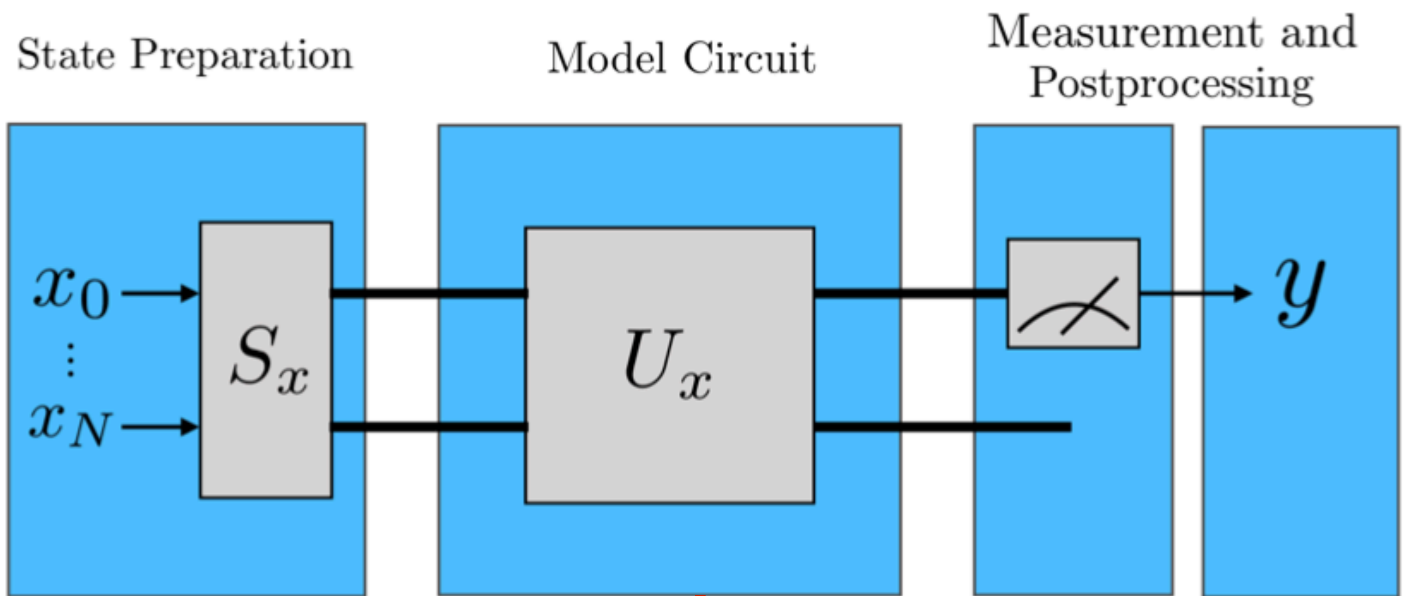
$$x \mapsto S_x|\phi\rangle = S_x|0\rangle^{\otimes n} = |x\rangle$$

e.g. angle encoding

$$|x\rangle = \bigotimes_{i=1}^{n} \cos(x_i)|0\rangle + \sin(x_i)|1\rangle$$



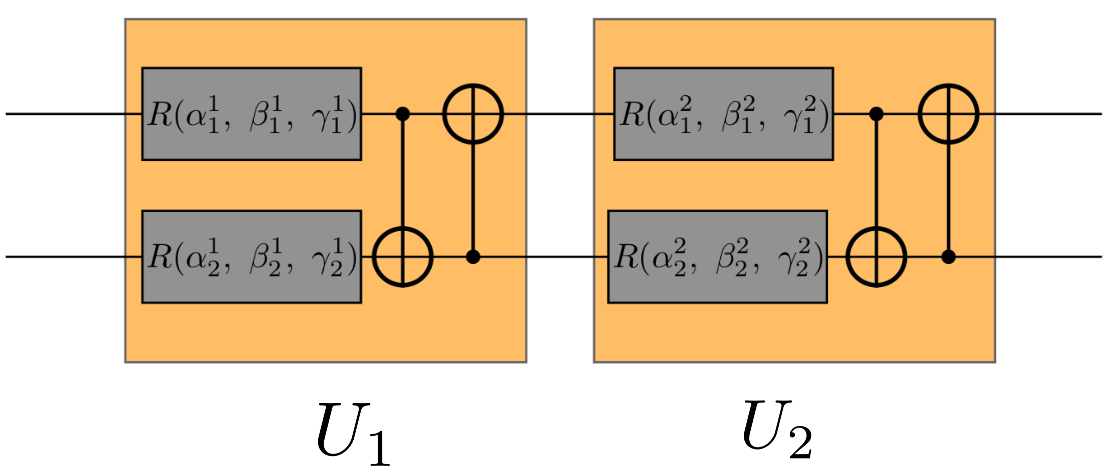
Quantum Machine Learning with a Variational Quantum Circuit

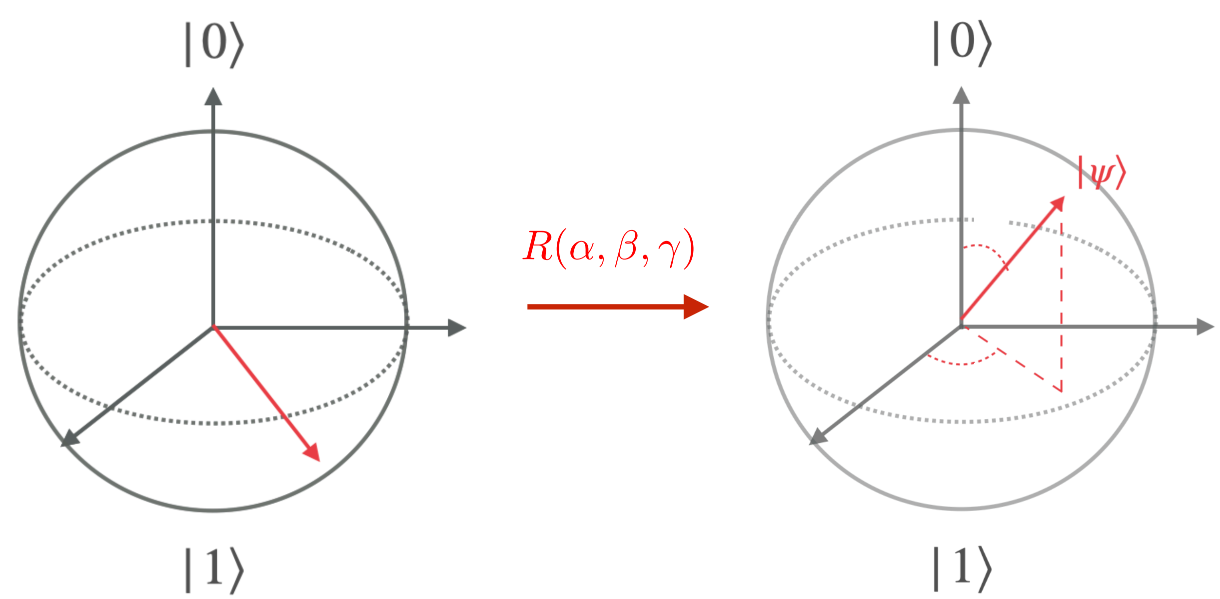


$$|\psi\rangle = U(w)|x\rangle \quad \text{with} \quad U(w) = U_{l_{\max}}(w_{l_{\max}})...U_l(w_l)...U_1(w_1)$$

model circuit ↗ · trainable parameters ↑ · prepared state ↖

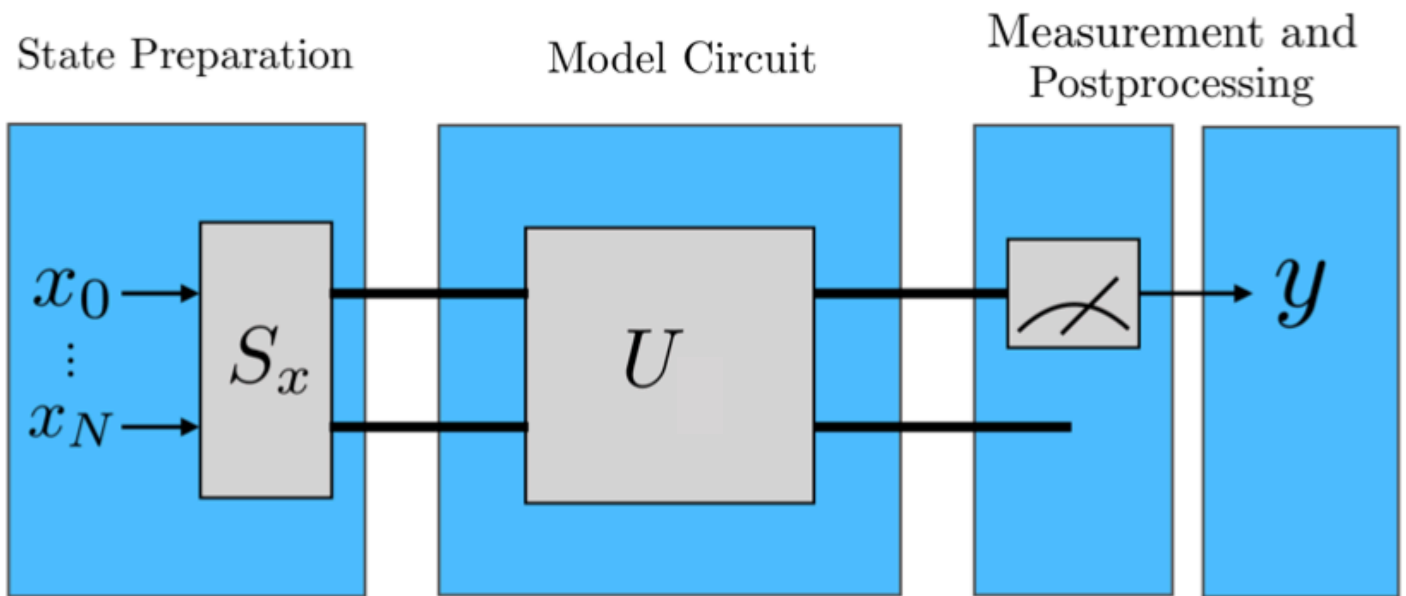
2-layer Variational Quantum Circuit





→ Rotation + CNOT -> Entanglement

Quantum Machine Learning with a Variational Quantum Circuit



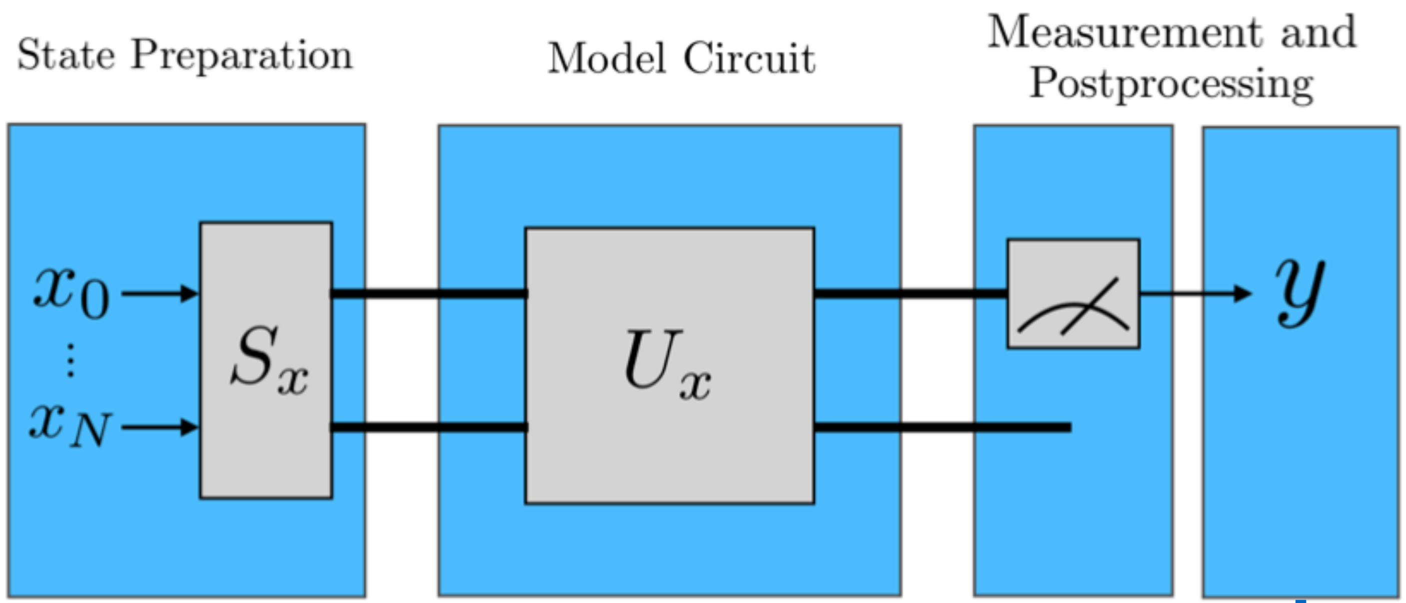
- Entangled state shares information across qubits
- Evaluate expectation value of qubits to construct loss

  for supervised S vs B classification one qubit sufficient

$$\mathbb{E}(\sigma_z) = \langle 0|S_x(x)^\dagger U(w)^\dagger \hat{O} U(w) S_x(x)|0\rangle = \pi(w,x) \quad \text{for} \quad \hat{O} = \sigma_z \otimes \mathbb{I}^{\otimes(n-1)}$$

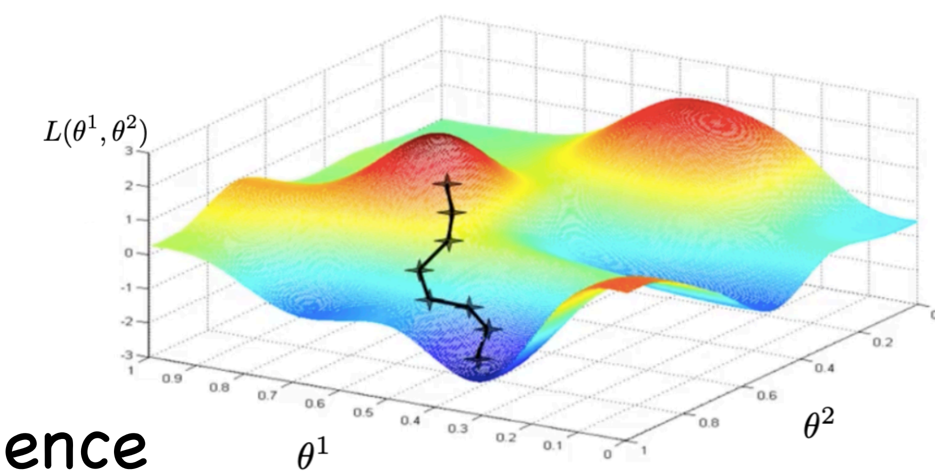
- Quantum network output: $f(w,b,x) = \pi(w,x) + b$
- Changing operator and loss => VQE, VQT, ... (simulate QFT)

Quantum Machine Learning with a Variational Quantum Circuit



- Hybrid approach (QC to calculate exp. value, CC to optimise U operator)
- Loss function $L = \frac{1}{n}\sum_{i=1}^{n}\left[y_i^{\text{truth}} - f(w,b,x_i)\right]^2$

  label (signal, bkg), supervised learning



- Quantum gradient descent - for fast convergence

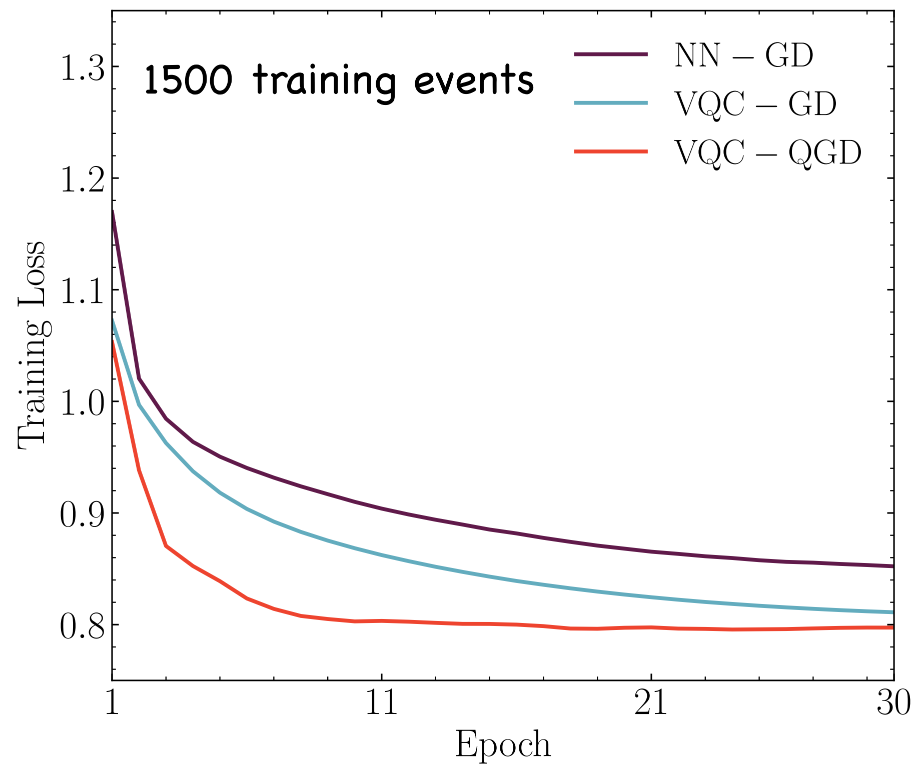
  Fubiny-Study metric underlies geometric structure of VQC parameter space: $\theta_{t+1} = \theta_t - \eta g^{+} \nabla L(\theta)$

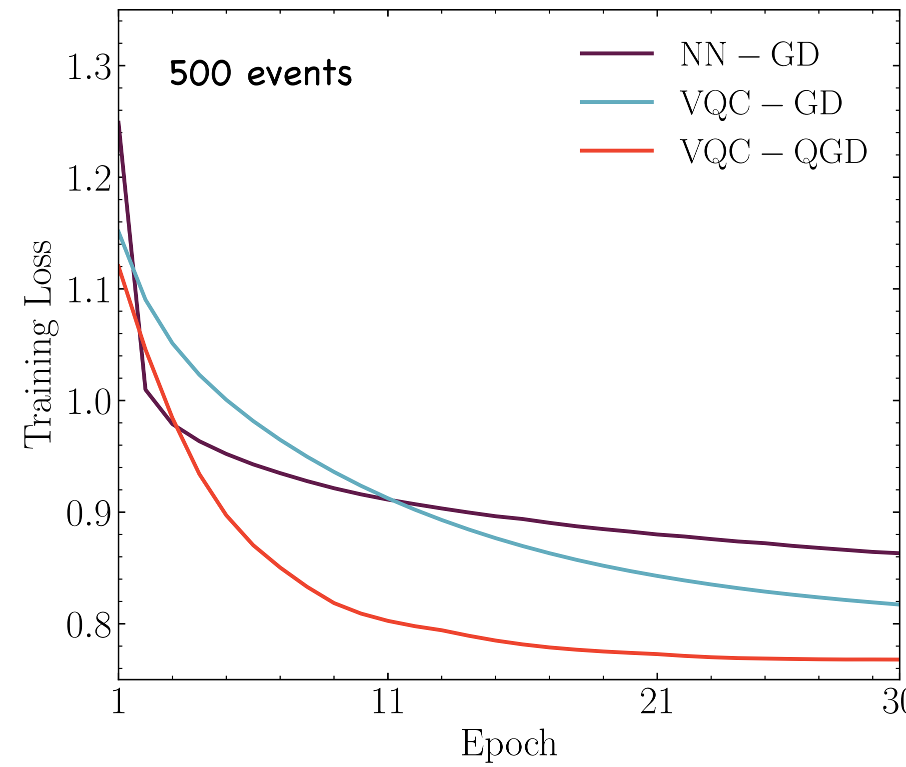
[Cheng '10]

[Blance, MS '20]

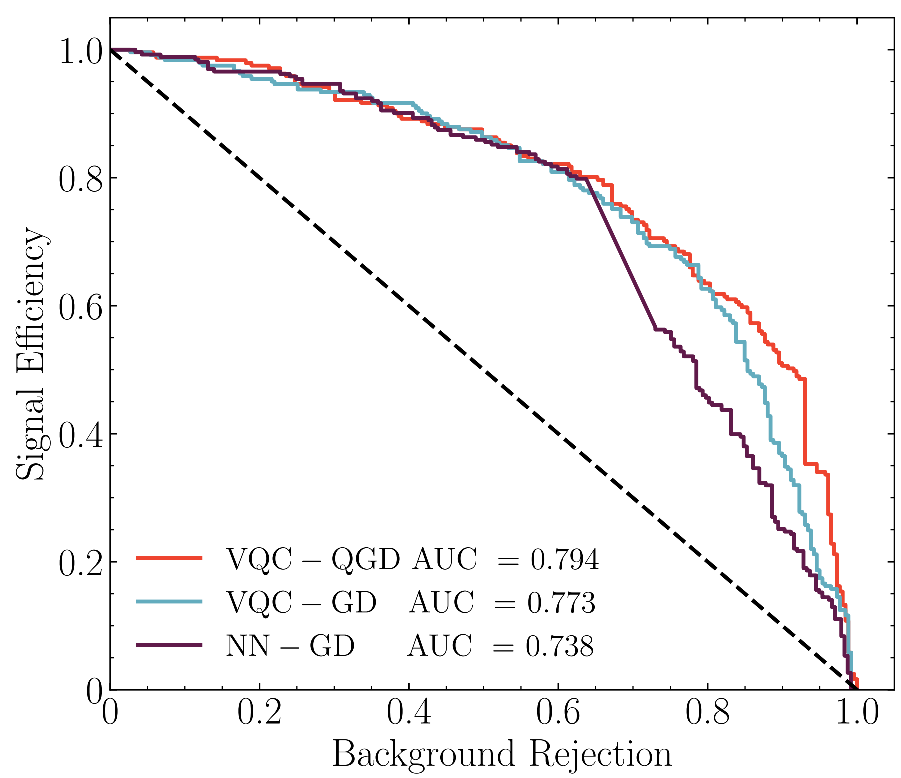
[Abbas et al '20]

Gate quantum machine learning in action





[Blance, MS '20]



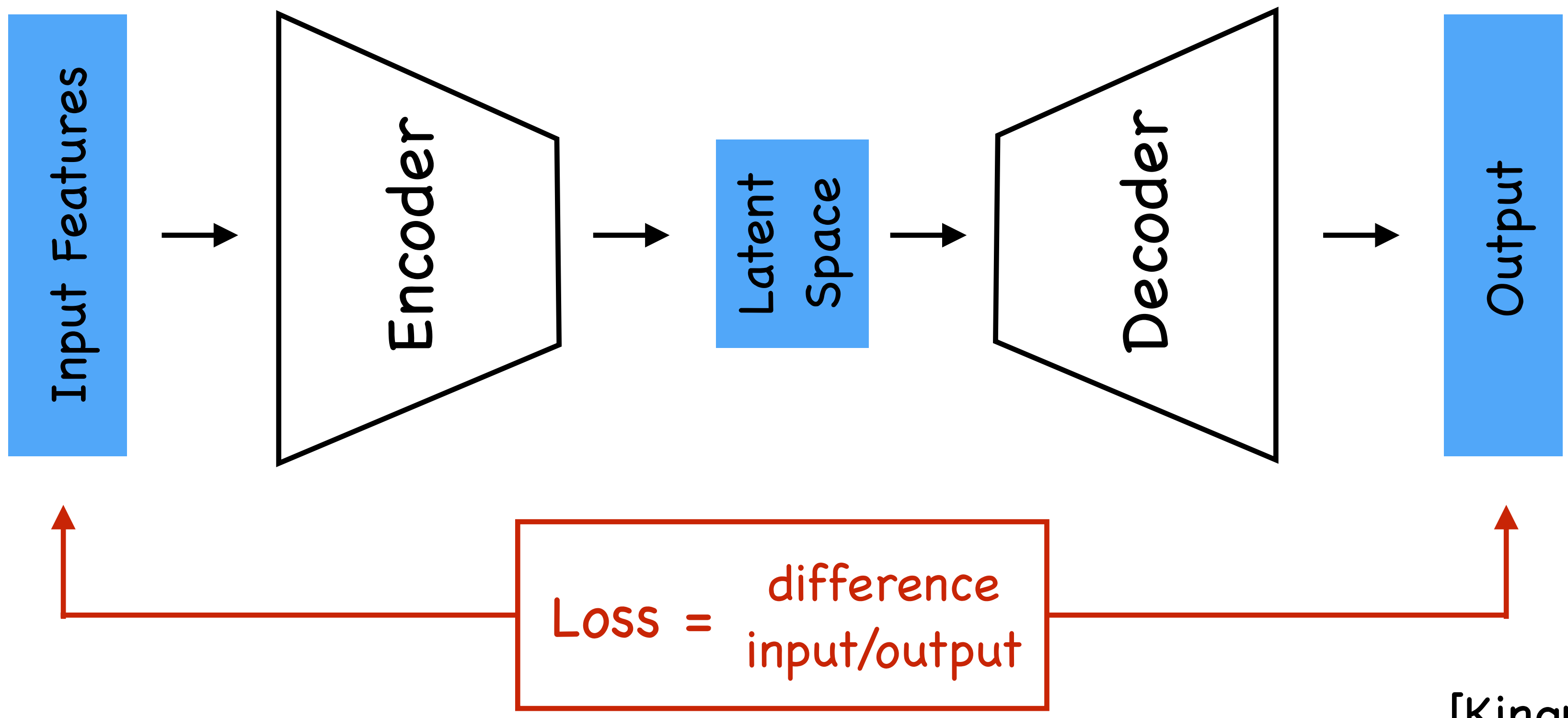
QC device vs simulator

Device	**Accuracy (%)**
PennyLane default.qubit	72.6
ibmq_qasm_simulator	72.6
ibmqx2	71.4

- Applied to $pp \to t\bar{t}$ vs $pp \to Z' \to t\bar{t}$ lept. top dec for 2d feature space only p_{T,b_1} and $\not{E}_T$

Autoencoder for unsupervised learning

Most popular NN-based anomaly detection method

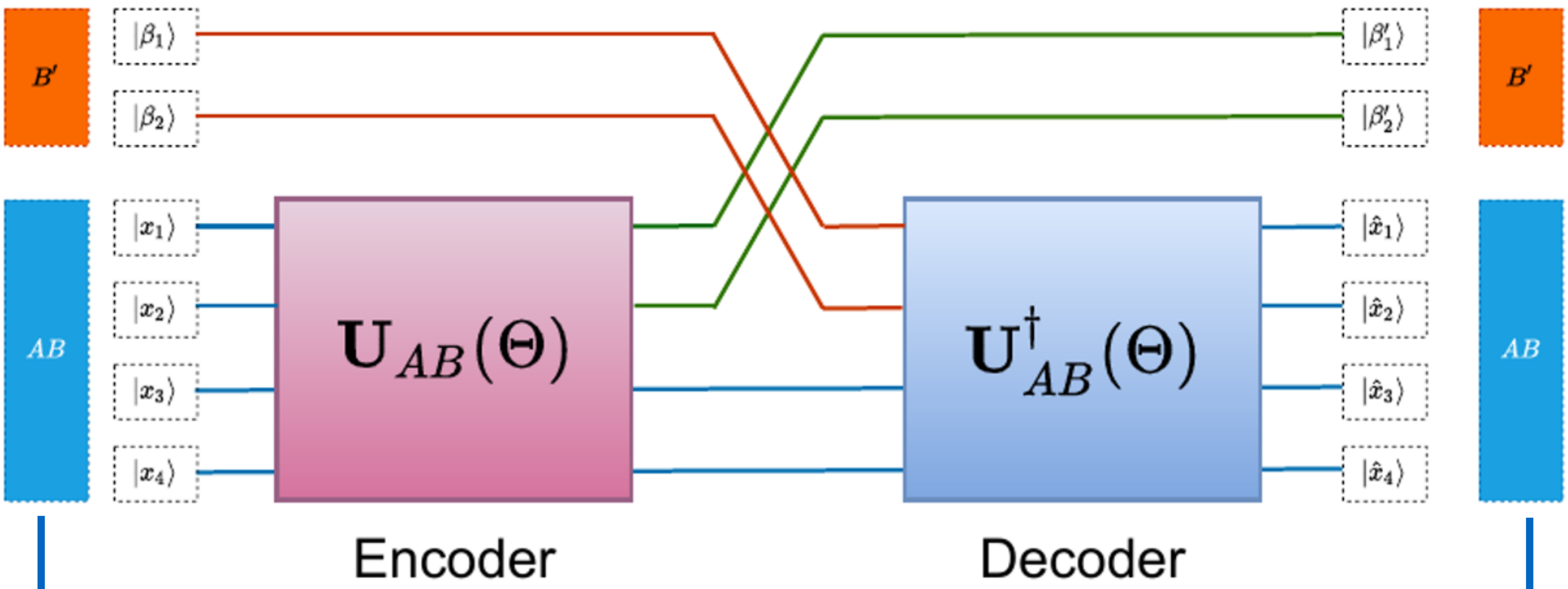


[Kingma, Welling '13]

- in first step input is encoded into information bottleneck
- between input/output layer and bottleneck can be several hidden layers (conv./deep NNs) -> highly non-linear
- after bottleneck decoding step
- Reconstructed output is then compared with input via loss-function (often MSE)
- NN is trained such that input and output high degree of similarity

Unsupervised learning with quantum-gate Autoencoder

[Ngairangbam, MS, Takeuchi '21]



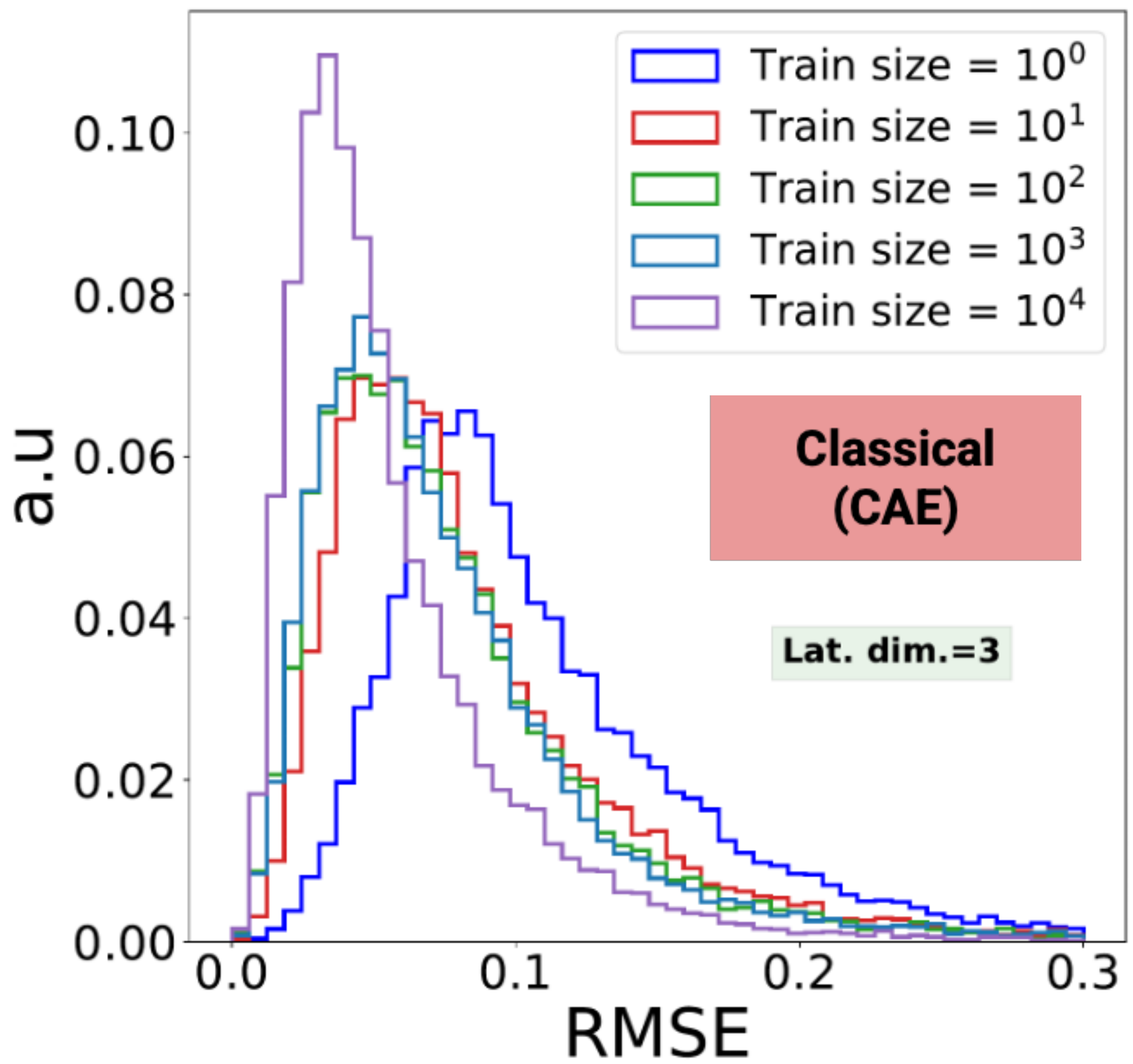
Quantum similarity measured via fidelity

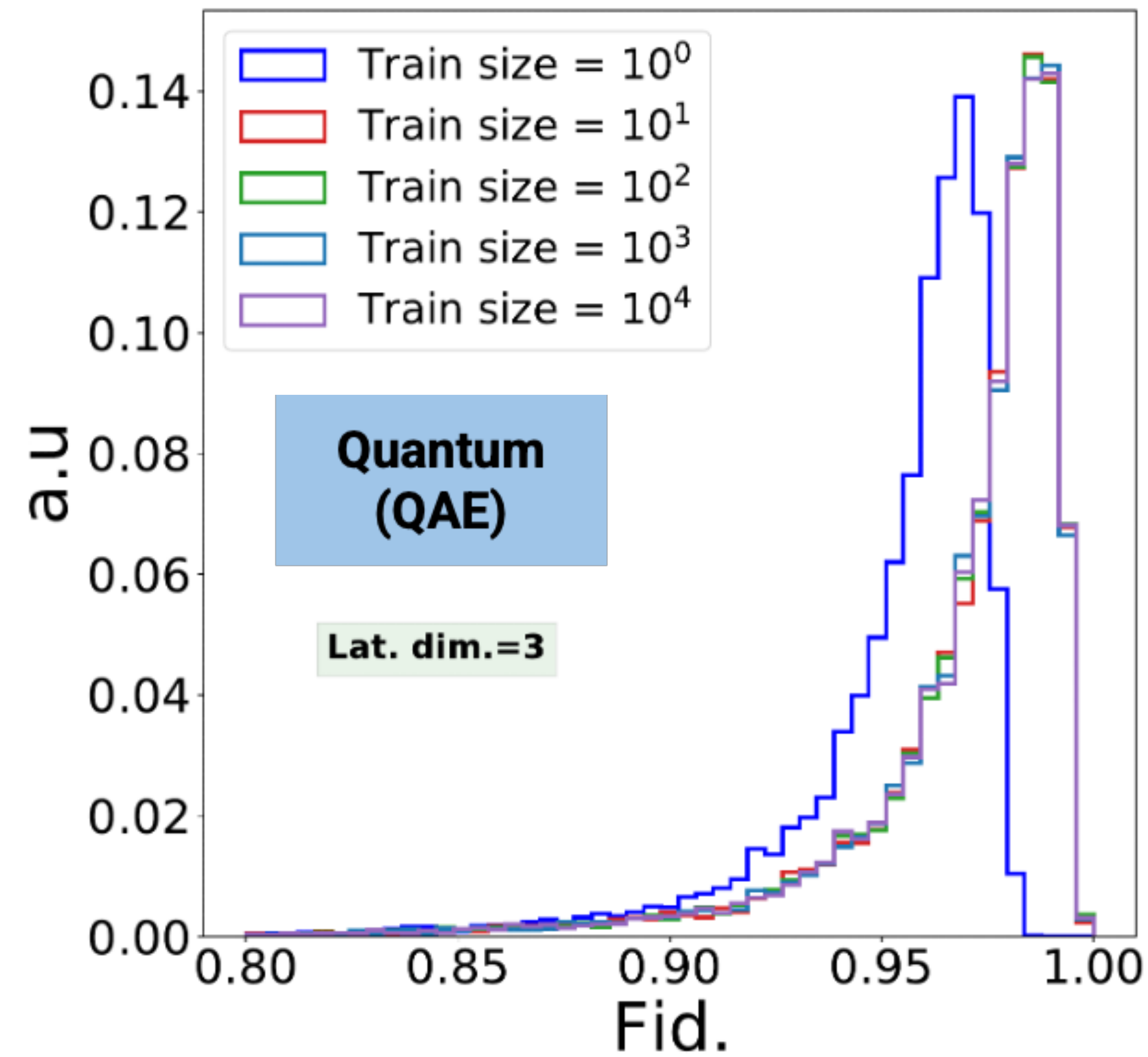
$$F(|\phi\rangle, |\psi\rangle) = F(|\psi\rangle, |\phi\rangle) = |\langle\phi|\psi\rangle|^2$$

Induce ***information bottleneck*** by **discarding states of B system** after encoding, and **replacing with reference states B'** with no connection with the encoder.

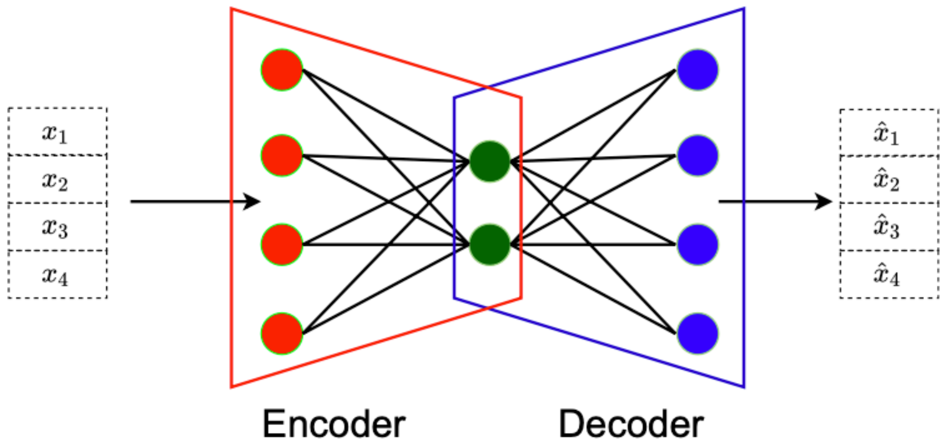
Results: Training size dependence

Dependence of (BG) test loss on training size

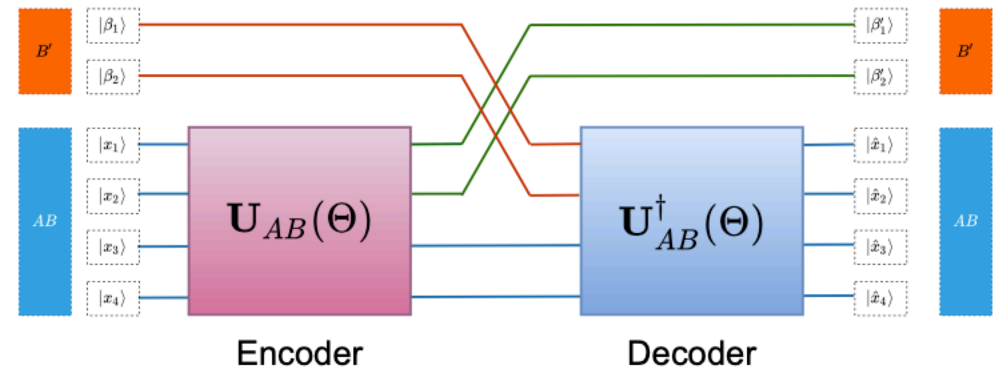


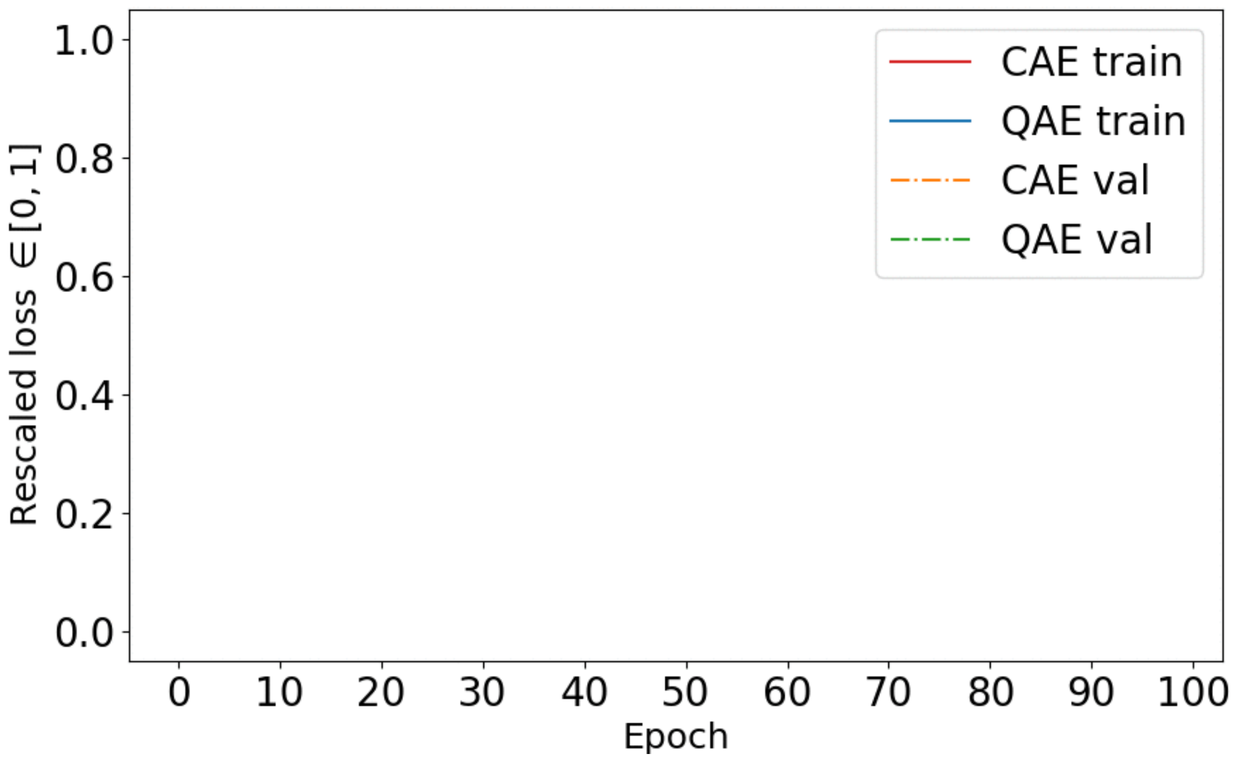


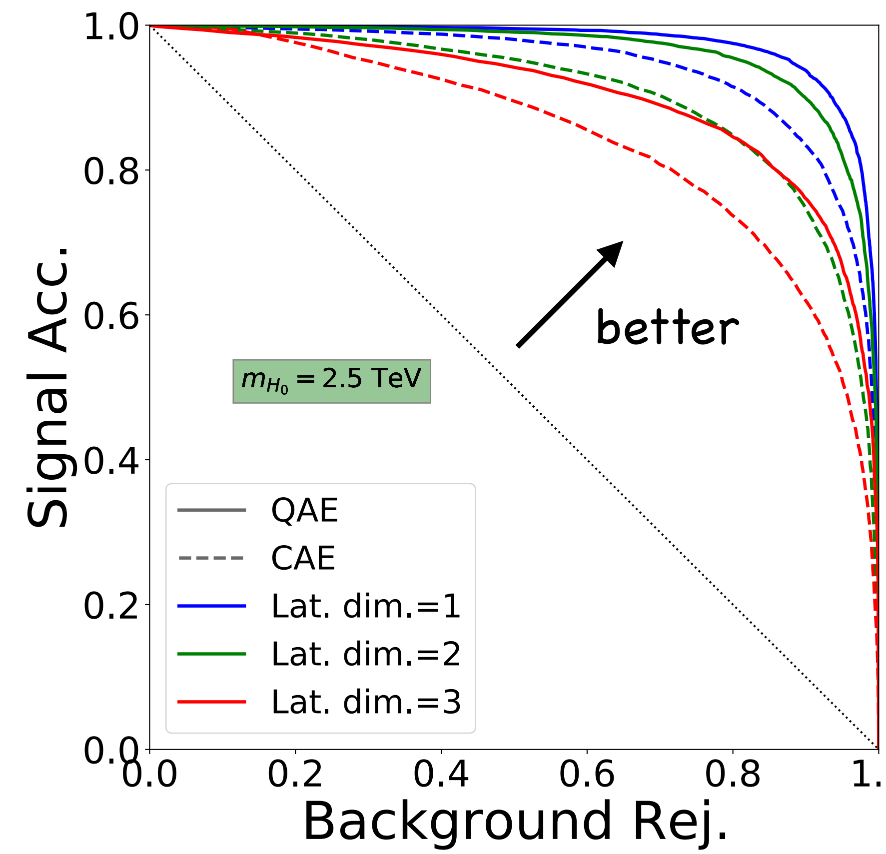
Classical autoencoder



Quantum autoencoder







→ Much faster training and better performance for Quantum autoencoder

→ In our test case, outcome prevails for much larger classical networks

Adiabatic quantum computing

- Adiabatic quantum computing (AQC) proposed as application of quantum adiabatic theorem to solve optimisation problems [Farhi, Goldstone, Gutmann '00]

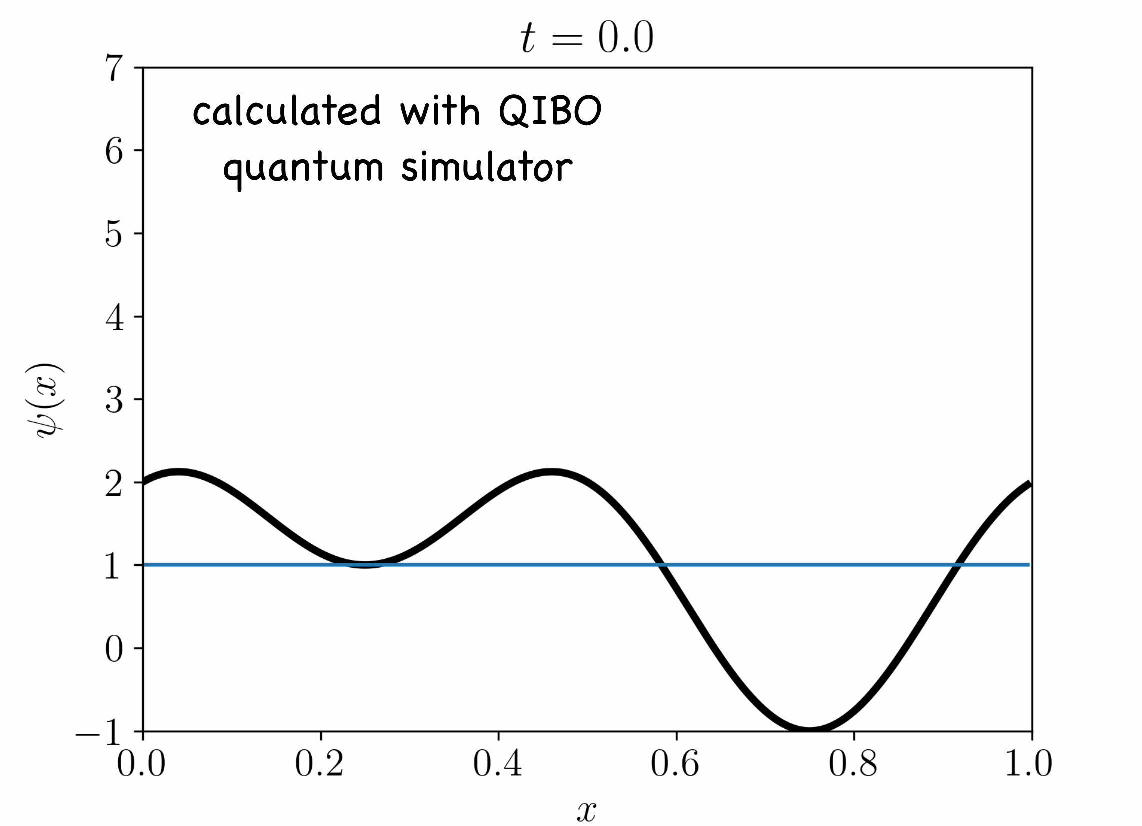
- Turns out to equivalent to quantum circuit model, i.e. it is universal [Aharonov, et al '07]

- States that if system prepared in ground state $|\psi_0\rangle$ of Hamiltonian $\mathcal{H}$

  If Hamiltonian changed smoothly and slowly enough system remains in ground state

  ➡ A time variation of the Hamiltonian from $\mathcal{H}_I$ to $\mathcal{H}_P$ is implemented according to:

$$\mathcal{H}(t) = (1 - s(t))\mathcal{H}_I + s(t)\mathcal{H}_P \quad t \in [0, T] \quad s : [0, \tau] \to [0, 1]$$



$$H = (1 - t)\,\frac{p^2}{2m^2} + t\ V(x)$$

↑ encode problem/optimisation task here

Quantum annealing: Non-universal but powerful?

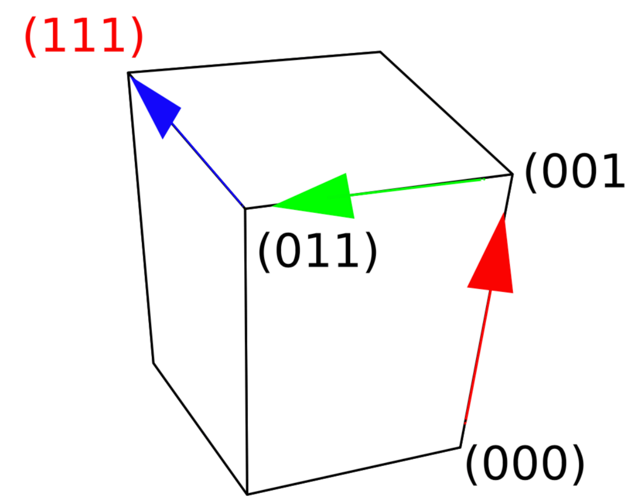
- Specific Hamiltonian. What does the "anneal" mean?

$$\mathcal{H}_{\mathrm{QA}}(t) = \sum_i \sum_j J_{ij}\sigma_i^Z \sigma_j^Z + \sum_i h_i \sigma_i^Z + \Delta(t)\sum_i \sigma_i^X$$

final Hamiltonian (encodes actual problem)

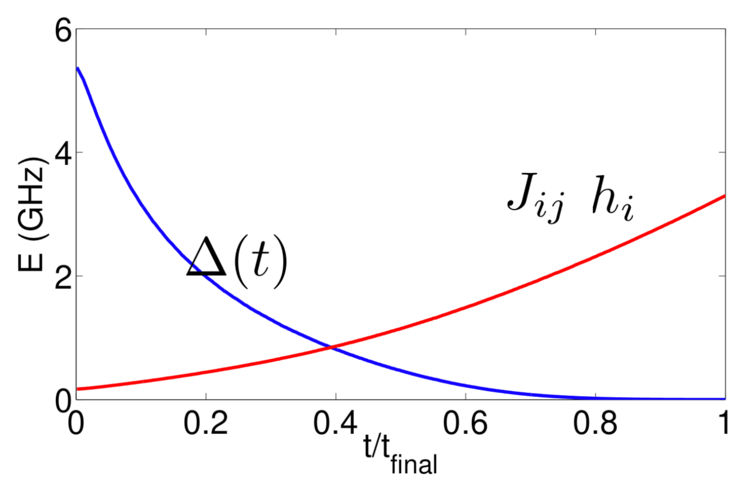
initial Hamiltonian (ground state = superposition of qubits with 0 and 1)

$\Delta(t)$ induces bit-hopping in the Hamming/Hilbert space



- Anneal idea: transition from ground state of initial Hamiltonian into ground state of problem Hamiltonian

- The idea is to dial this parameter to land in the global minimum (i.e. the solution) of some "problem space" described by J, h:

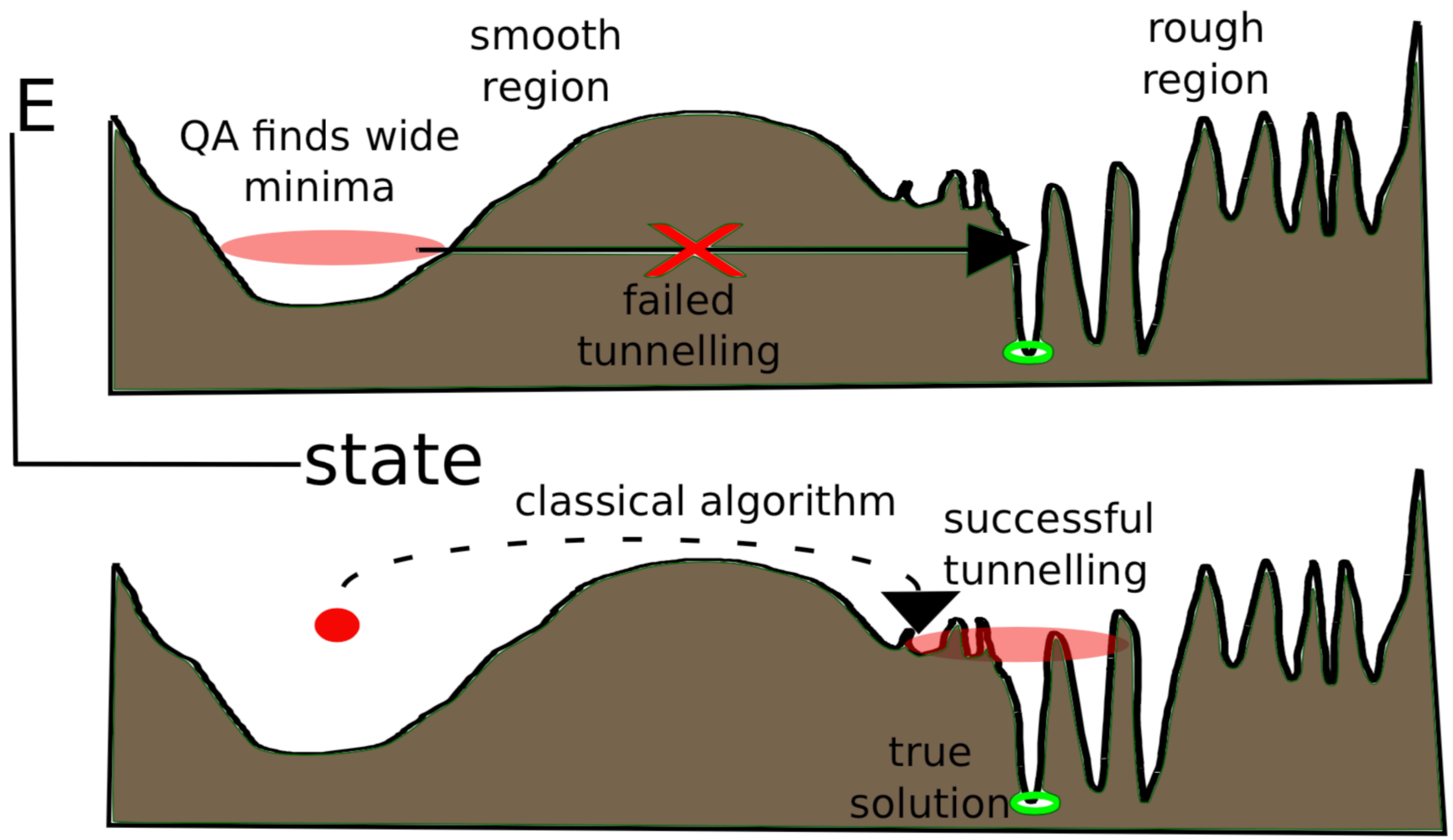


Thermal (classical) and Quantum Annealing are complementary:

- Thermal tunnelling is fast over broad shallow potentials $\sim e^{-\mathrm{height}/T}$
  (Quantum "tunnelling" is exponentially slow)

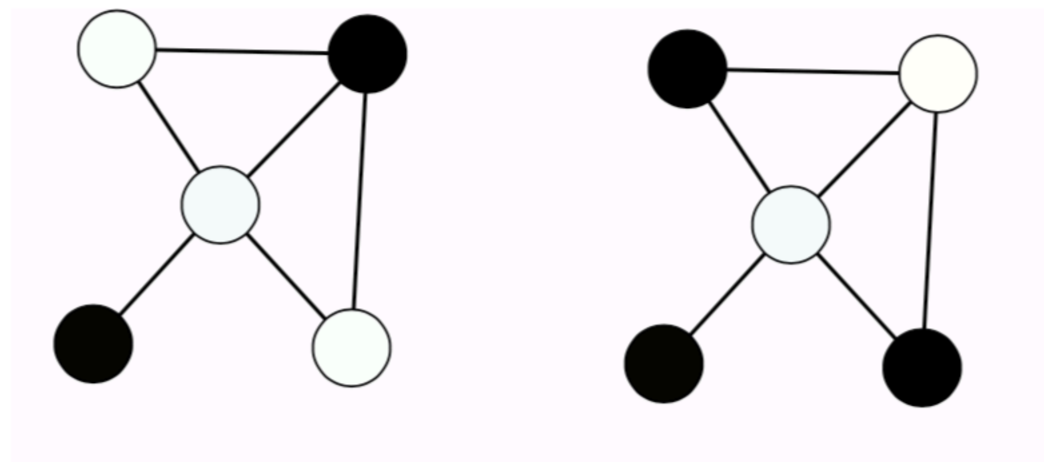
- Quantum tunnelling is fast through tall thin potentials $\sim e^{-\sqrt{\mathrm{height}}\times \mathrm{width}/\hbar}$
  (Thermal "tunnelling" is exponentially slow - Boltzmann suppression)

- Hybrid approach can be useful depending on solution landscape



How to encode a problem on an Ising model

Example 1: how many vertices on a graph can we colour so that none touch?



NP problem

Let non-coloured vertices have $\sigma_i^Z = -1$ and coloured ones have $\sigma_i^Z = +1$

Add a reward for every coloured vertex, and for each link between vertices i,j we add a penalty if there are two +1 eigenvalues:

$$\mathcal{H} = -\Lambda \sum_i \sigma_i^Z + \sum_{\text{linked pairs } \{i,j\}} \left[\sigma_i^Z + \sigma_j^Z + \sigma_i^Z \sigma_j^Z\right]$$

Example 2:
- N^2 students sit exam in a square room with NxN desks 1.5m apart.
- Half the students (A) have a virus while half of them (B) do not.

➡ How can they be arranged to minimise the number of infections due to <2m social distancing?

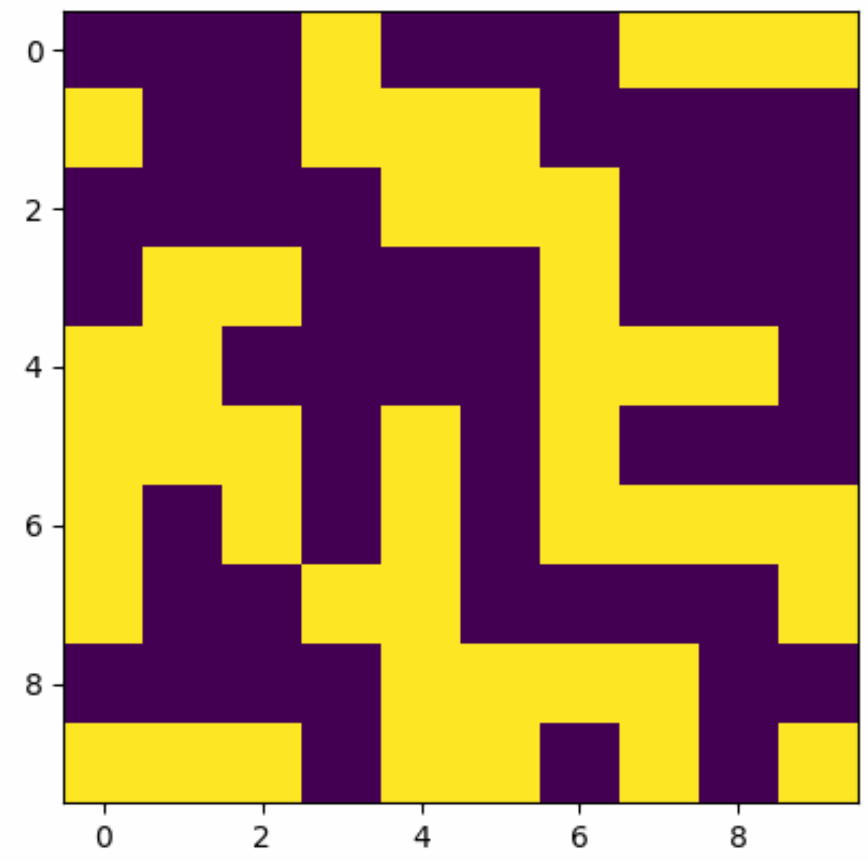
There are N^2 spins $\sigma^Z_{l\,N+j}$ arranged in rows and columns. We do not care if A>=<A or B>=<B, but if A>=<B then we put a penalty of 2+ on the Hamiltonian (ferromagnetic coupling) :

$$\mathcal{H} = \sum_{\ell m=1}^{N} \sum_{ij=1}^{N} \left(\delta_{\ell m}(\delta_{(i+1)j} + \delta_{(i-1)j}) + \delta_{ij}(\delta_{(\ell+1)m} + \delta_{(\ell-1)m})\right) \left[1 - \sigma^Z_{\ell N+i}\sigma^Z_{mN+j}\right]$$

Finally we need to apply constraint that #A=#B (no spontaneous healing/self-infection):

$$\mathcal{H}^{(\mathrm{constr})} = \Lambda\,(\#A - \#B)^2 \quad = \Lambda \left(\sum_{\ell,i}^{N} \sigma^Z_{\ell N+i}\right)^2 \quad = \Lambda \sum_{\ell m=1}^{N} \sum_{ij=1}^{N} \sigma^Z_{\ell N+i}\sigma^Z_{mN+j}$$

- Example 2 done with classical thermal annealing using the Metropolis algorithm.



- We find 2 degenerate solutions.

- Finding solutions easy for human, due to symmetry, but difficult for computer

➡ configuration space 2^100

➡ non-convex optimisation

➡ discrete problem (no gradient)

- Quantum annealing provides result in $\mathcal{O}(10\ \mu s)$

A quantum laboratory for QFT and QML

- going beyond the reach of classical computers -

- Using the spin-chain approach for field theories discussed before, we can encode a QFT on a quantum annealer and study its dynamics directly.

[Abel, MS '20]

- To show that the system is a true and genuine quantum system we investigate if the state can tunnel from a meta-stable vacuum into a the true vacuum.

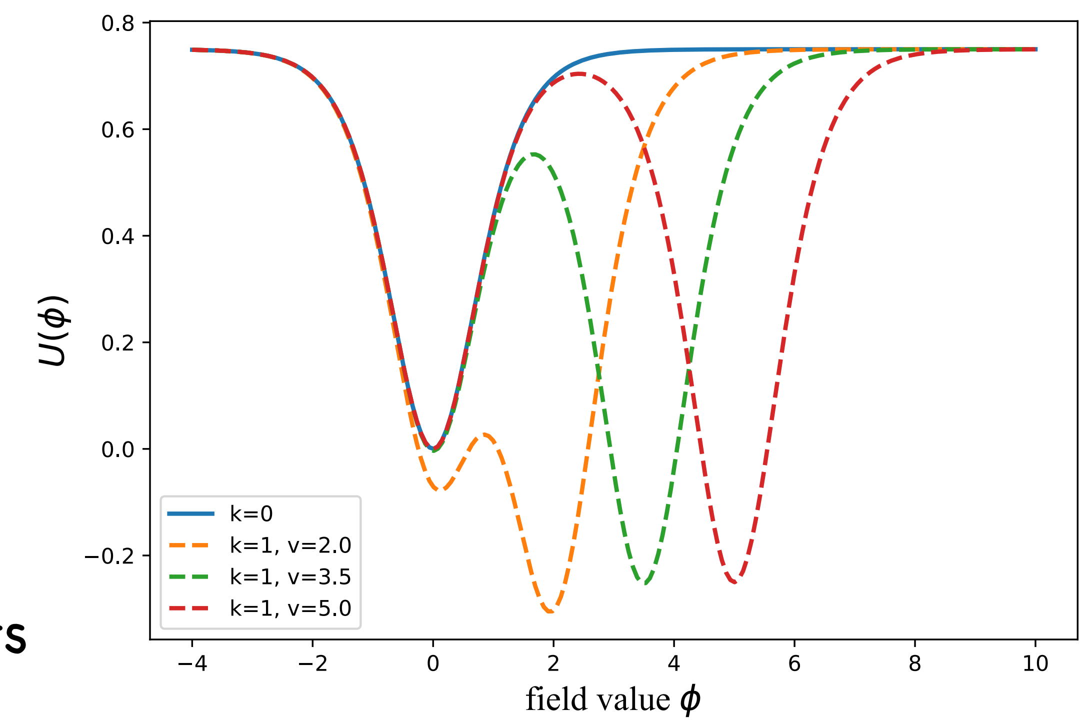
- Choose a potential of interest:

$$U(\phi) = \frac{3}{4}\tanh^2\phi - k(t)\,\mathrm{sech}^2\left(c(\phi - v)\right)$$

time dependent

where $\phi = \eta/\eta_0$

$\phi(t)$ is the field and c, v are dimless constants



- For real-time evolution of field theory on QA see [Fromm, Philipsen, Winterowd '22]

The tunnelling probability in a QFT is calculated by evaluating the path-integral in Euclidean space around the action's critical points using the steepest gradient-descent method

$$\langle \eta_i | \eta_f \rangle_E = \int \mathcal{D}\delta\eta \, e^{-\hbar^{-1} \int dt \left(\frac{m(\dot{\eta}_{cl}+\delta\dot{\eta})^2}{2} + U(\eta_{cl}+\delta\eta) - E_0 \right)} = A e^{-\hbar^{-1} S_{E,cl}}$$

quantum annealer

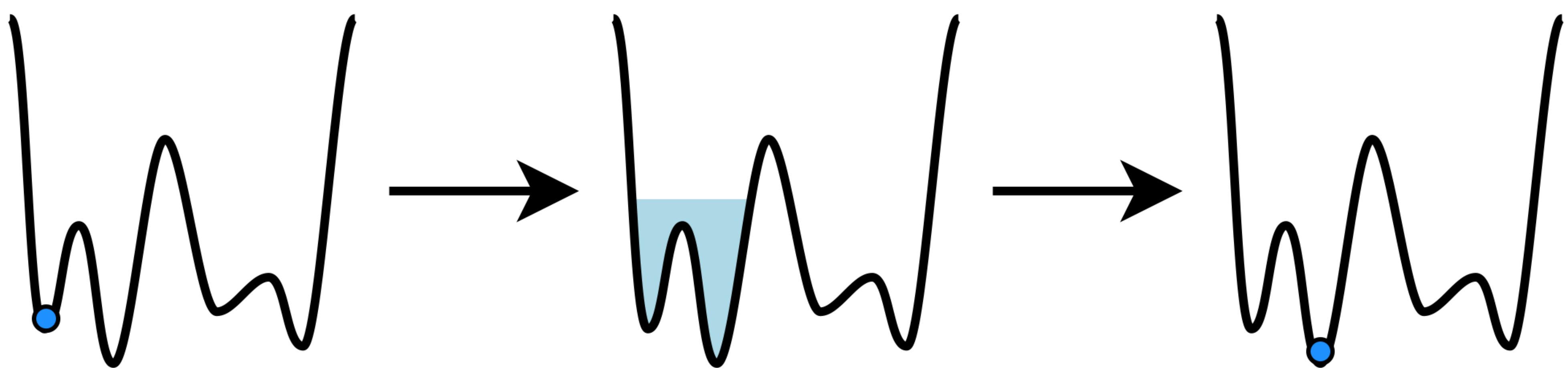
For the tunnelling rate $\Gamma = |\langle \eta_i | \eta_f \rangle_E|^2 \approx e^{-2\hbar^{-1} S_{E,cl}}$ with $S_{E,cl} = \int_{\eta_+}^{\eta_e} d\eta \sqrt{2m(U - E_0)}$

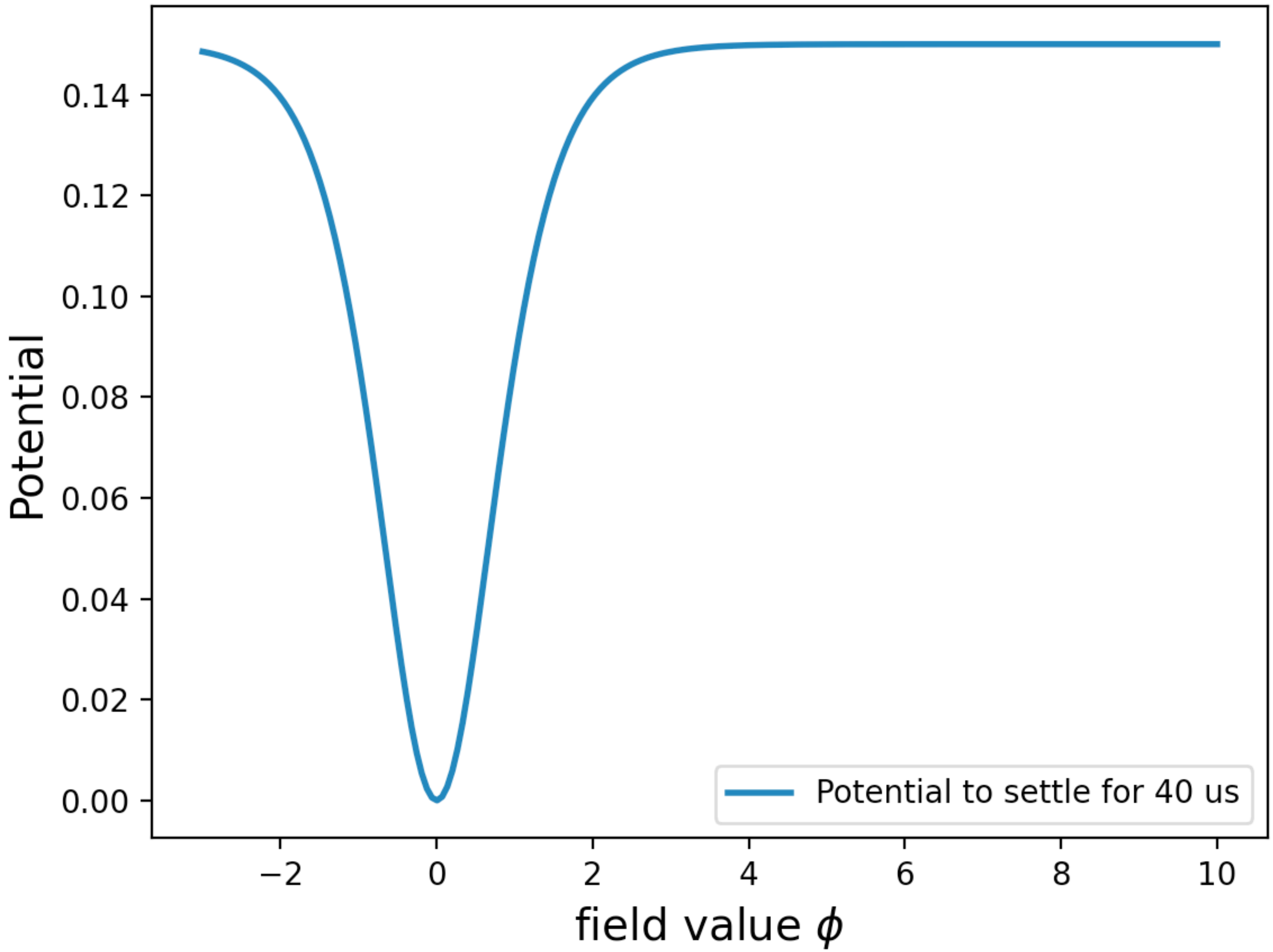
Exponent is object of interest: $\hbar^{-1} S_E \approx \gamma^{-\frac{1}{2}} \int_{\phi_+}^{\phi_e} \sqrt{\frac{3}{4} \tanh^2 \phi - \operatorname{sech}^2(\phi - v)} \, d\phi$ with $\gamma \stackrel{\text{def}}{=} \hbar^2 / 2m\eta_0^2$

$$\log \Gamma \approx -2\hbar^{-1} S_E \approx \sqrt{\frac{3}{\gamma}} \left(\frac{5}{3} - v \right)$$

D-Wave reverse annealing

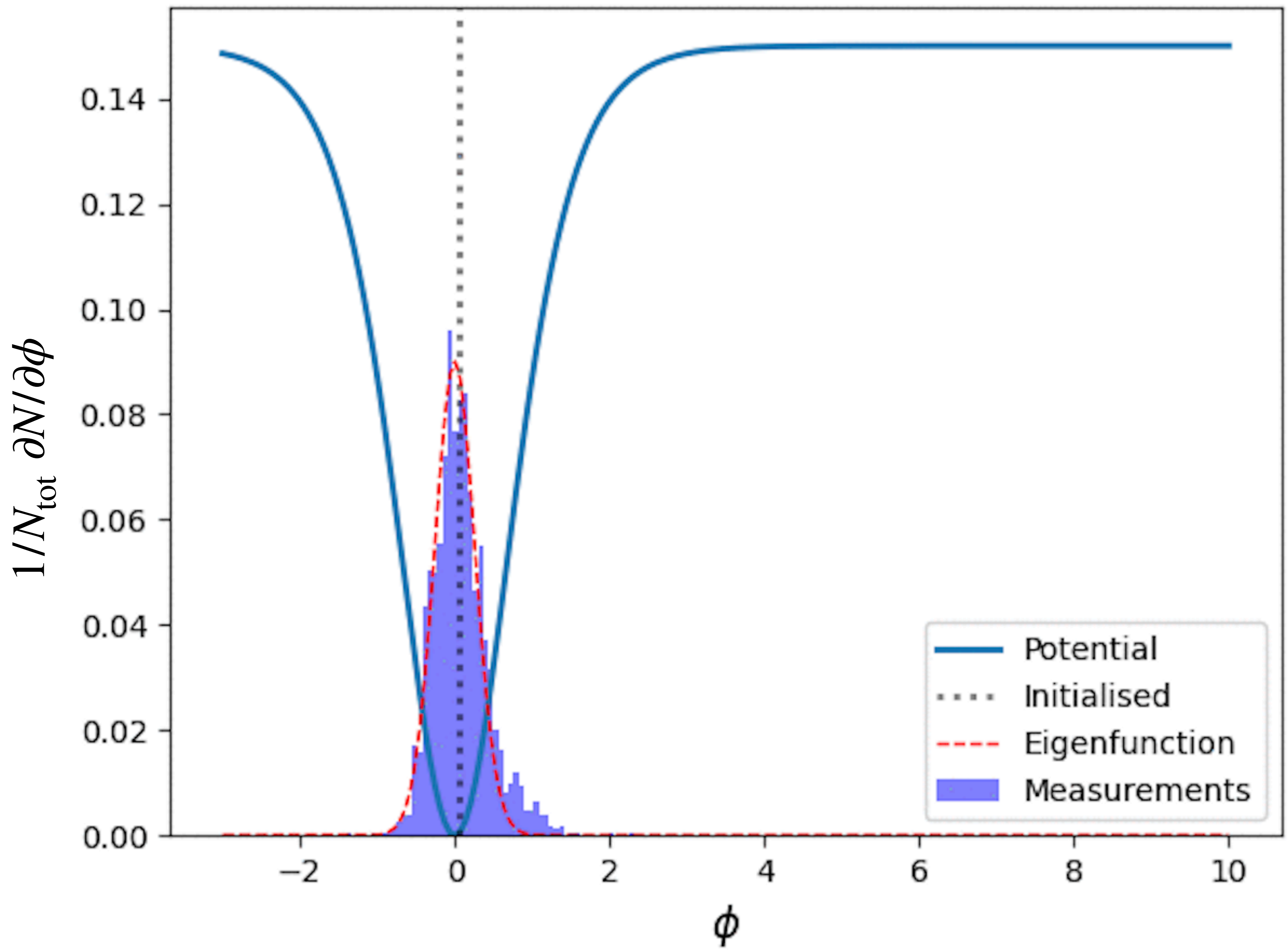
starts at sq=1 (classical) -> sq < 1 (quantum) -> measurement in sq=1 (classical)

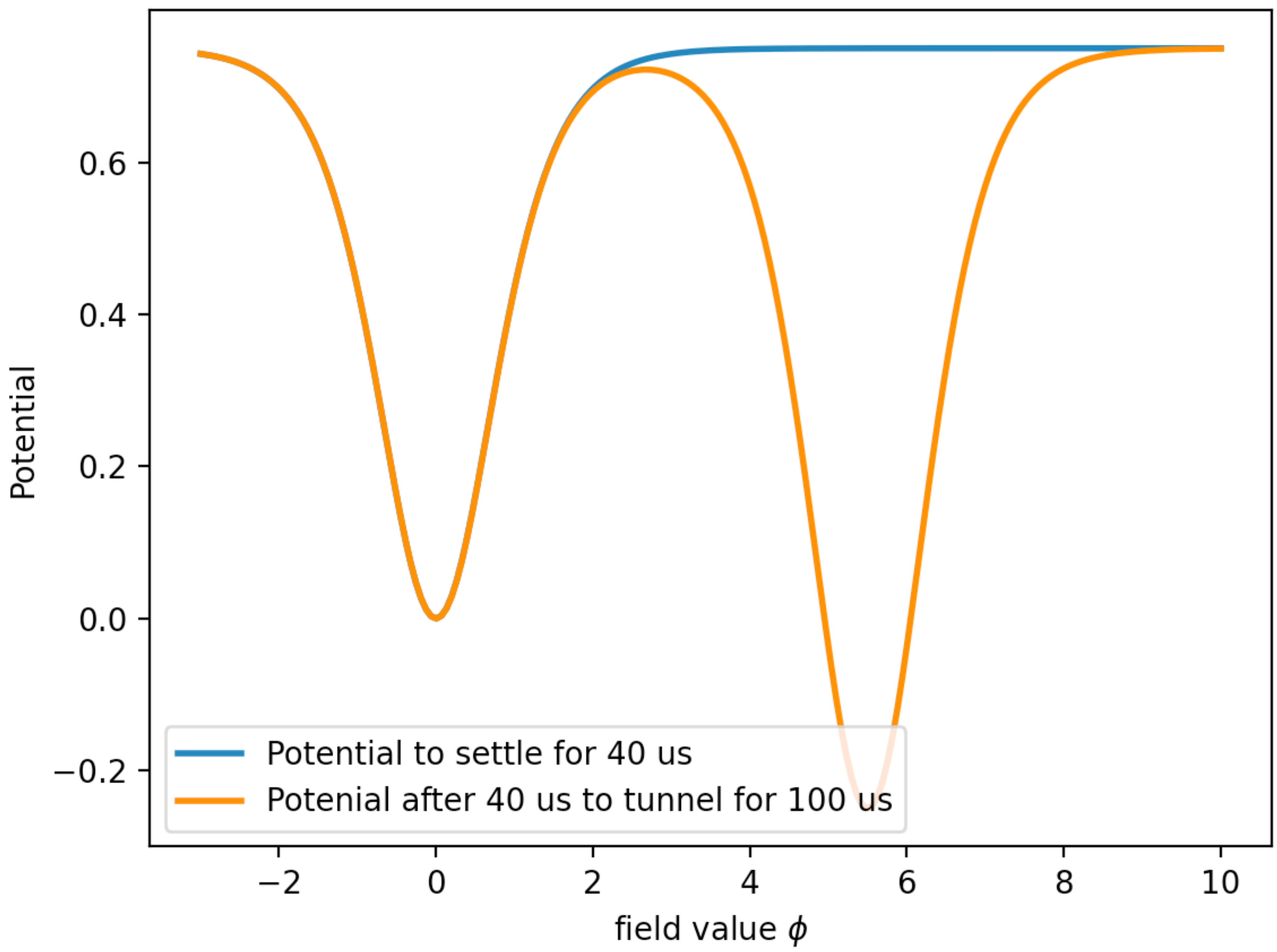


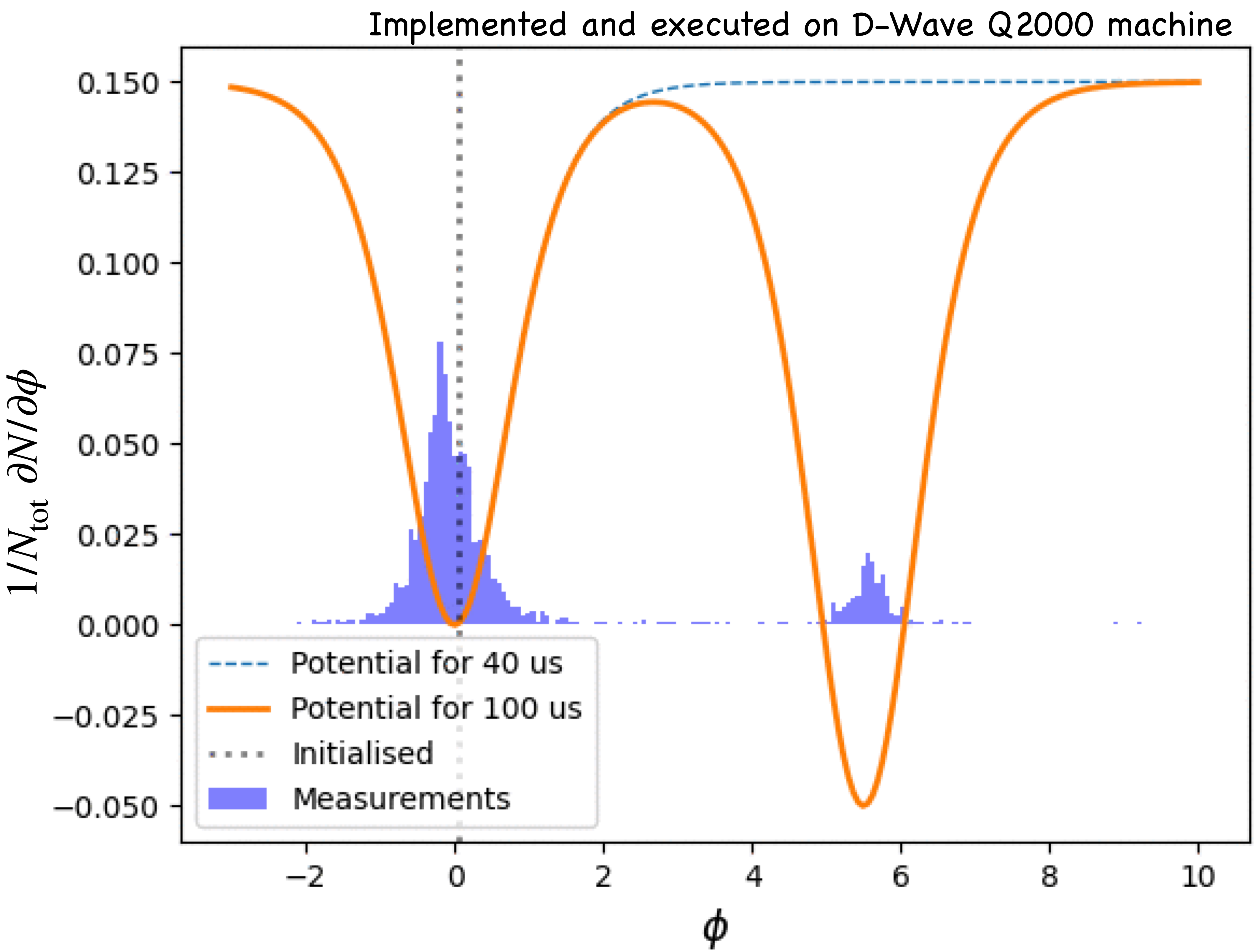


0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Potential
−2
0
2
4
6
8
10
field value ϕ
Potential to settle for 40 us

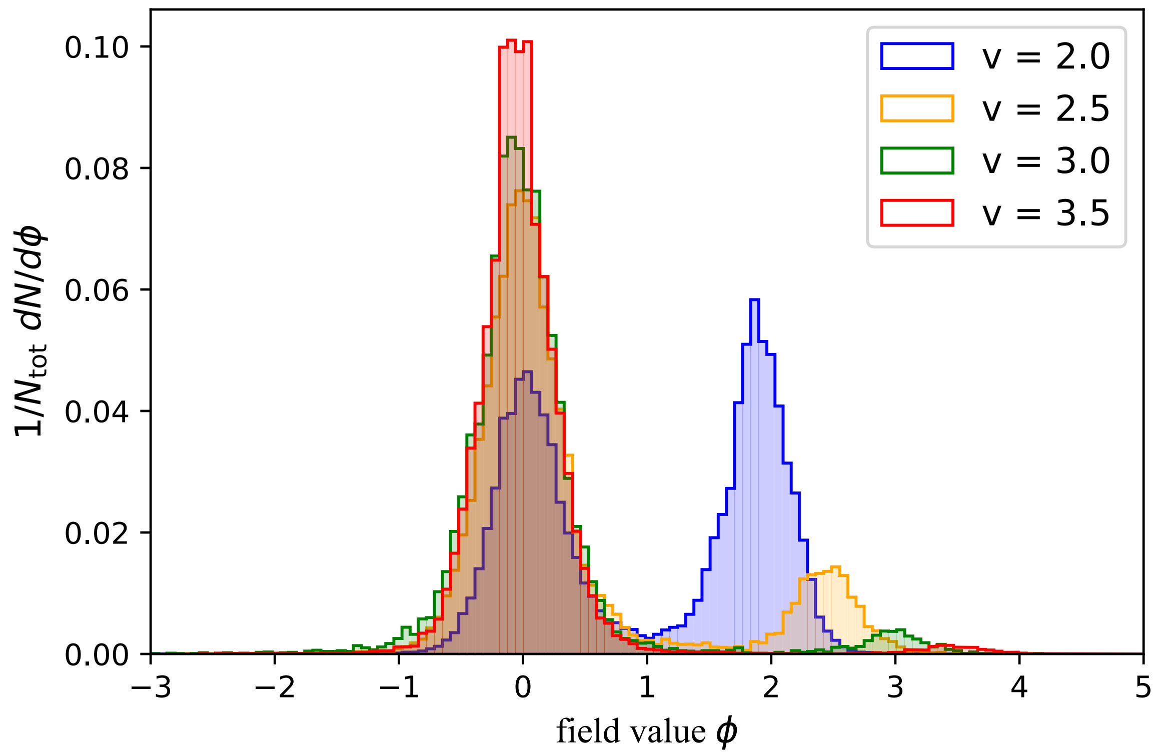
Implemented and executed on D-Wave Q2000 machine




0.6
0.4
0.2
0.0
−0.2
Potential
Potential to settle for 40 us
Potenial after 40 us to tunnel for 100 us
−2
0
2
4
6
8
10
field value ϕ

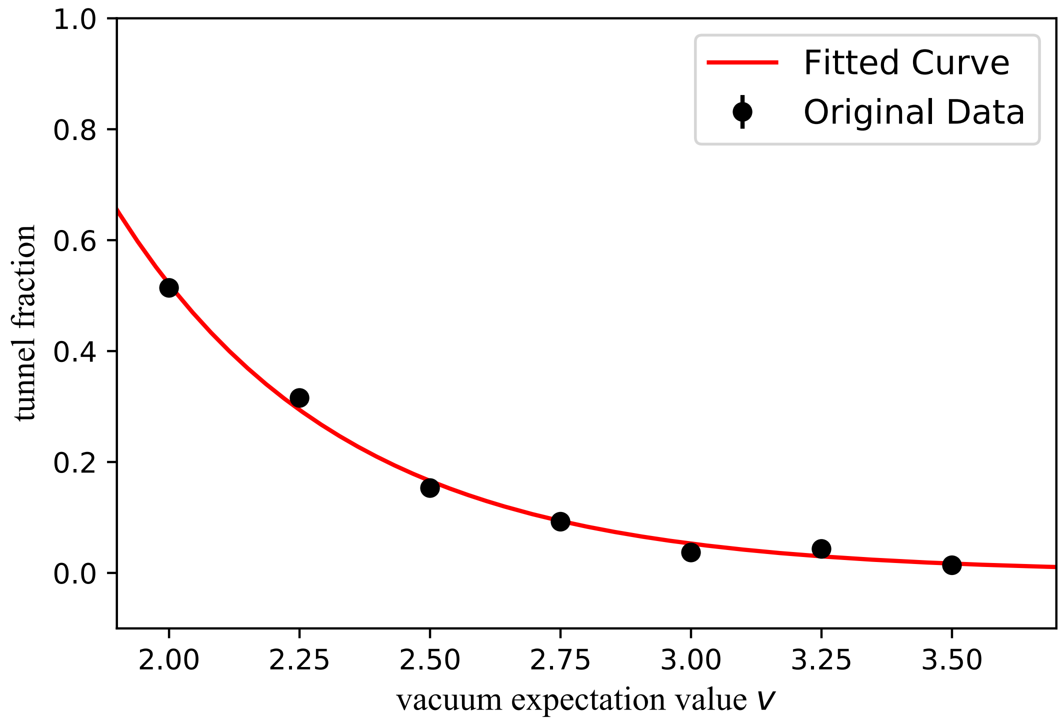

Implemented and executed on D-Wave Q2000 machine
0.150
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
−0.050
−2
0
2
4
6
8
10
ϕ
$1/N_{\text{tot}}\ \partial N/\partial\phi$
Potential for 40 us
Potential for 100 us
Initialised
Measurements

Results: it decays with v as expected



Perform tunnelling for

$t_{\text{tunnel}} = 100\mu s$ at $s_q = 0.7$

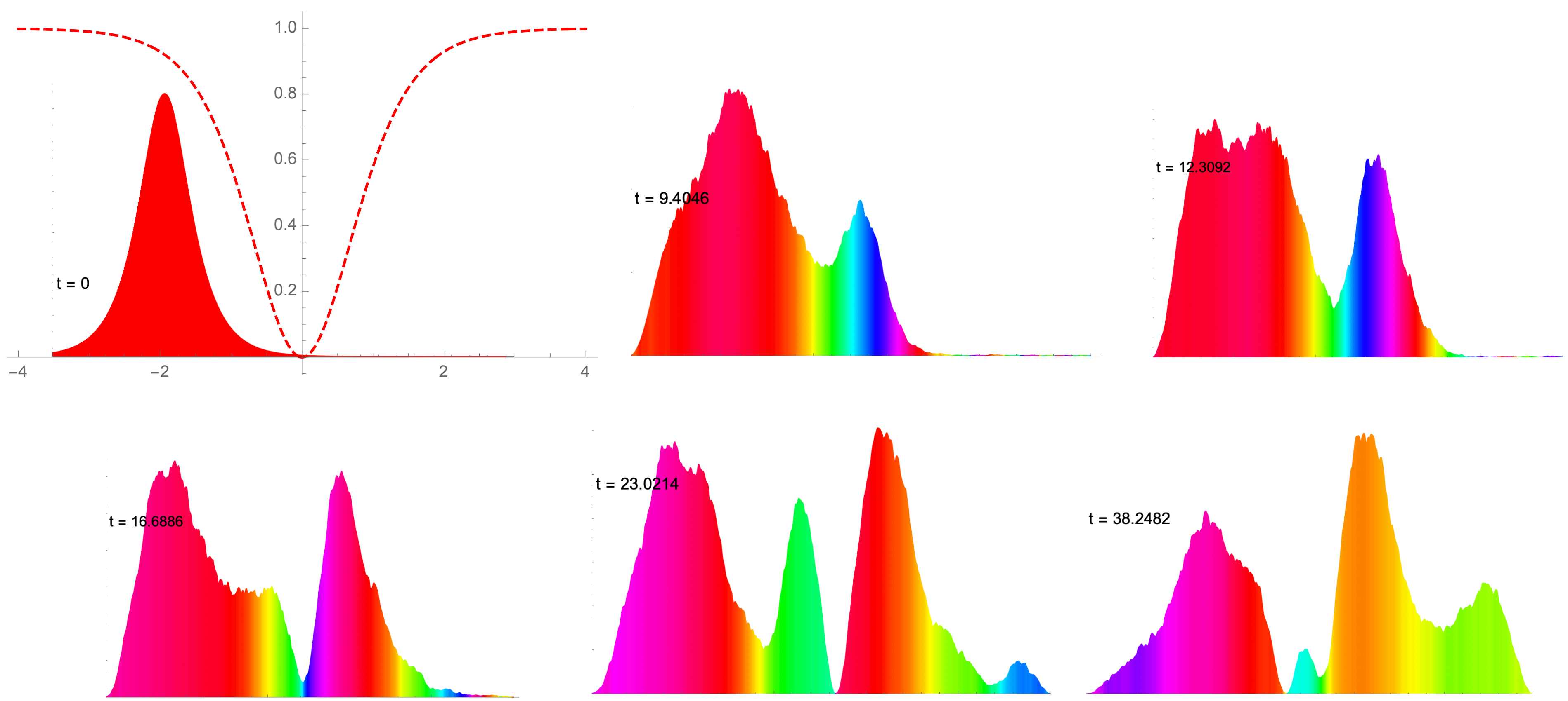


Theory: $\log\Gamma = 3.0 \times (1.66 - v)$

Exp: $\log\Gamma = 2.29 \times (1.71 - v)$

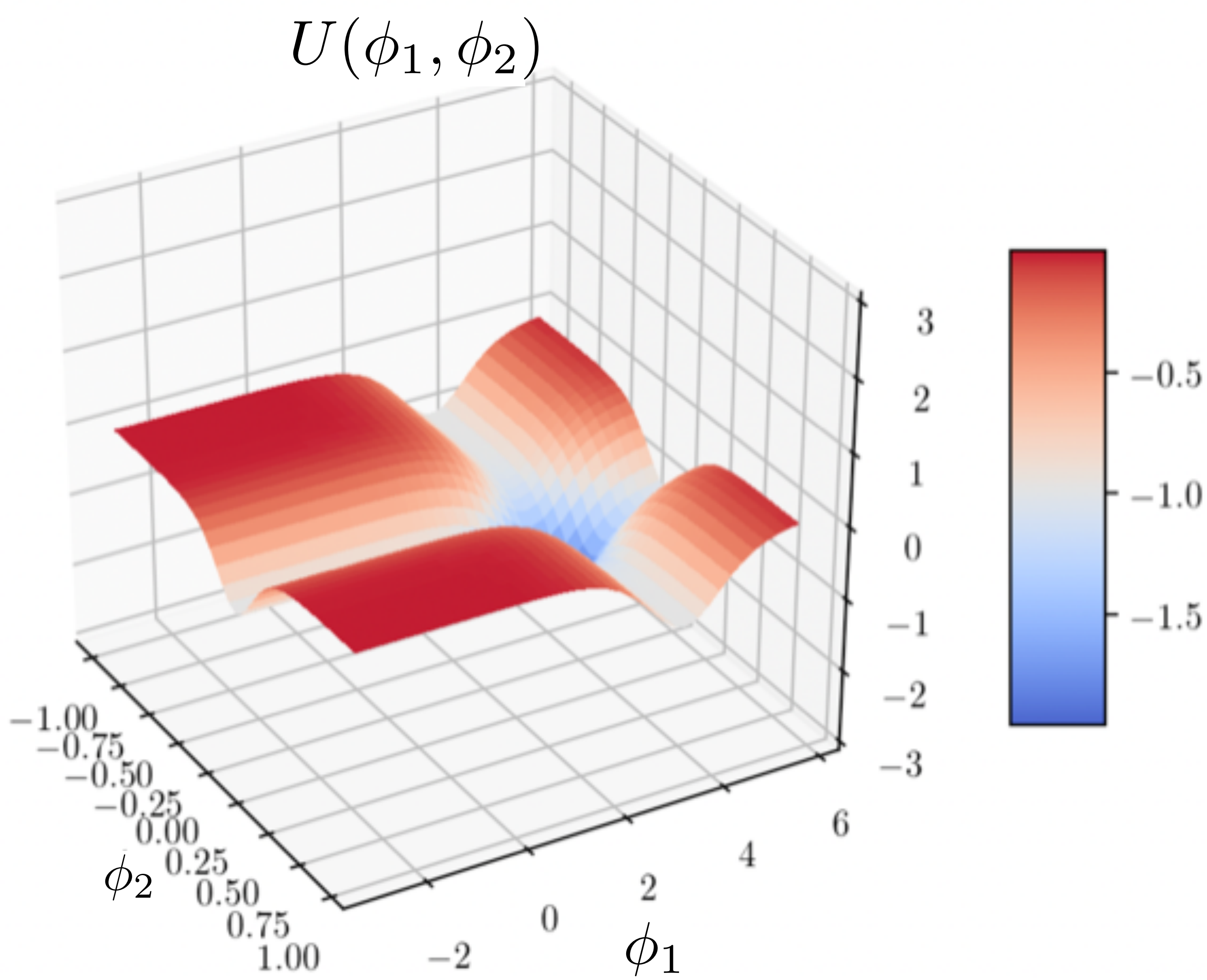
Also dynamics has characteristic behaviour. For example it still "tunnels" to the bottom of a potential even if there is no barrier: i.e. the wave function leaks across, rather than rolling as a lump —

Numerically solving S.E. we find (this takes an hour!)

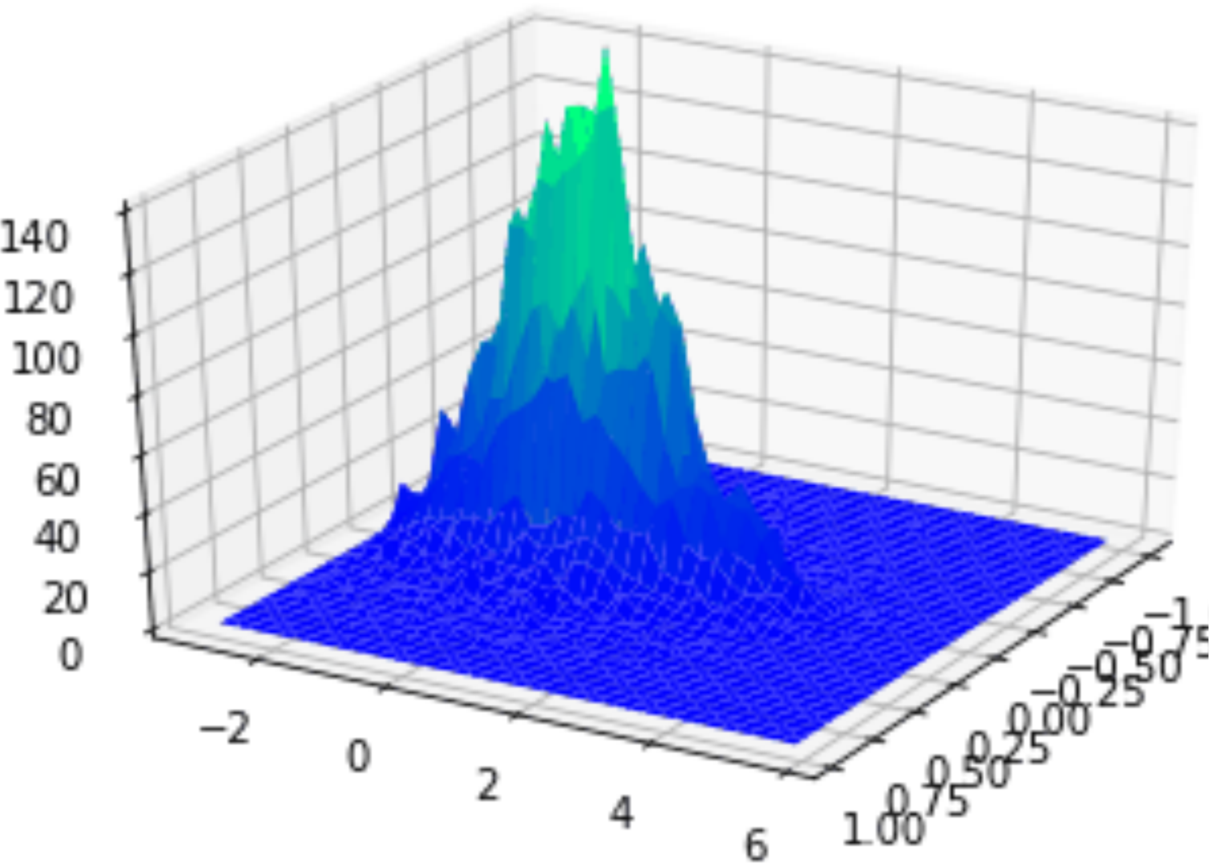


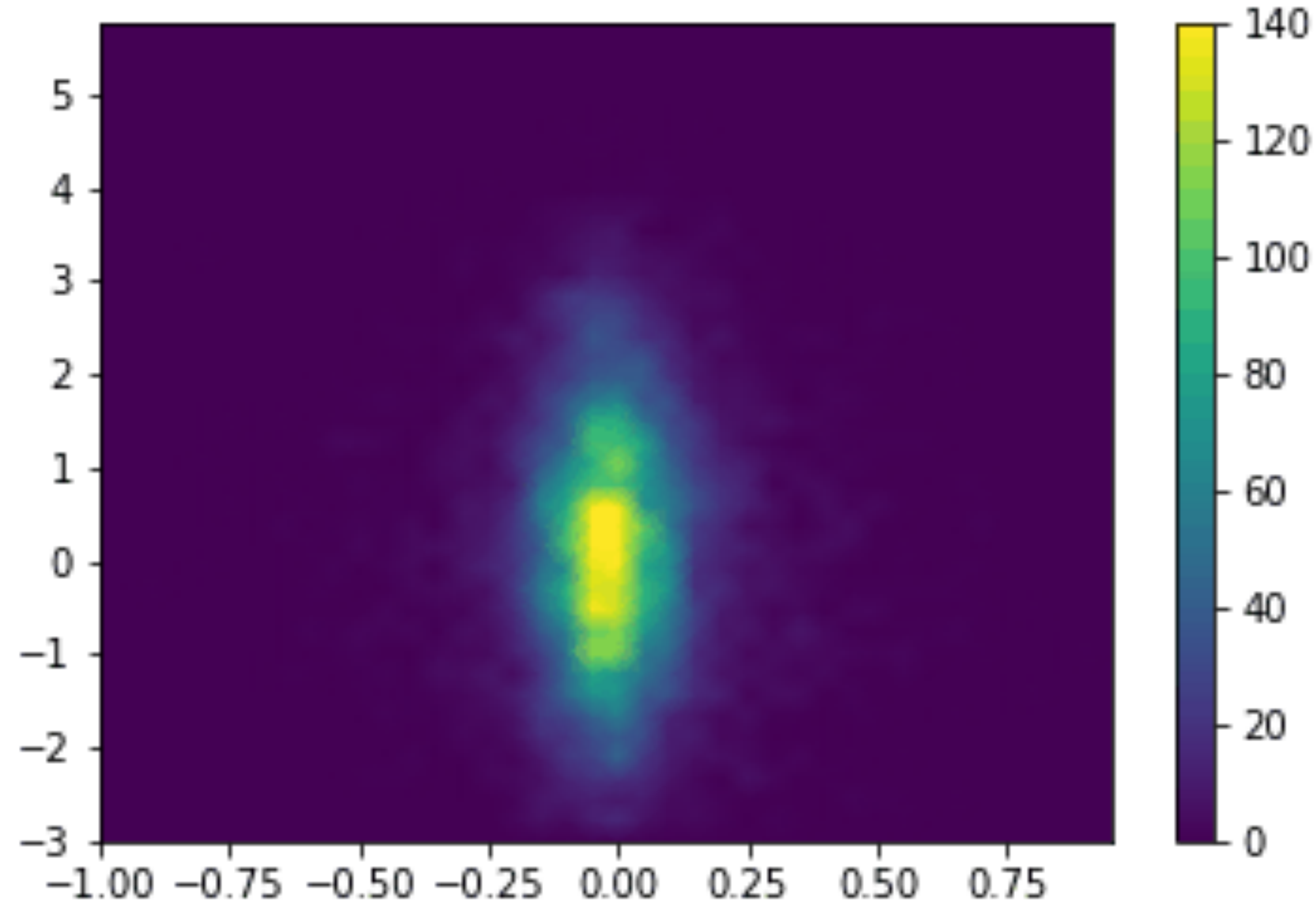
Also dynamics has characteristic behaviour. For example it still transits to the bottom of a potential even if there is no barrier i.e. the wave function leaks across, rather than rolling as a lump

2D example potential



Also dynamics has characteristic behaviour. For example it still transits to the bottom of a potential even if there is no barrier i.e. the wave function leaks across, rather than rolling as a lump



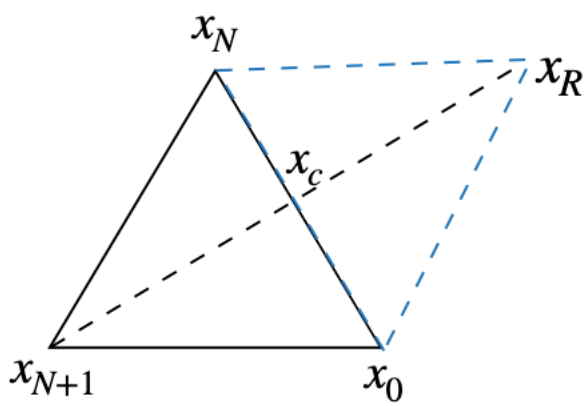


Optimisation comparison quantum vs classical

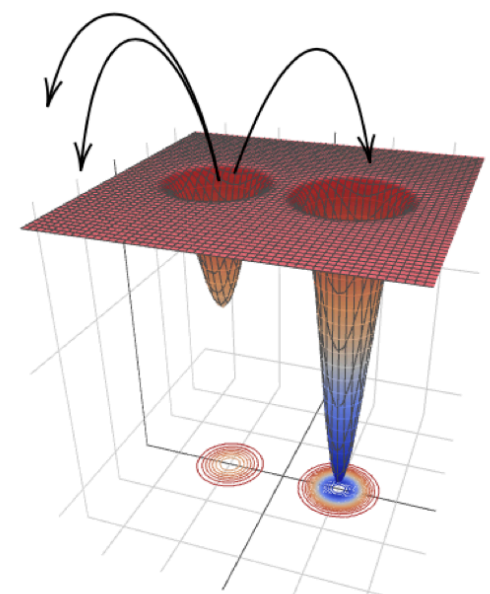
gradient descent

$$x_{i+1} = x_i - \nabla f(x_i)$$

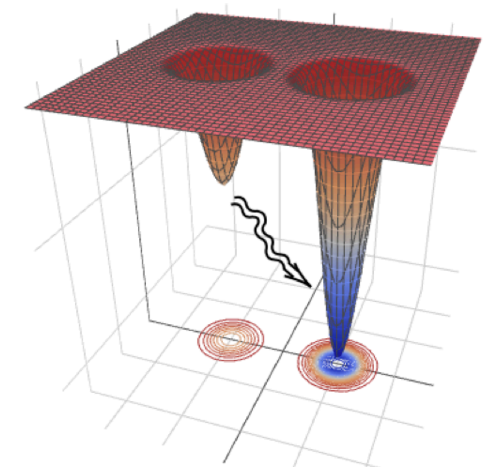
Nelder-Mead



Thermal Annealing

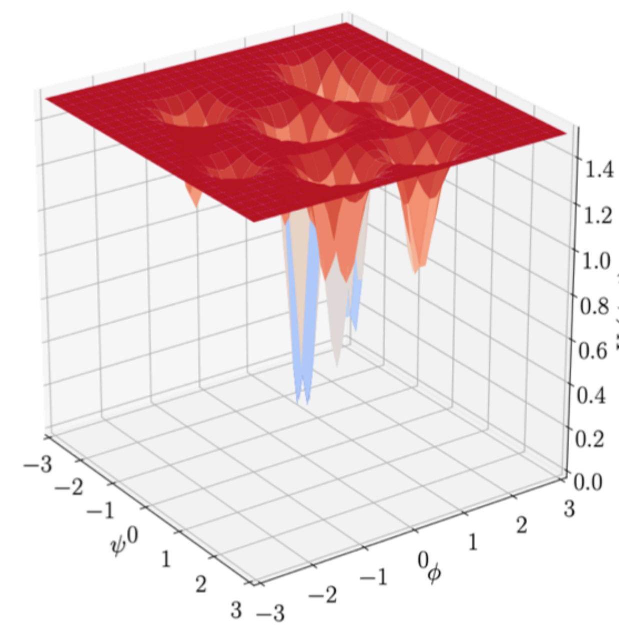


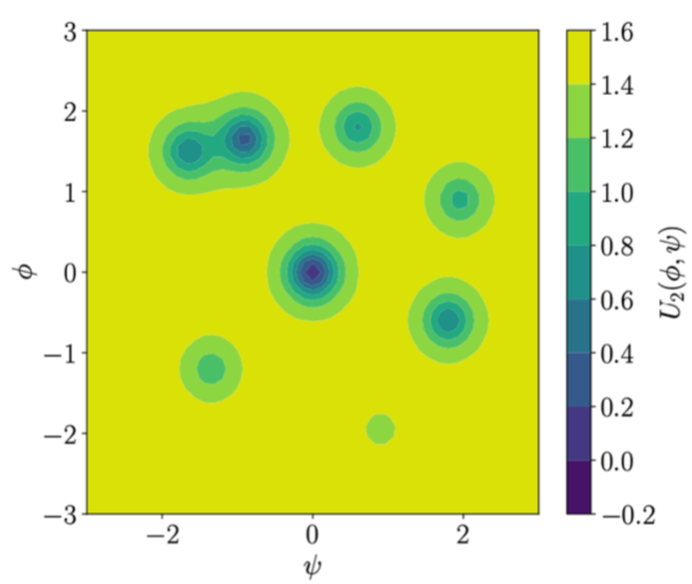
Quantum Annealing



Applied to several examples in [Abel, Blance, MS '21], let's show one here:

Multi-well potential



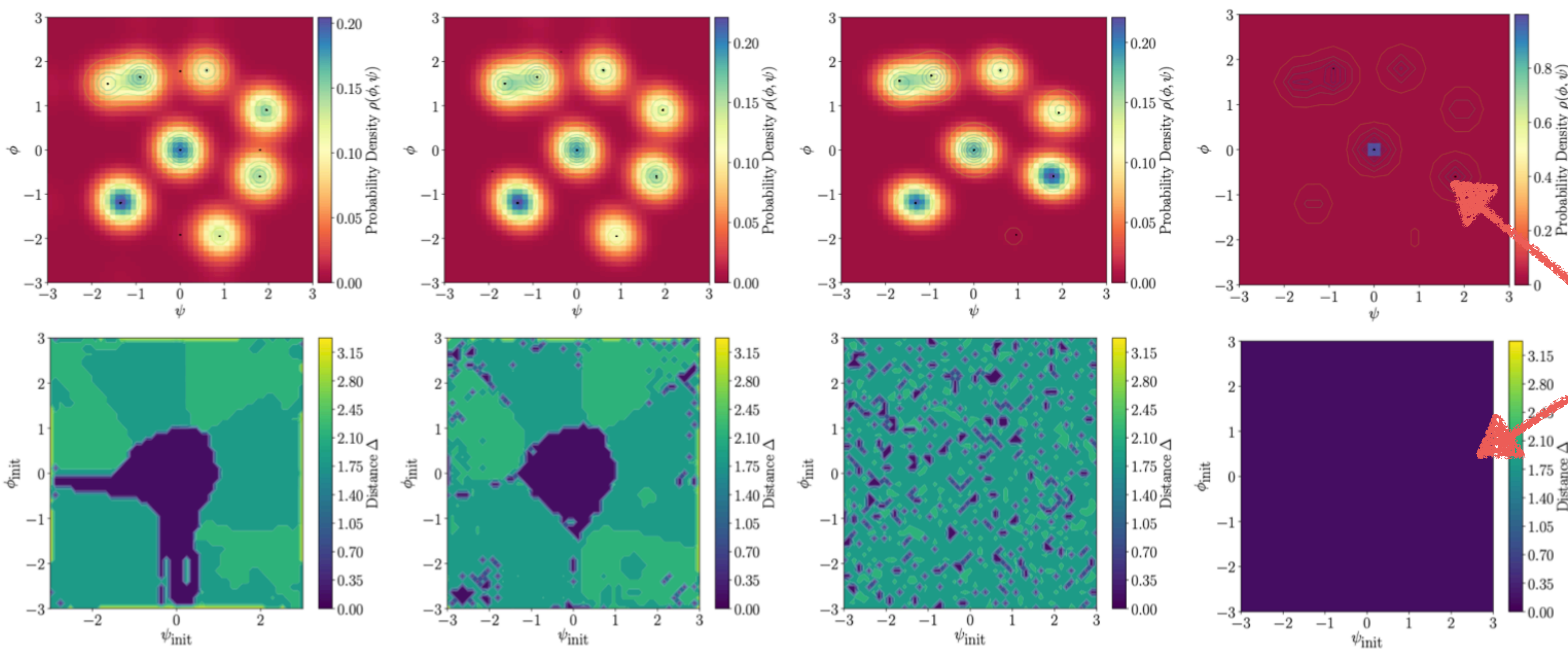


Results for Multi-well potential

- Quantum algorithms finds global minimum of potential reliably and fast!

Method	Time/run (μs)
Nelder-Mead	4900
Gradient Descent	2900
Thermal Annealing	5×10^5
Quantum Annealing	115

[Abel, Blance, MS '21]



(a) Nelder-Mead (b) Gradient descent (c) Thermal annealing (d) Quantum annealing

Quantum annealer almost never gets stuck in wrong minimum

QA is depth savvy, i.e. works qualitatively different

→ Clear advantage

Completely Quantum Neural Networks

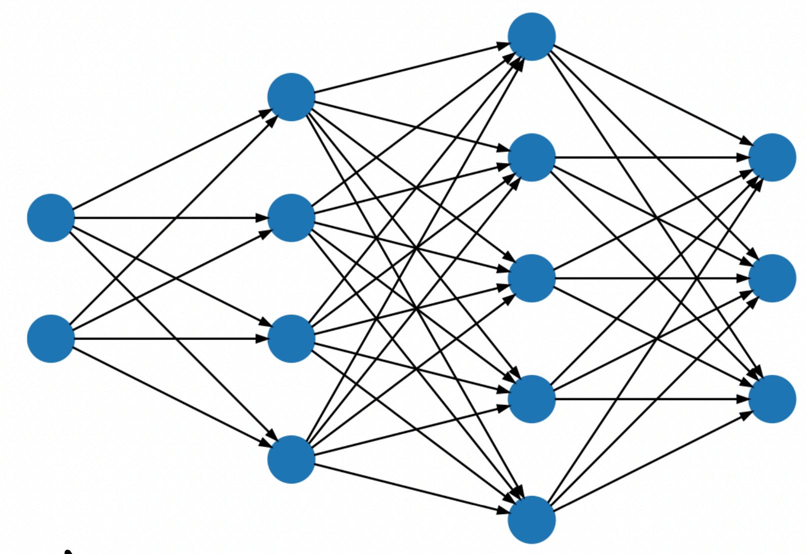
Structure of node i, in layer L $$L_i(x) = g\left(\sum_i w_{ij} x_i + b_i\right)$$

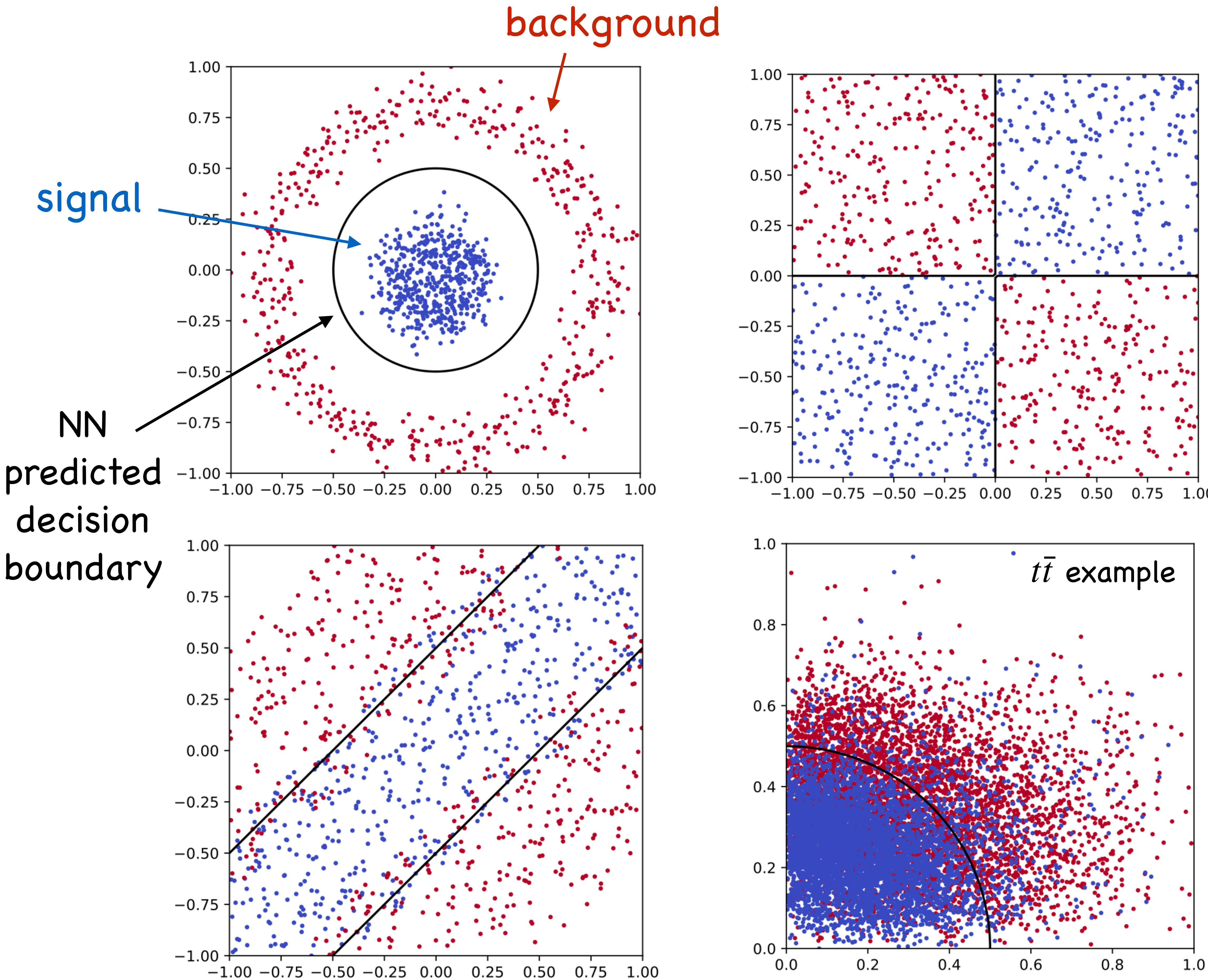
Network output in final layer $$Y = L^{(n)} \circ \ldots \circ L^{(0)}$$

Loss function $$\mathcal{L}(Y) = \frac{1}{N_d} \sum_a |y_a - Y(x_a)|^2$$

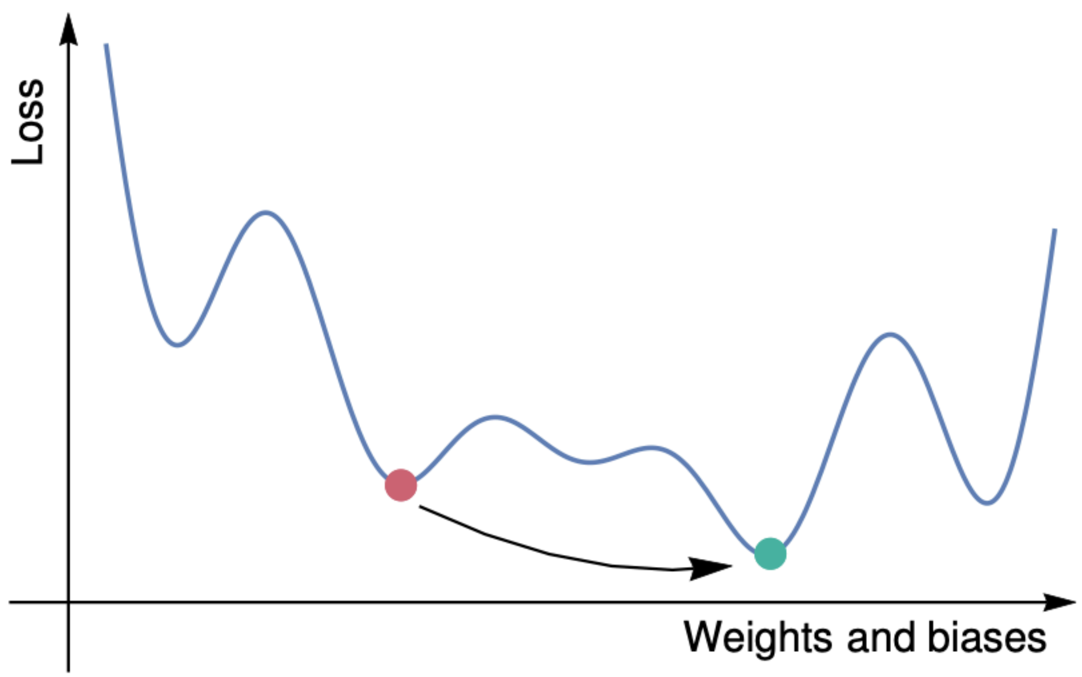
[Abel, Criado, MS '22]

- Developed binary encoding of weights (discretised)
- Polynomial approximation of activation function
- Reduction of binary higher-order polynomials into quadratic ones (Ising model)

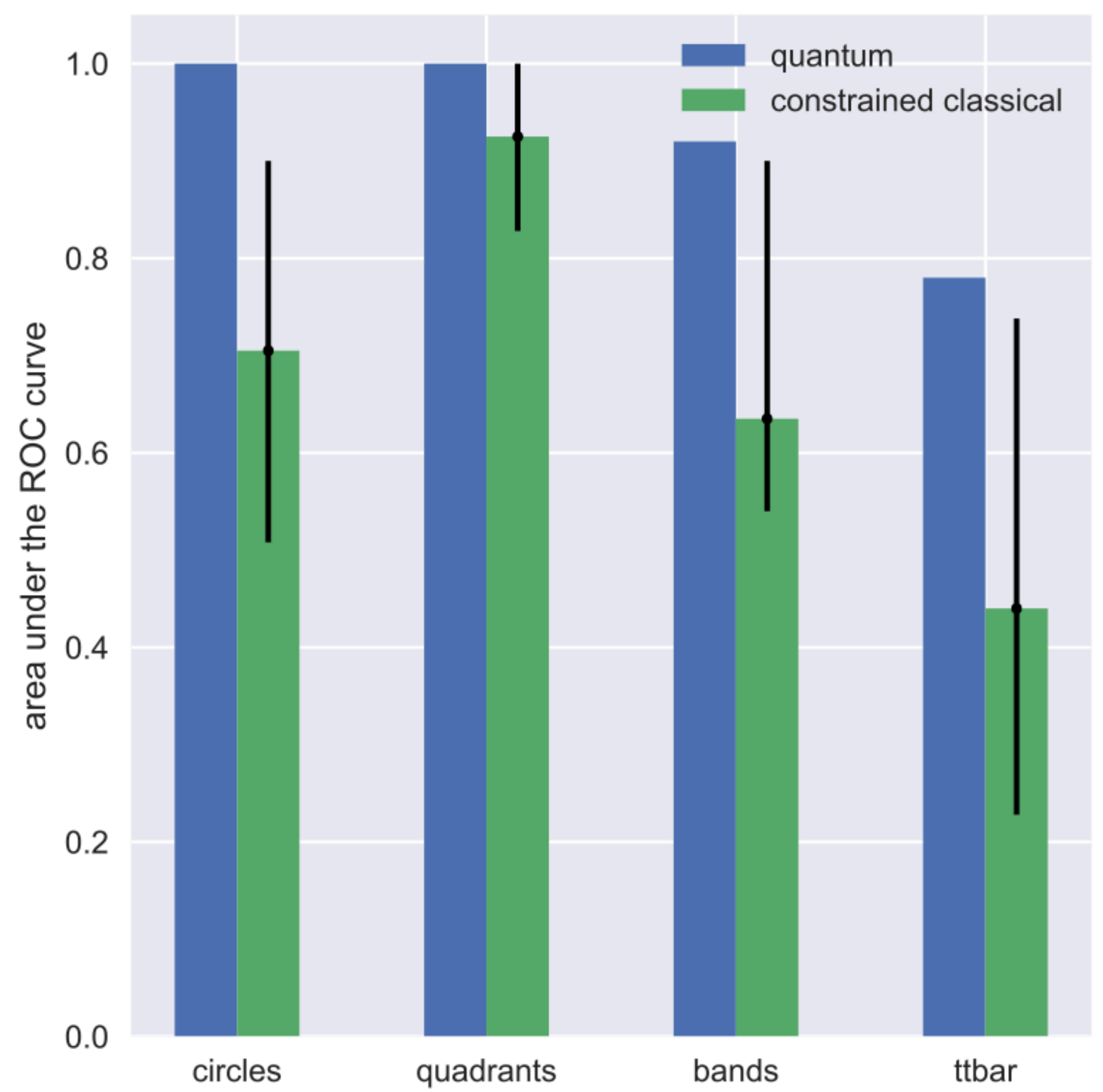



background
signal
NN
predicted
decision
boundary
$t\bar{t}$ example

Completely Quantum Neural Networks



Reliable and very fast ground-state finder of loss function



Optimal network training

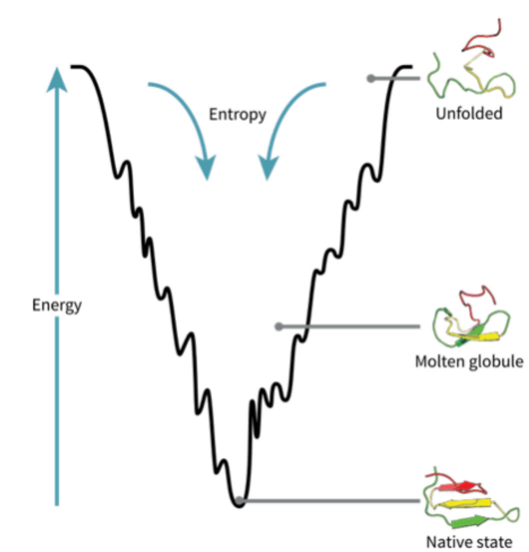
Application to differential equations and variational methods

Define your mathematical task as an **optimisation problem**

$$\mathcal{F}_m(\vec{x}, \phi_m(\vec{x}), \nabla\phi_m(\vec{x}), \cdots, \nabla^j\phi_m(\vec{x})) = 0$$

Build the full function, here a DE into the loss function, incl boundary conditions

$$\mathcal{L}(\{w, \vec{b}\}) = \frac{1}{i_{\max}} \sum_{i,m} \hat{\mathcal{F}}_m(\vec{x}^i, \hat{\phi}_m(\vec{x}^i), \cdots, \nabla^j\hat{\phi}_m(\vec{x}^i))^2 + \sum_{\mathrm{B.C.}} (\nabla^p\hat{\phi}_m(\vec{x}_b) - K(\vec{x}_b))^2 \ ,$$



[Piscopo, MS, Waite ’19]

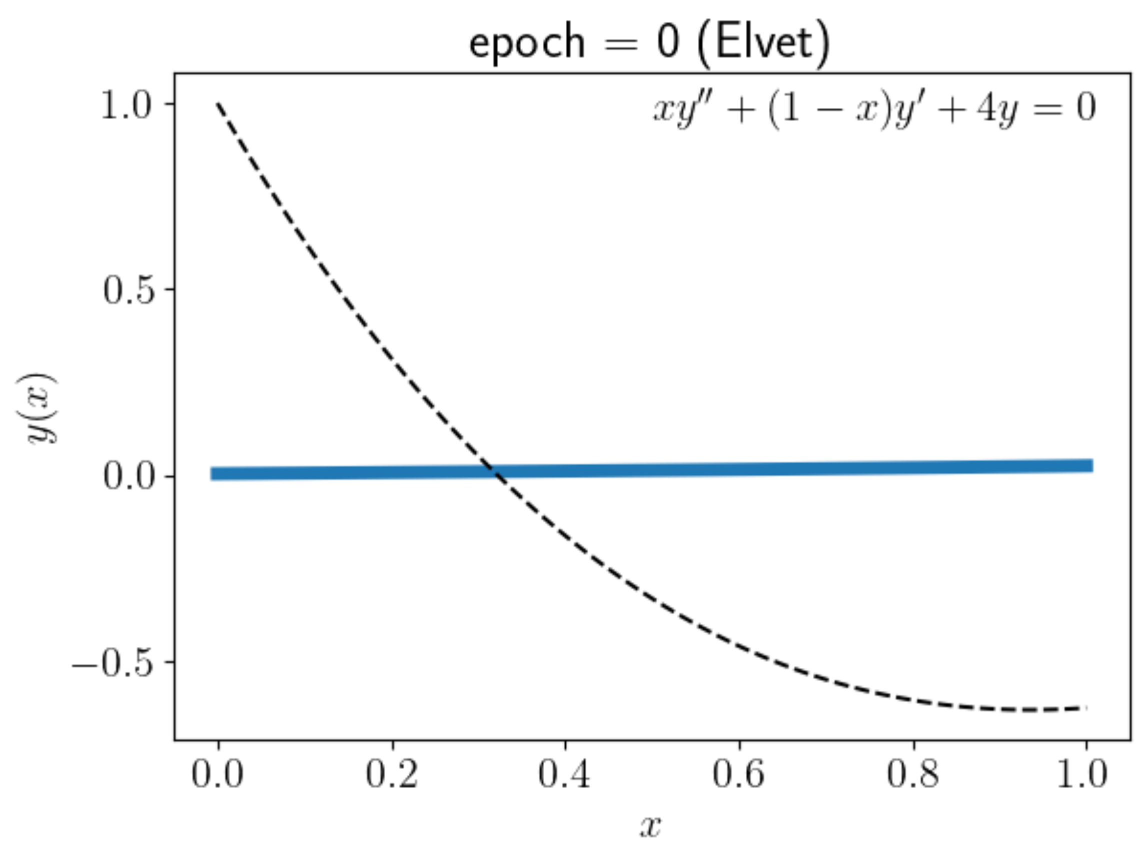
identify trial solution with network output $\hat{\phi}_m(\vec{x}) \equiv \check{N}_m(\vec{x}, \{w, \vec{b}\})$

QADE: Solving differential equations with a quantum annealer

[Criado, MS '22]

Example Laguerre differential equation:

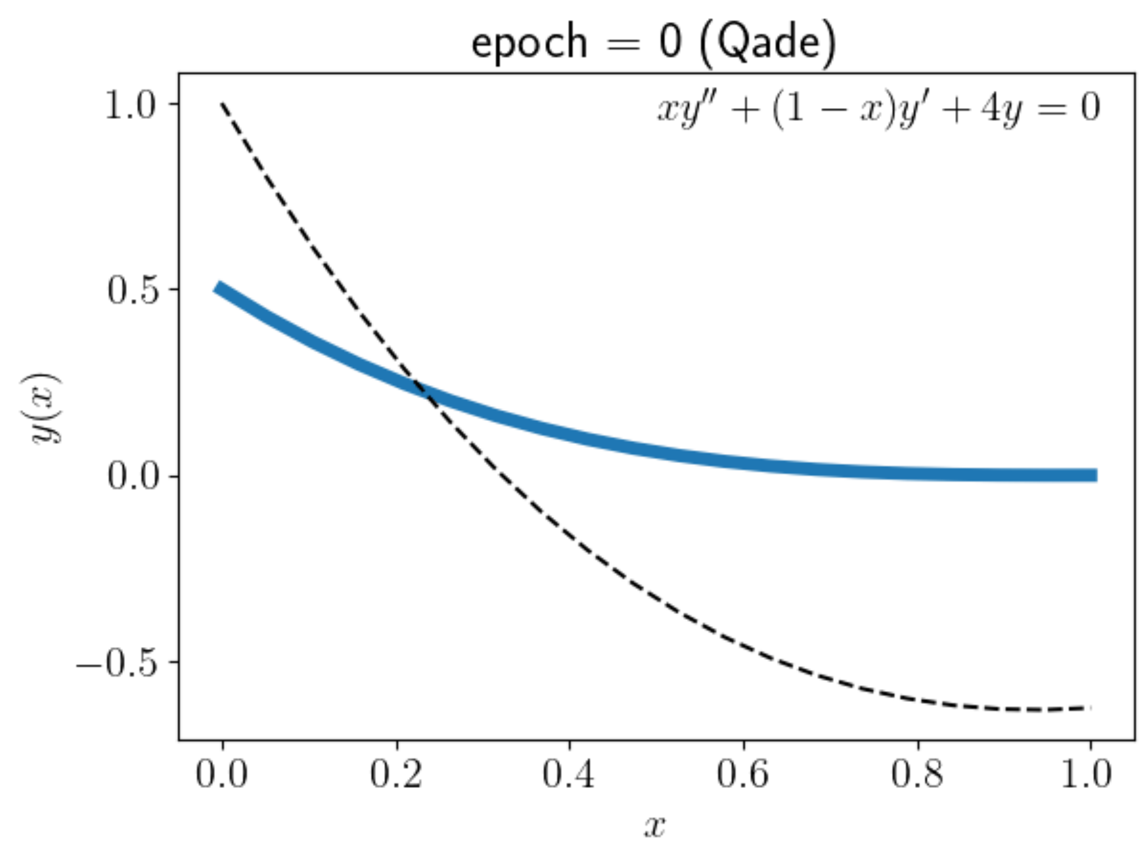
$$xy'' + (1-x)y' + 4y = 0 \text{ with } y(0) = 1 \text{ and } y(1) = L_4(1)$$



Classical Neural Network

[Piscopo, MS, Waite '19] [Araz, Criado, MS '21]

https://gitlab.com/elvet/elvet



Quantum algorithm

http://gitlab.com/jccriado/qade

QFitter

Example Higgs EFT fit: [Criado, Kogler, MS '22]

$$\mathcal{L} = \frac{c_{u3} y_t}{v^2}(\phi^\dagger\phi)(\bar{q}_L\tilde{\phi}u_R) + \frac{c_{d3} y_b}{v^2}(\phi^\dagger\phi)(\bar{q}_L\phi d_R)$$
$$+ \frac{i c_W g}{2m_W^2}(\phi^\dagger\sigma^a D^\mu\phi)D^\nu W^a_{\mu\nu} + \frac{c_H}{4v^2}\left(\partial_\mu(\phi^\dagger\phi)\right)^2$$
$$+ \frac{c_\gamma (g')^2}{2m_W^2}(\phi^\dagger\phi)B_{\mu\nu}B^{\mu\nu} + \frac{c_g g_S^2}{2m_W^2}(\phi^\dagger\phi)G^a_{\mu\nu}G^{a\mu\nu}$$
$$+ \frac{i c_{HW} g}{4m_W^2}(\phi^\dagger\sigma^a D^\mu\phi)D^\nu W^a_{\mu\nu}$$
$$+ \frac{i c_{HB} g'}{4m_W^2}(\phi^\dagger D^\mu\phi)D^\nu B_{\mu\nu} + \text{h.c.}$$

$$\chi^2 = \sum_{ij} V_a C^{-1}_{ab} V_b \qquad V_a = O_a^{(\text{exp})} - O_a^{(\text{th})}(c)$$

- Fast and reliable state-of-the-art Higgs, ELW, … fits
- Convergence no problem for non-convex $\Delta\chi^2 = \chi^2 - \chi^2_{\text{min}}$ functions

Formulation	Method	Fit time	c_{HW}	c_H	c_g	c_γ	χ^2
Standard	Minuit (initial $c_{HW} = 0$)	2.0 s	-0.009	0.100	1.4×10^{-5}	3.2×10^{-6}	4110
	Minuit (initial $c_{HW} = -0.05$)	2.4 s	-0.050	0.039	-9.7×10^{-6}	-1.0×10^{-4}	135
	Simulated annealing (initial $c_{HW} = 0$)	642 s	-0.009	0.100	1.4×10^{-5}	3.7×10^{-6}	4110
	Simulated annealing (initial $c_{HW} = -0.05$)	644 s	-0.009	0.100	1.4×10^{-5}	3.7×10^{-6}	4110
QUBO	Simulated annealing (Class A)	6.4 s	-0.012	-0.054	-3.0×10^{-5}	3.9×10^{-5}	3910
	Simulated annealing (Class B)	6.4 s	-0.045	-0.175	-3.7×10^{-5}	1.8×10^{-4}	228
	Quantum annealing	0.2 s	-0.047	-0.050	1.9×10^{-5}	7.5×10^{-7}	68

Training NNs using Adiabatic QC

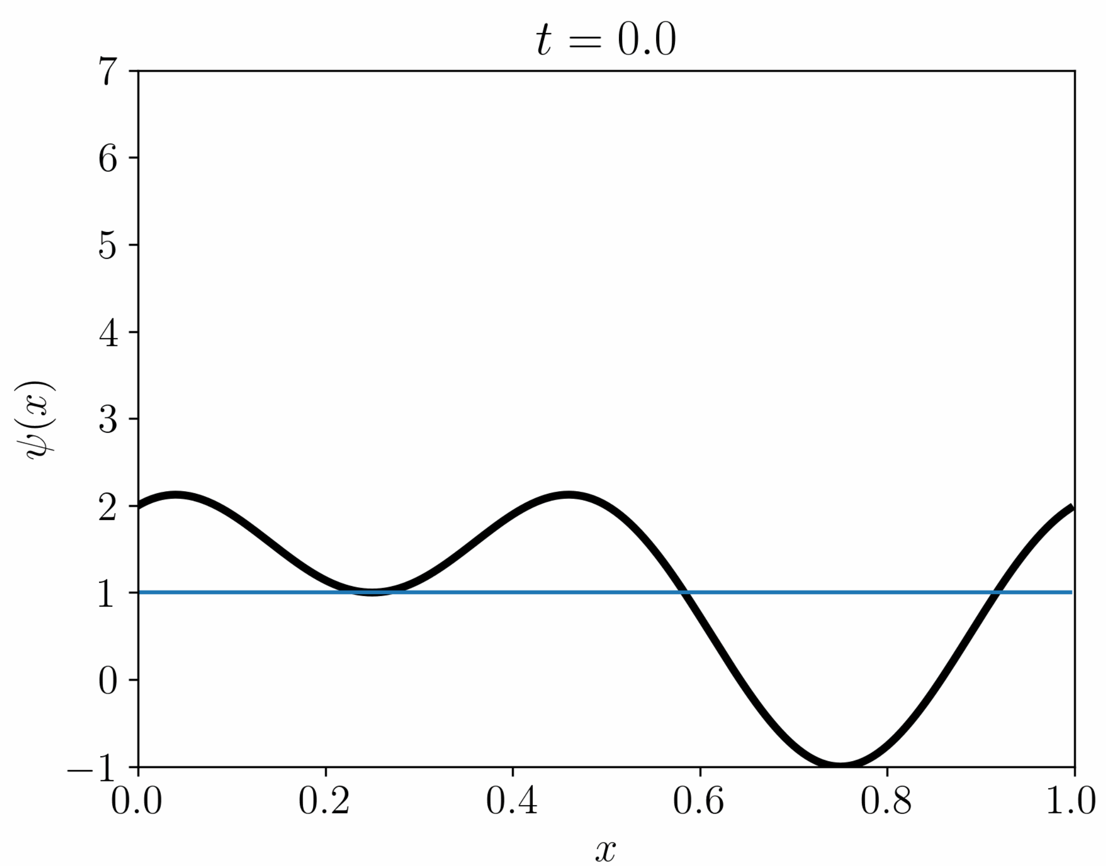
[Abel, Criado, MS '23]

- Applicable to digital quantum computers, i.e. quantum gate computers. Not limited to Ising model

O(1000) qubits for Ising model

O(10) qubits for AQC - prop. #weights

- # of gate operations in AQC scales polynomially with NN width and exp with depth
- Gradient-free optimisation -> particularly important for discrete/binary NN



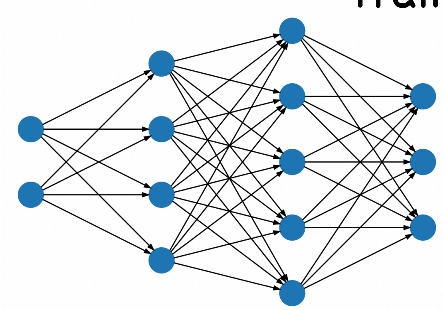
measure $\psi(x)^2$

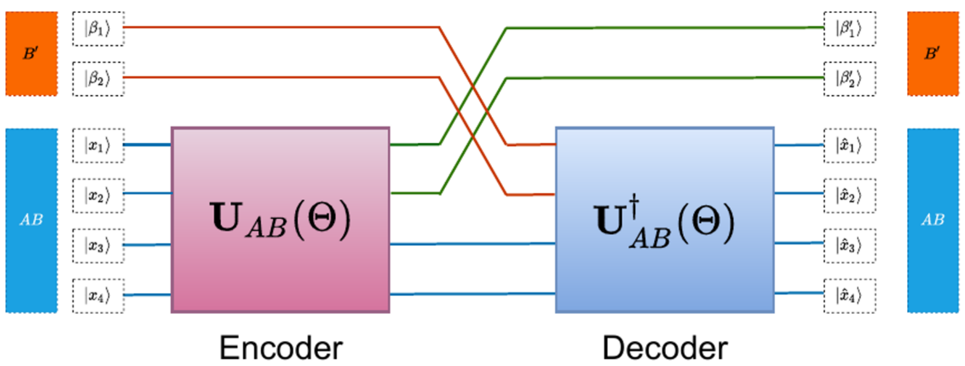
extract optimal weights x

$$H = (1-t)\,\frac{p^2}{2m^2} + t\;V(x)$$

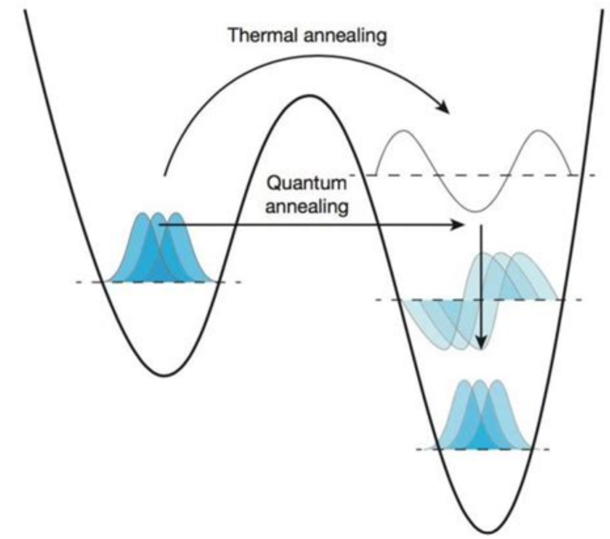
$$\text{Loss} = \frac{1}{N}\sum_i^N \phi(x,i) - \kappa_i \;^2$$

NN output with trainable weights x





Summary



- Quantum Computing is exciting research area that rapidly expands, supported through private and public sector. Many algorithms to be invented.

  ➡ Can exploit QM prop: entanglement, superposition principle and tunnelling

- HEP is inherently quantum mechanical, thus description in terms of quantum computing should be advantageous

  ➡ Suitable theory description needed for QC devices

  ➡ Path to an application yielding quantum advantage

- For quantum advantage in real-world applications need development of technical realisation of quantum computers (size, fault tolerance, type of operations,...)