THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES

Quantum Computing for High-Energy Physics and Data Analysis

Michael Spannowsky

IPPP, Durham University

How do classical computers work?

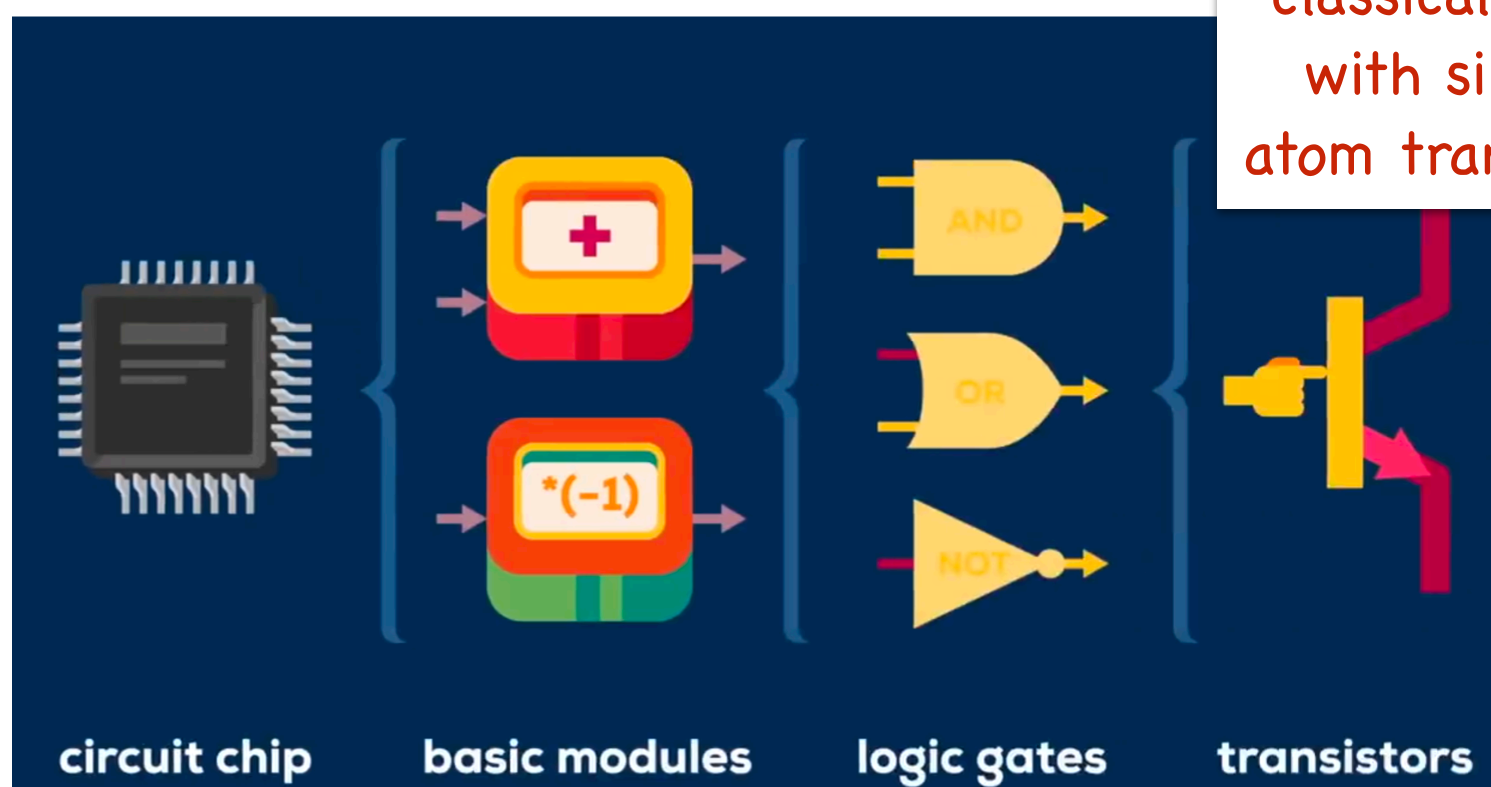
Classical computers are made from simple individual units

Reaching classical limit with single atom transistor

A transistor is the simplest form of data processing unit in computers

-> just a switch to block or open the path for information coming through

-> information 0 or 1



$2^2 = 2 \times 2 \longleftrightarrow$

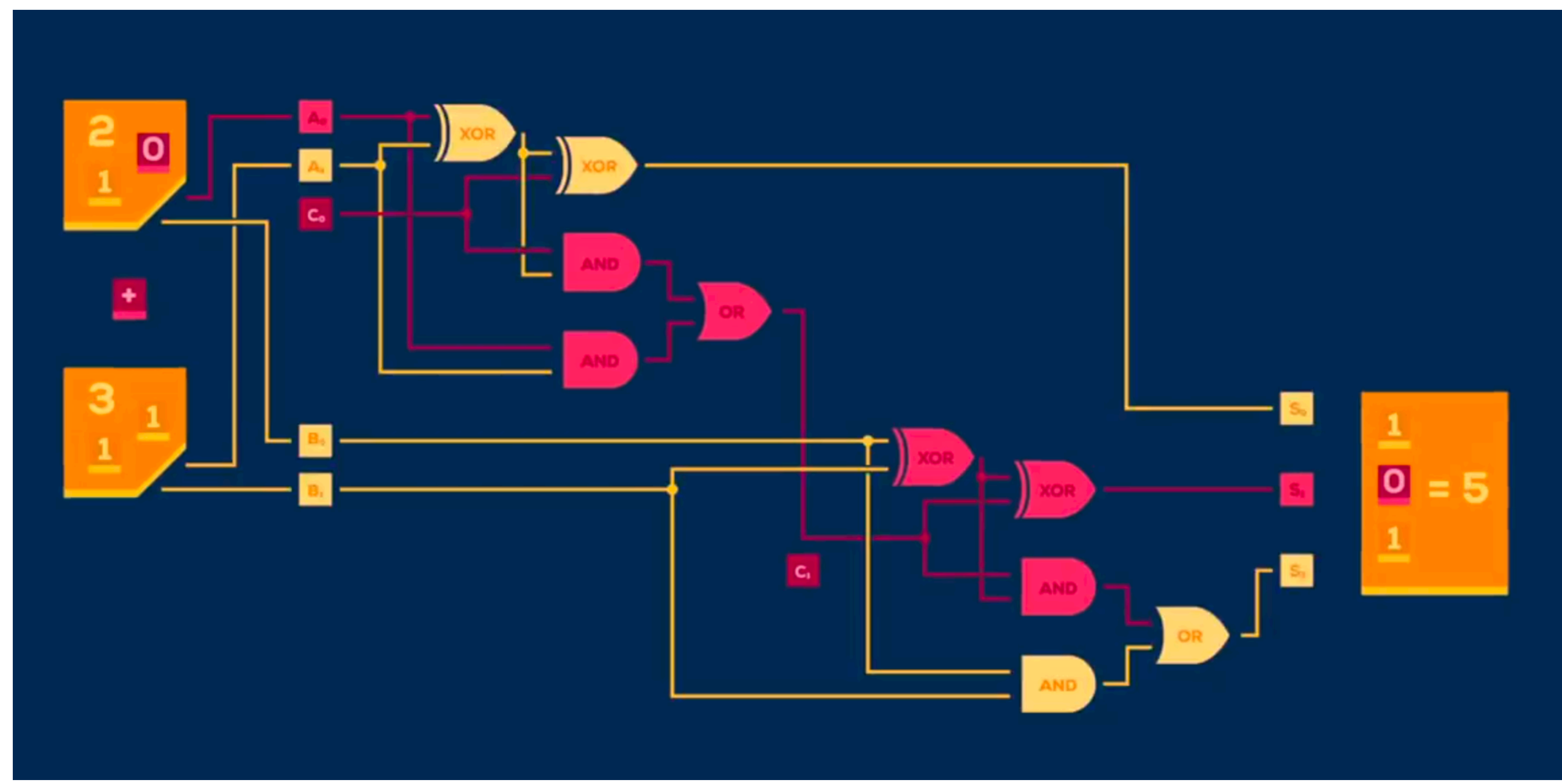
0	0
0	1
1	0
1	1

$2^7 = 2 \times 2 \times 2 \times 2 \times 2 \times 2 \times 2 = 128$

complexity of system grows exponentially with # bits

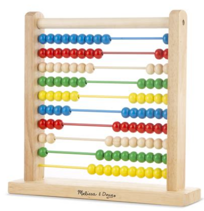
that way one can perform calculations, e.g. adding up two numbers that are encoded in binary code

once you can add, you can multiply etc



once you scale up, you can perform outstandingly difficult calculations, e.g simulate evolution of our Universe

Example for addition in binary code on the algorithmic level:



convert into different representation

define algebraic procedure on new representation

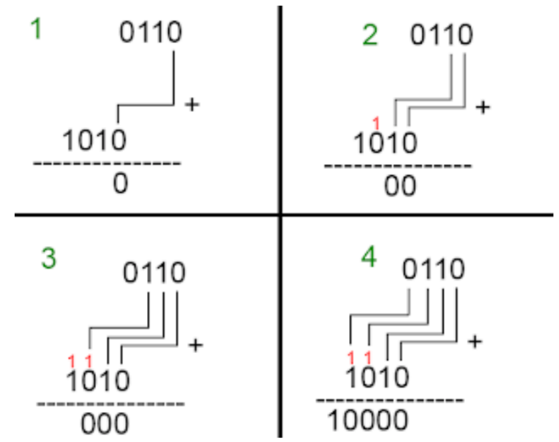
obtain result in new representation

convert back

6+10 → Binary

0110
+ 1010

→



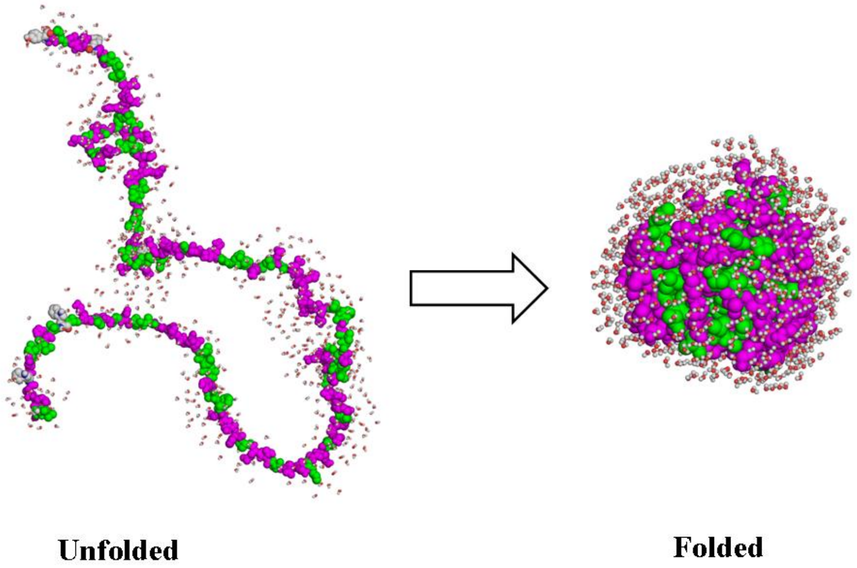
→ 10000 → 16

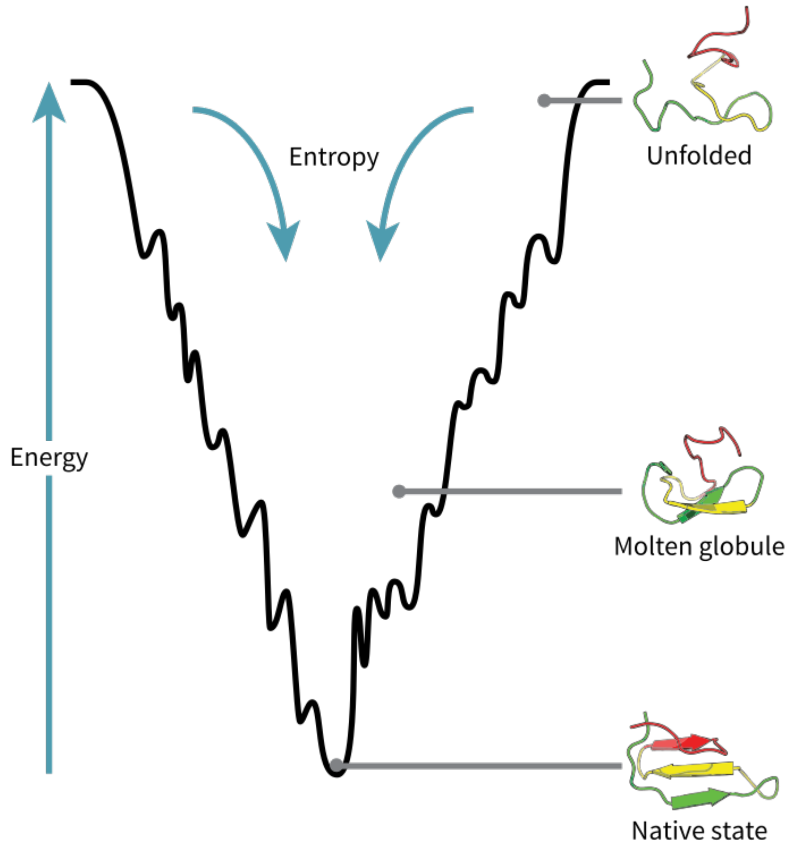
- Note, final solution manifold consists of 2^5 states

- However, convergence to ‘correct’ result very fast, as algorithm provides most direct path to solution state

- Puzzling: For this example, algebraic operation on original representation much simpler for human mind.

Protein-folding and Levinthal's Paradox





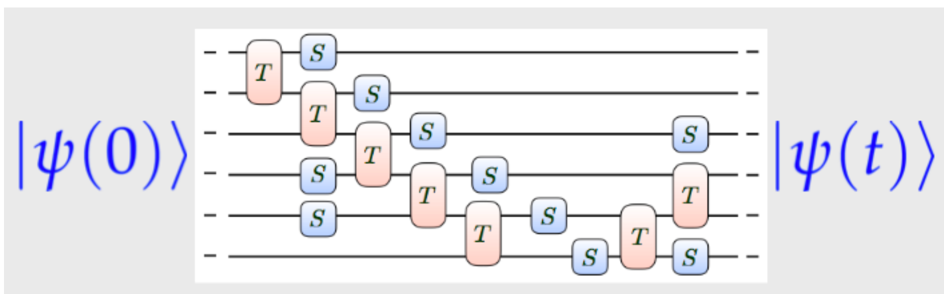
- Elongated proteins fold to same state within microseconds
- Some proteins have 3^{300} conformations
- <u>Levinthal's Paradox (1969)</u>:
  Sequential sampling of states would take longer than lifetime of Universe (even if only nanoseconds per state spent)
- Solution: No sequential sampling, but rapid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

→ Optimisation is Life

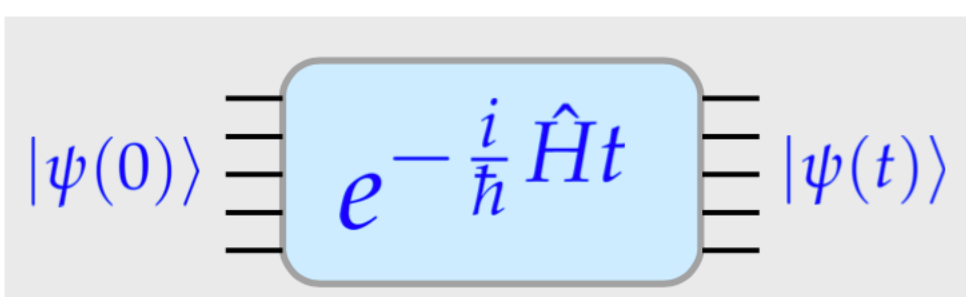
→ Solution of mathematical problem can be found quickly if encoded in ground state of complex system

Digital vs Analog simulations

- Digital: Express problem in digits and numbers. Level of abstraction, but results in universal computing



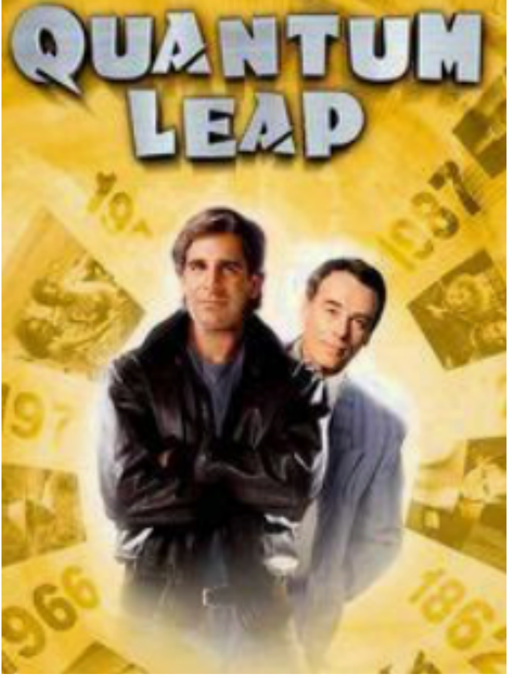
- Analog: Encode problem in the constituents of the system. Requires match between engineerable interactions and model



"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?

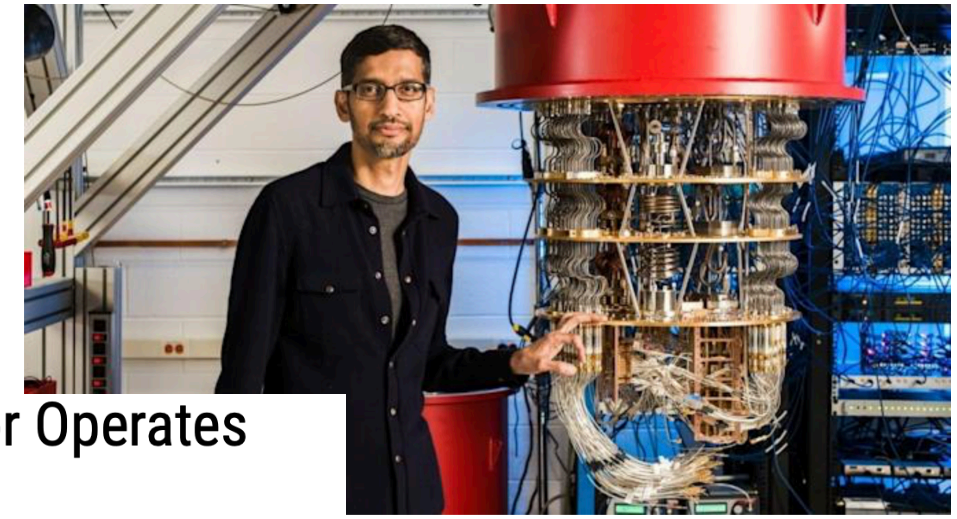
Beginning of a scientific journey that accelerated in recent years tremendously....



The Morning After: Google claims 'quantum supremacy'

And a controversial 'Ghost in the Shell' trailer.

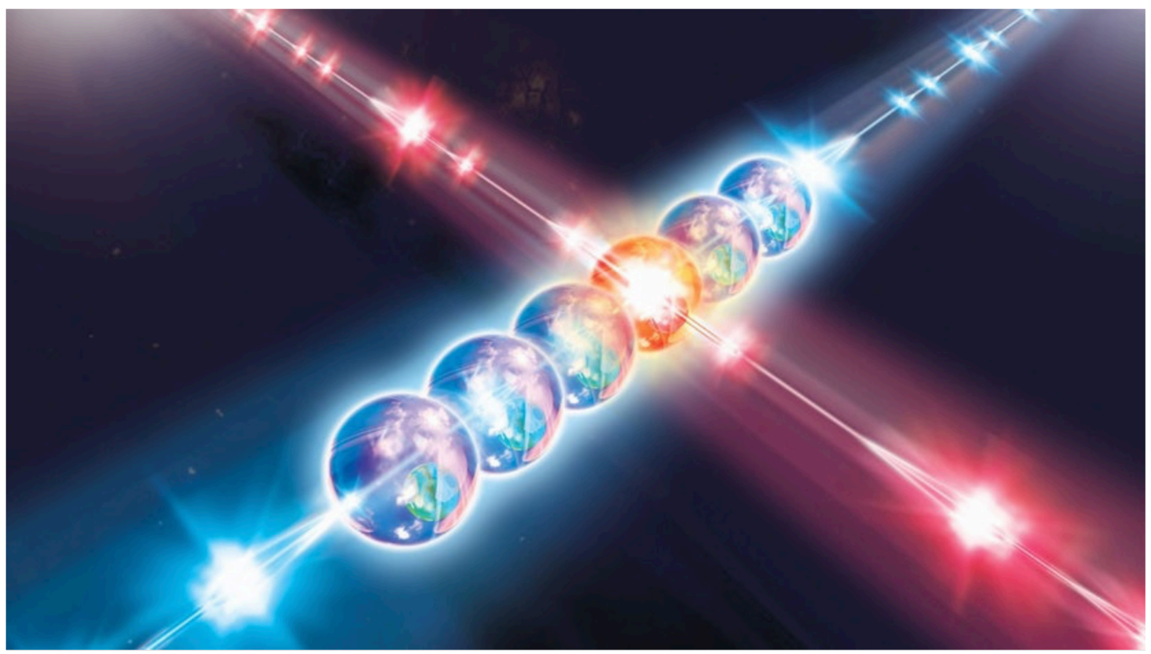
R. Lawler
@Rjcc
October 24th, 2019



First Quantum Computer Simulator Operates The Speed Of Light

Share

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



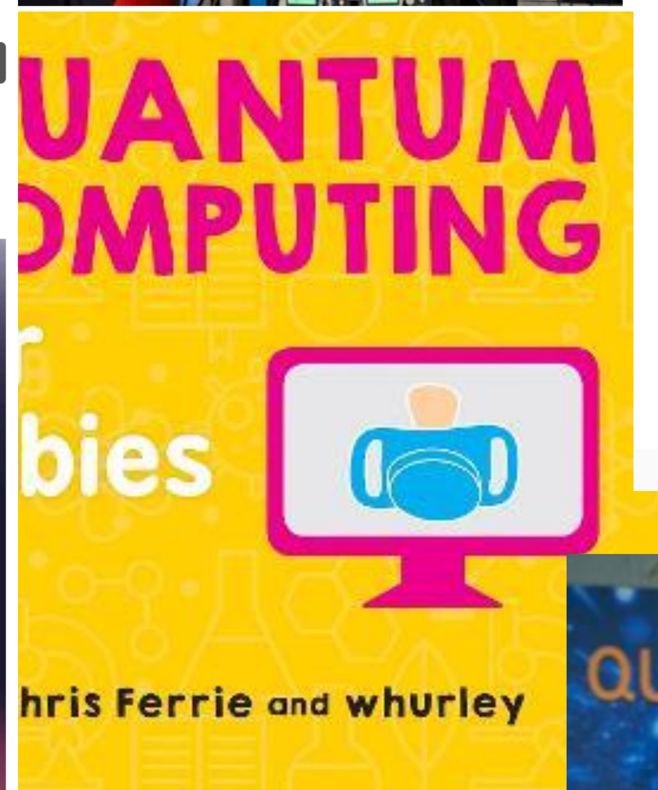
Master in Elektrotechnik, Informatik, Robotik, Maschinenwesen o. ä. (w/m/d)
German Aerospace Center (DLR) · Oberpfaffenhofen, Bavaria, Germany (On-site)
4 company alumni

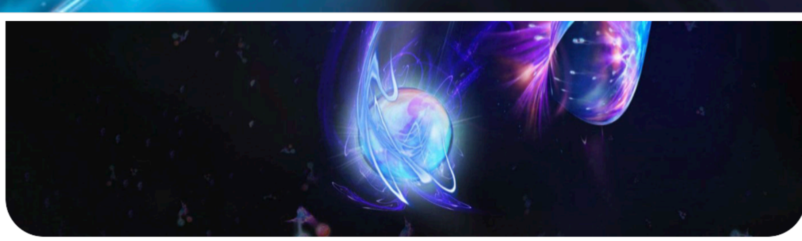
Professor Cyber Security im Online Fernstudium (m/w/d)
IU International University of Applied Sciences · Germany (Remote)
Actively recruiting

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



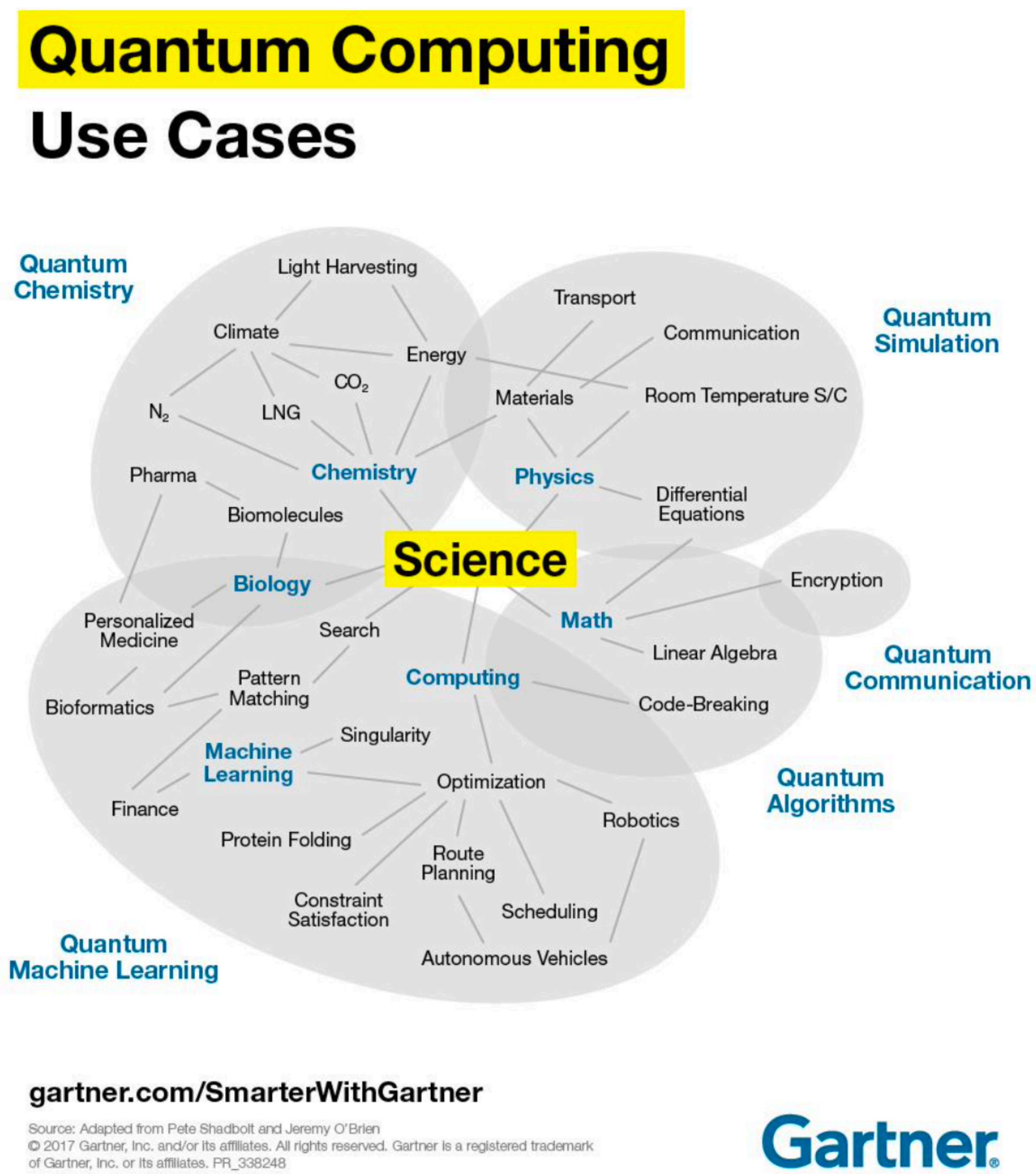


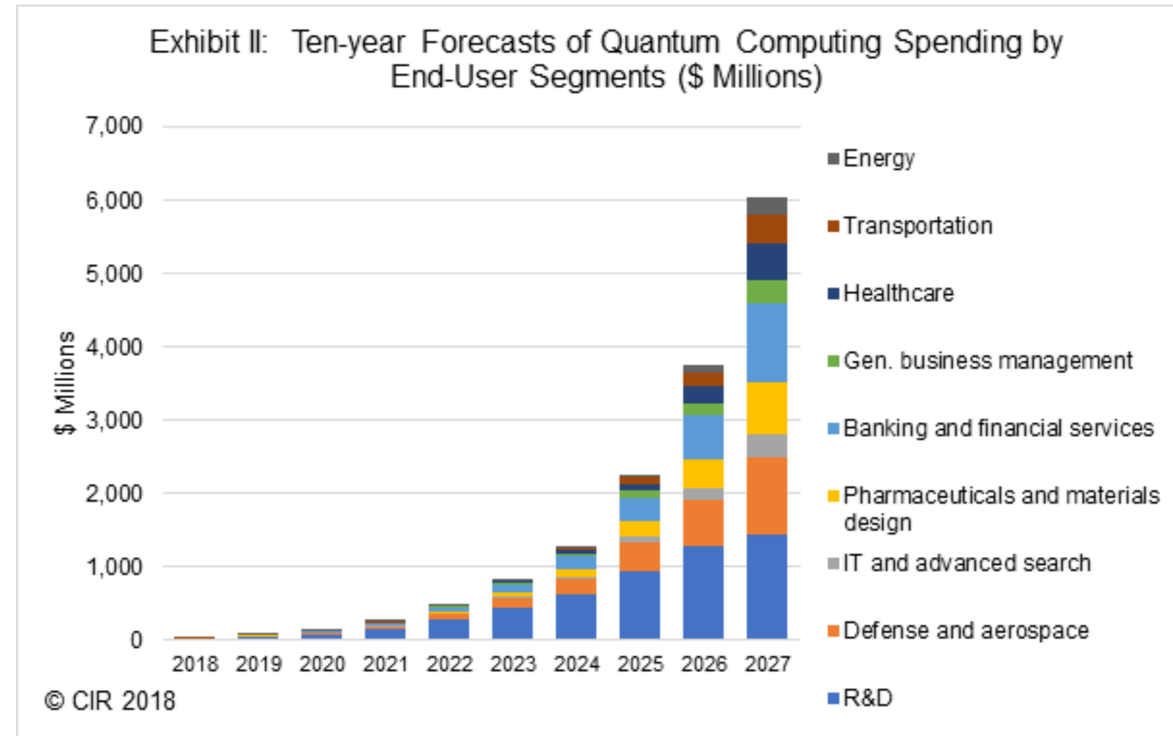
uantum Computers Will Be Incredibly Useful For

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





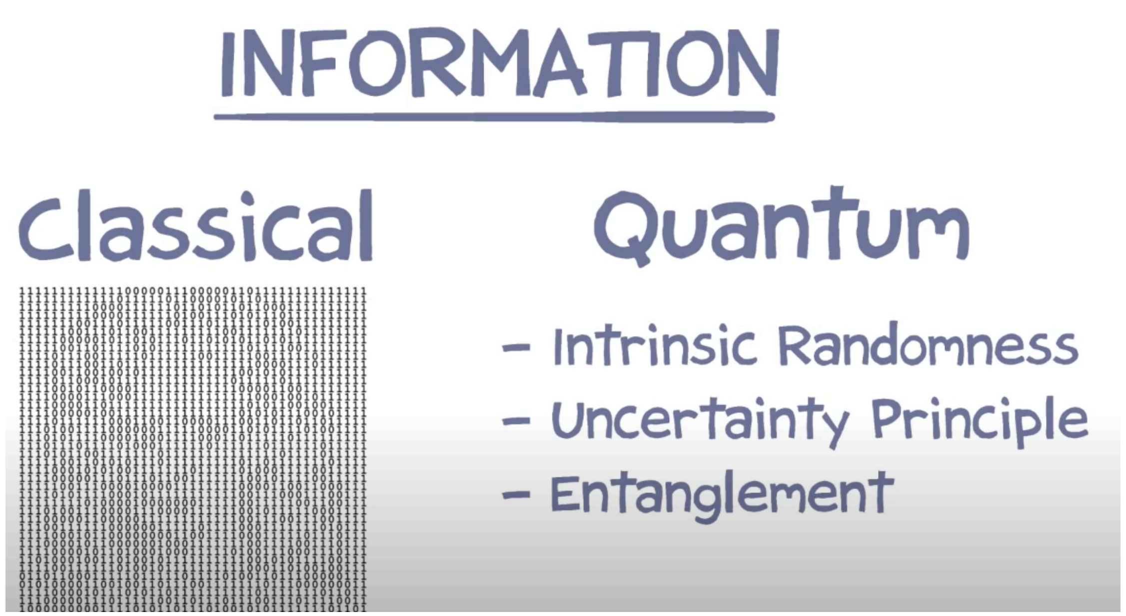
Significant financial investment expected across many sectors

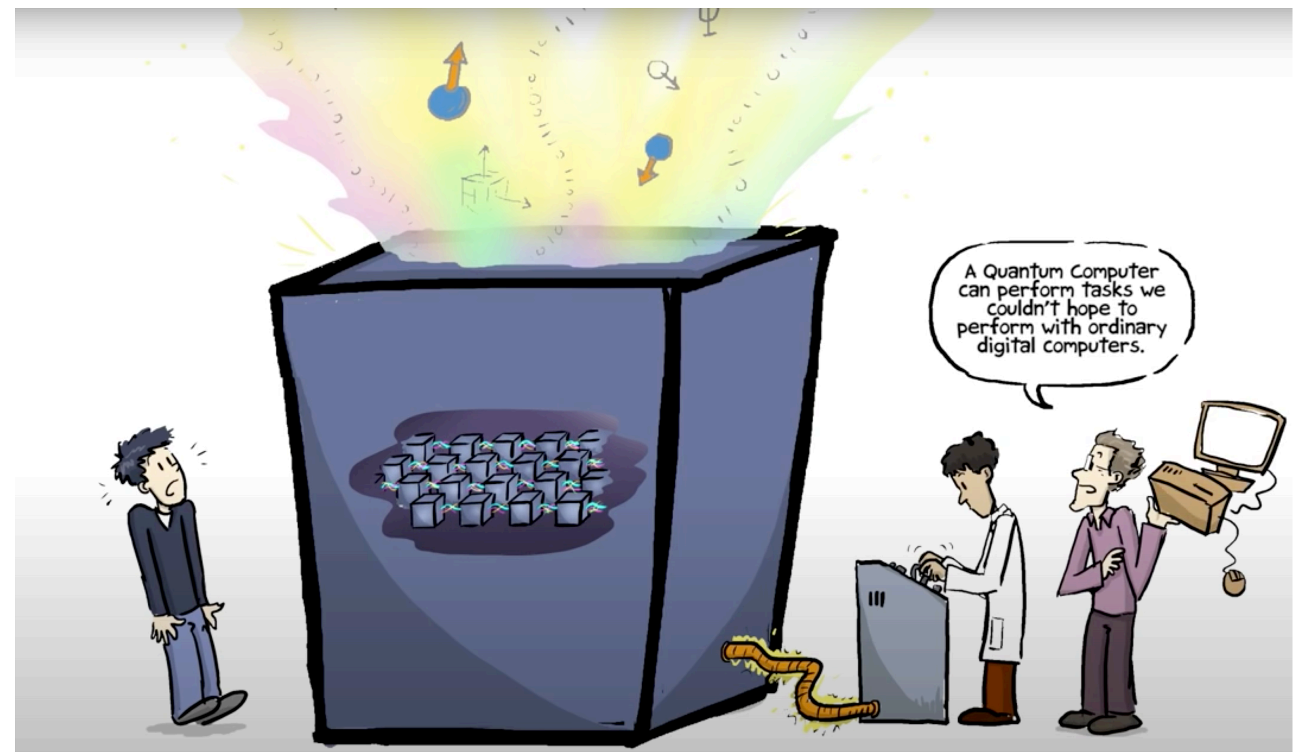
In US, already now higher financial investment from private than public sector

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

Basic motivation for Quantum Computing

"Can we take the quantum mechanical properties of microscopic objects and scale them up to larger quantum systems while harnessing their quantum prowess?"

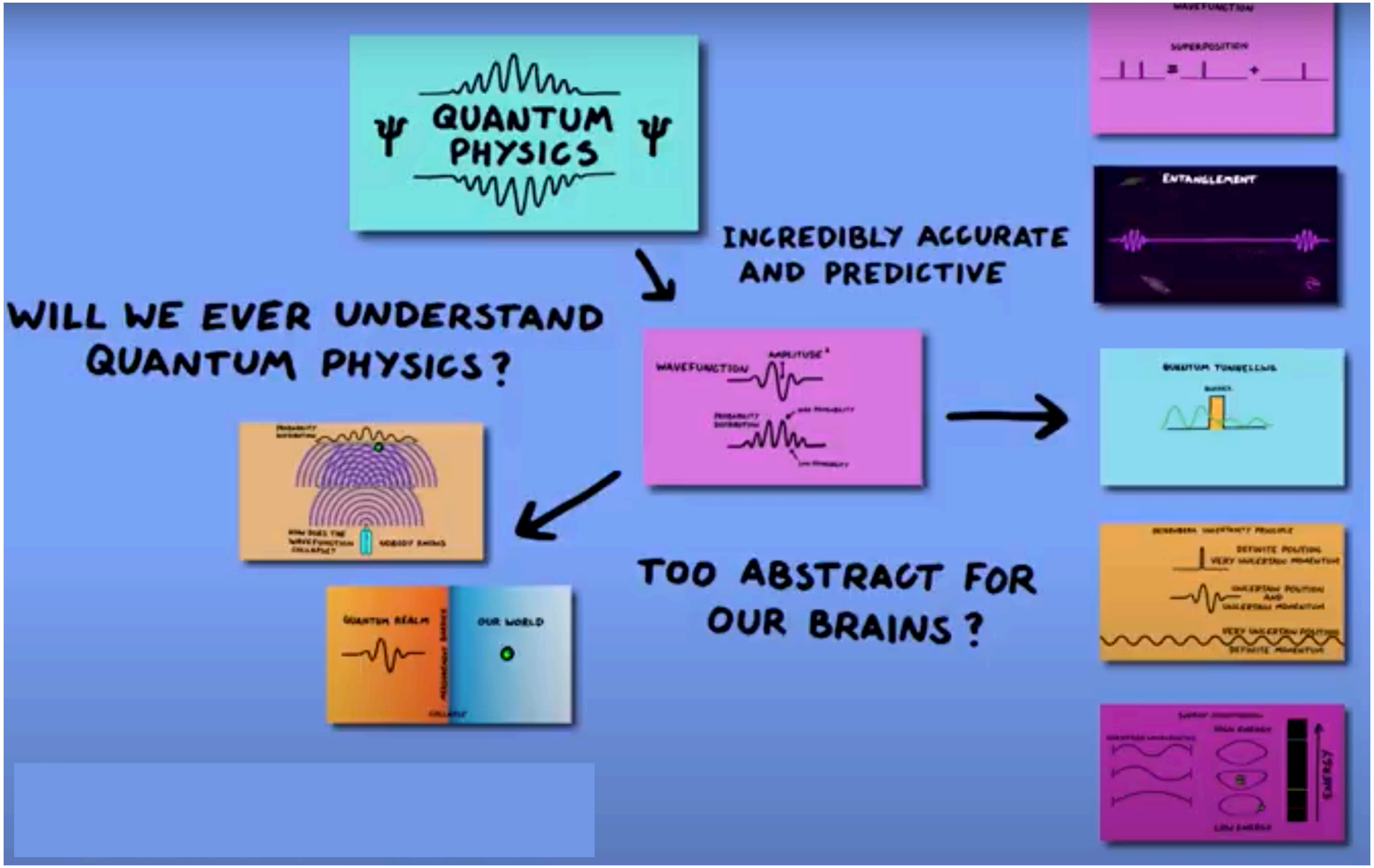




For some specialised task quantum supremacy has been shown

Disclaimer: nobody today thinks that quantum computers will universally replace classical computers

The quantum mechanical principles on which the algorithms have to rely to have a chance for a quantum advantage are



Superposition

Entanglement

Tunneling

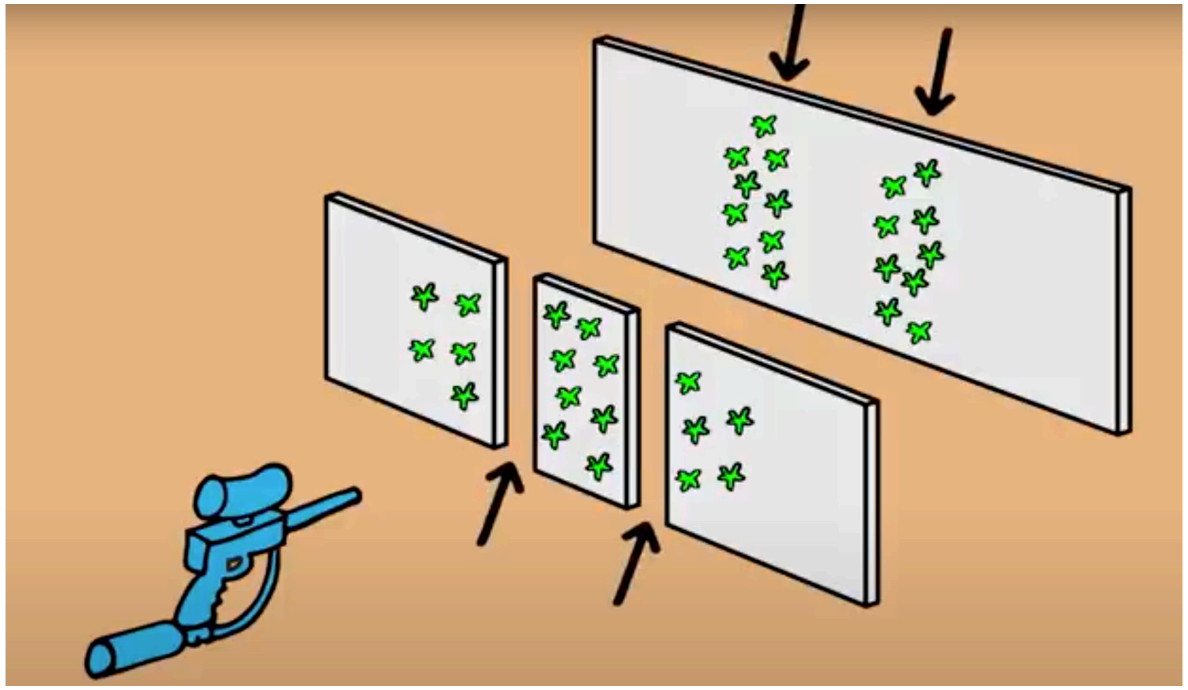
Heisenberg principle

Quantisation

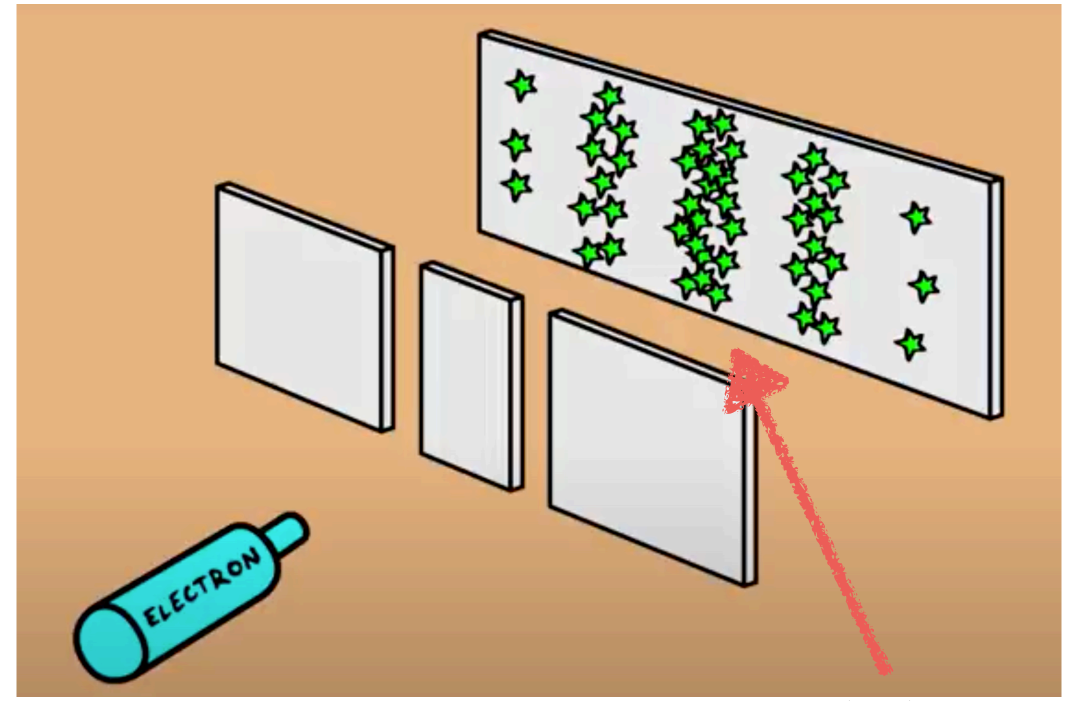
Configuration space sampling

→ Required to go beyond classical computing

Classical result double slit



double slit result for quantum object



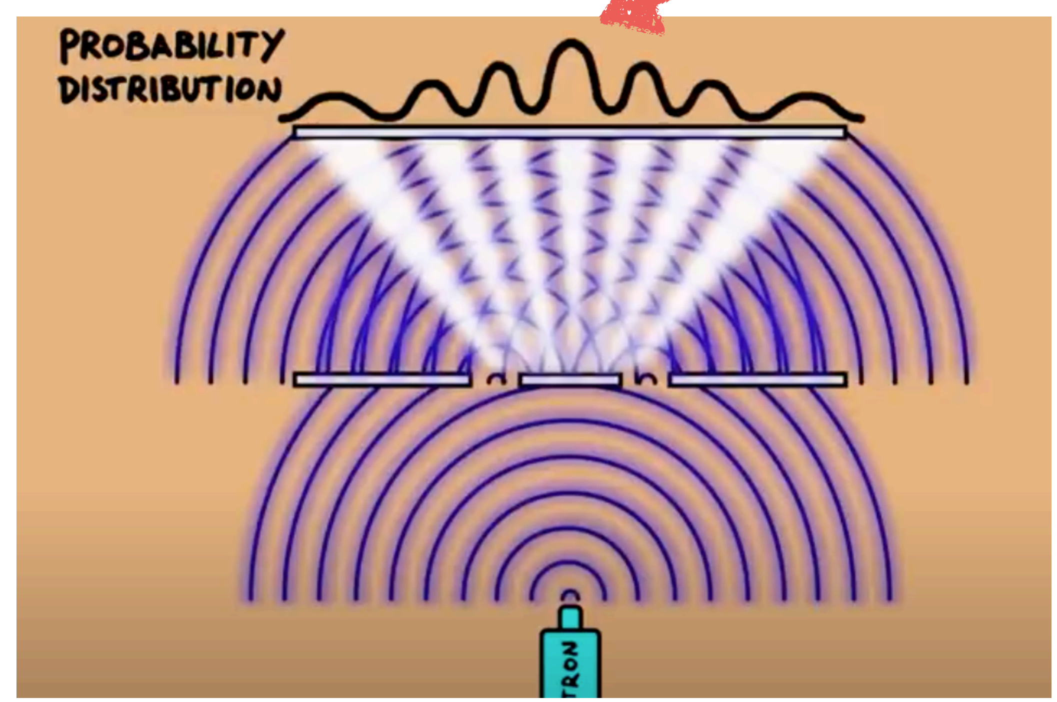
highest probability in the middle (behind shield)

- Shows that electrons (or any quantum mechanically described object) is described by a wave.

→ measurement collapses wave function, i.e. the electrons position is defined by one number x

$$\psi_{\text{total}} = \psi_1 + \psi_2$$

$$|\psi|^2_{\text{total}} = |\psi_1|^2 + |\psi_2|^2 + 2\text{Re}(\psi_1 \psi_2^*)$$

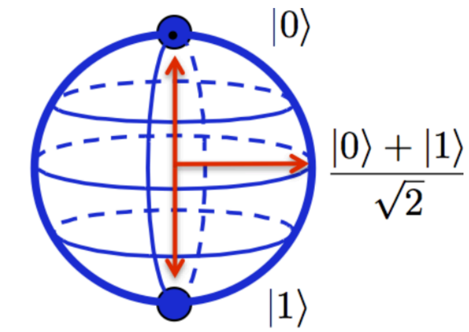


Interference pattern arises even if electrons are emitted one at a time

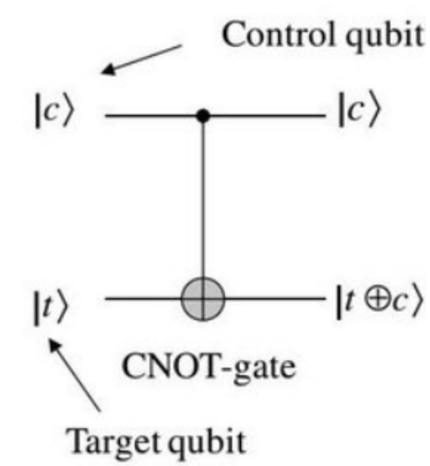
Thus, need transition form classical to quantum:

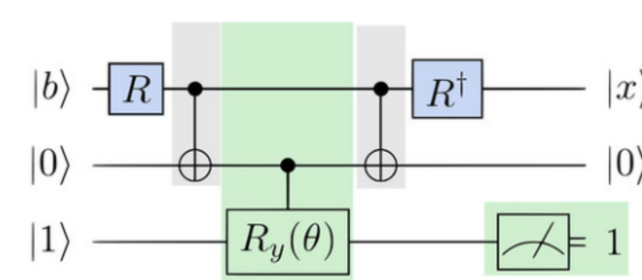
Classical Bit

Classical		Quantum
bits	⟷	qubits
gates	⟷	quantum gates
algorithms	⟷	quantum algorithms



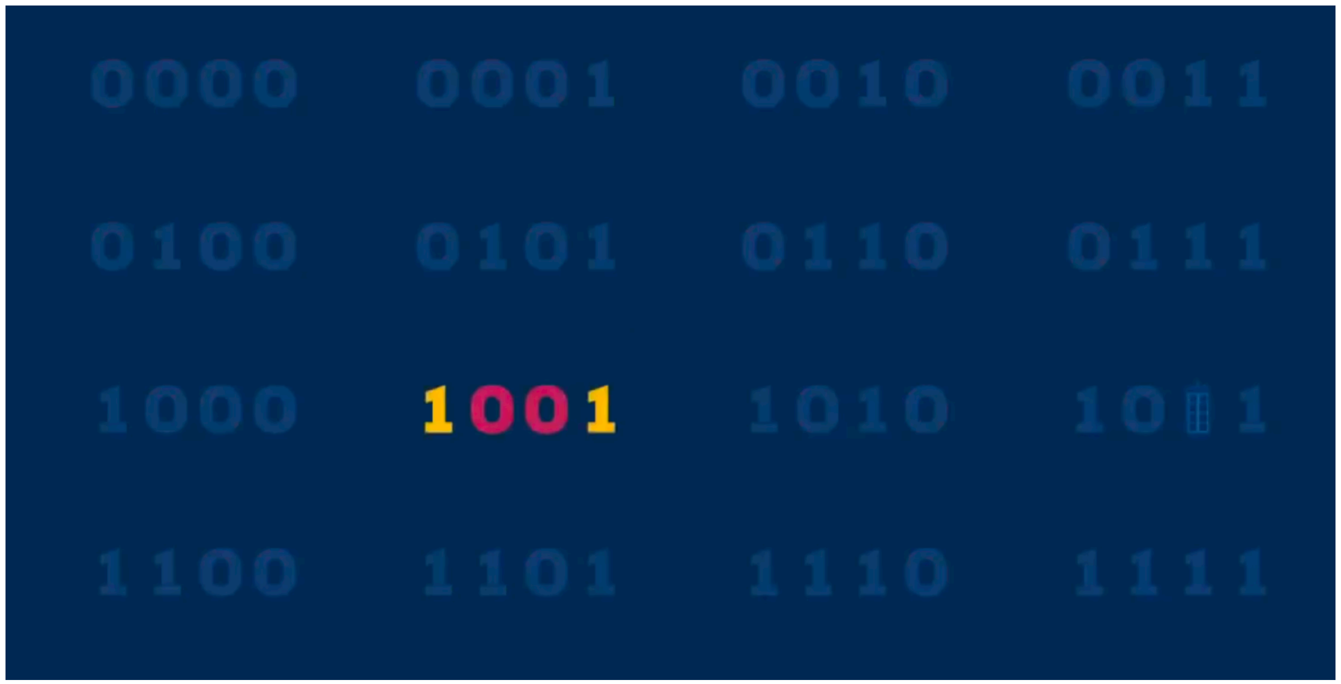
Qubit



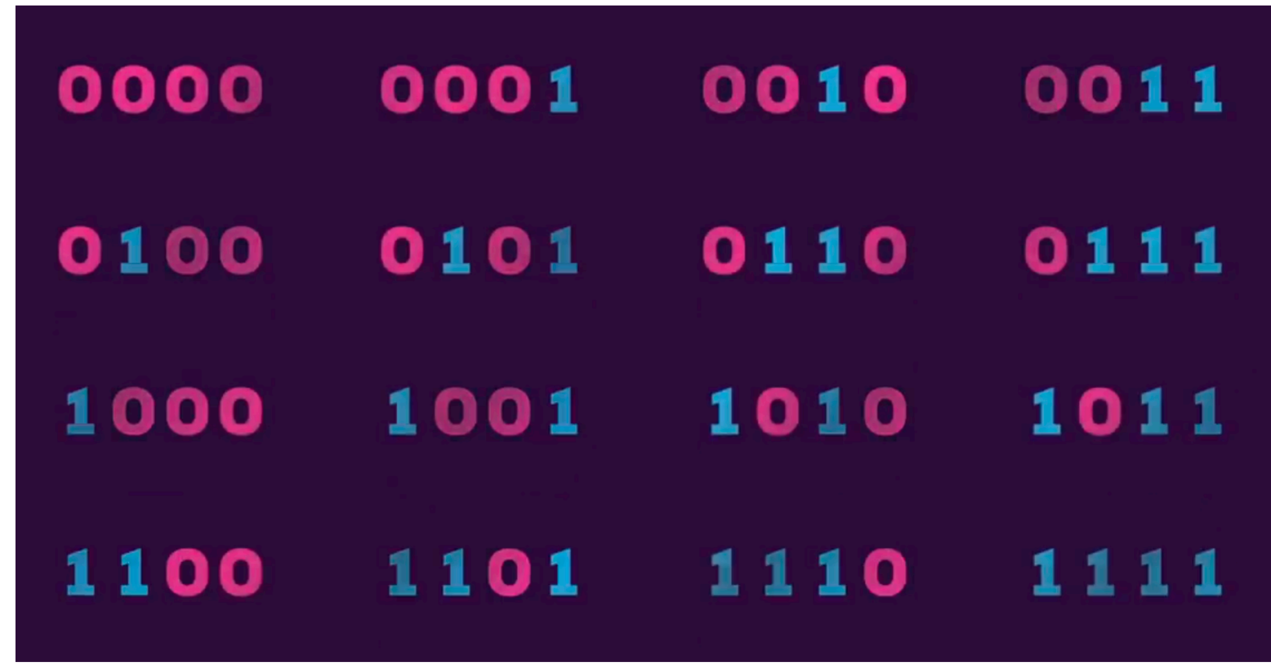


How can these quantum principles help to improve computations?

classical
system is in one state out of 16



quantum (superposition)
can be in all states at same time



- Configuration space here 16=2^4 states.
- Computations can be performed simultaneously on the whole configuration space. **-> can be much faster than classically**
- A measurement of the quantum system after the computations are performed results in the observation of one of these configurations, with a probability that corresponds to the computational processes

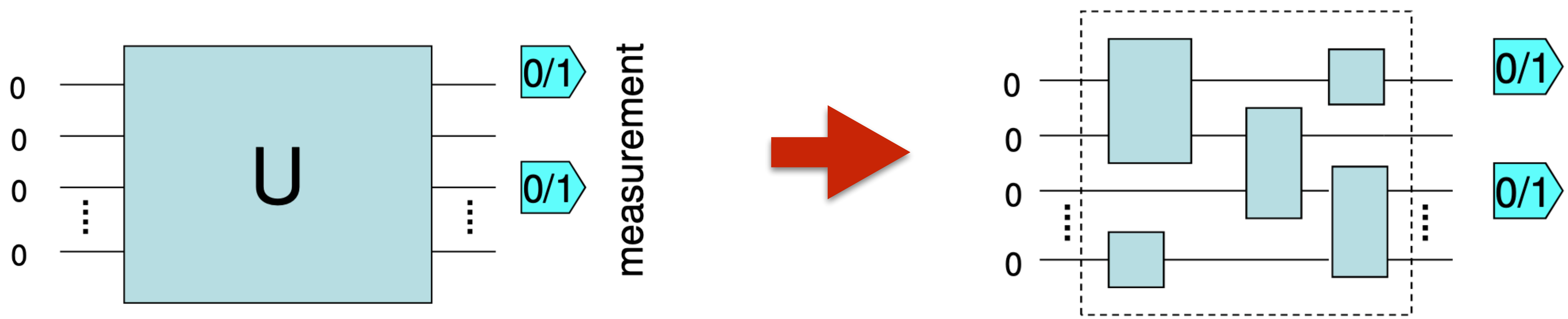
- General structure of any QC algorithm:

operator acts on Hilbert space states $U\|x\rangle = \|\Psi_1\rangle$	→	measurement of observable $\hat{U}$ corresponds to exp. value of operator U $\left\langle \hat{U} \right\rangle_\Psi = \frac{\langle\Psi\|U\|\Psi\rangle}{\langle\Psi\|\Psi\rangle}$

↓

Need to encode Hilbert space and operator suitable for quantum system	←	statistical statement need to evaluate often

↓



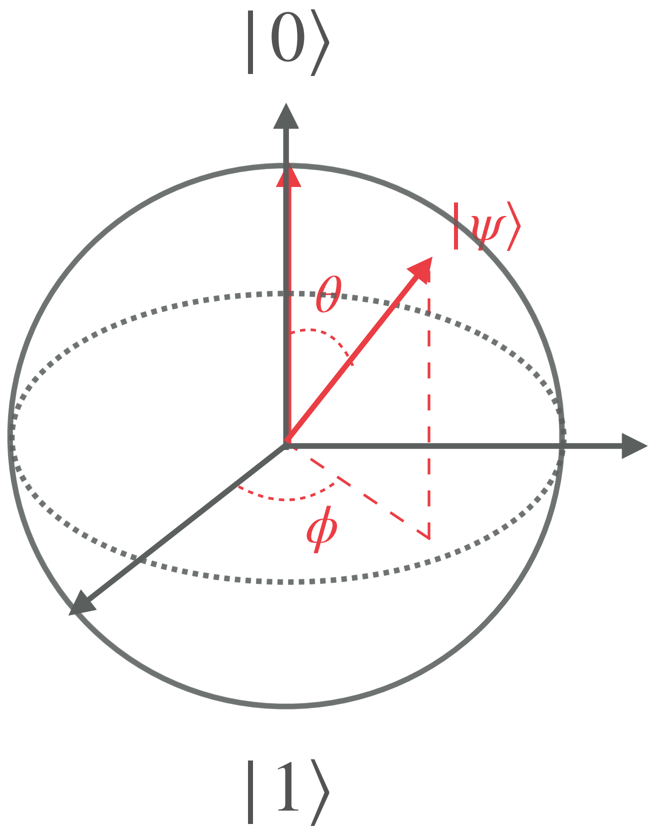
U

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

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

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

$|0\rangle$

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

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

$|1\rangle$

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

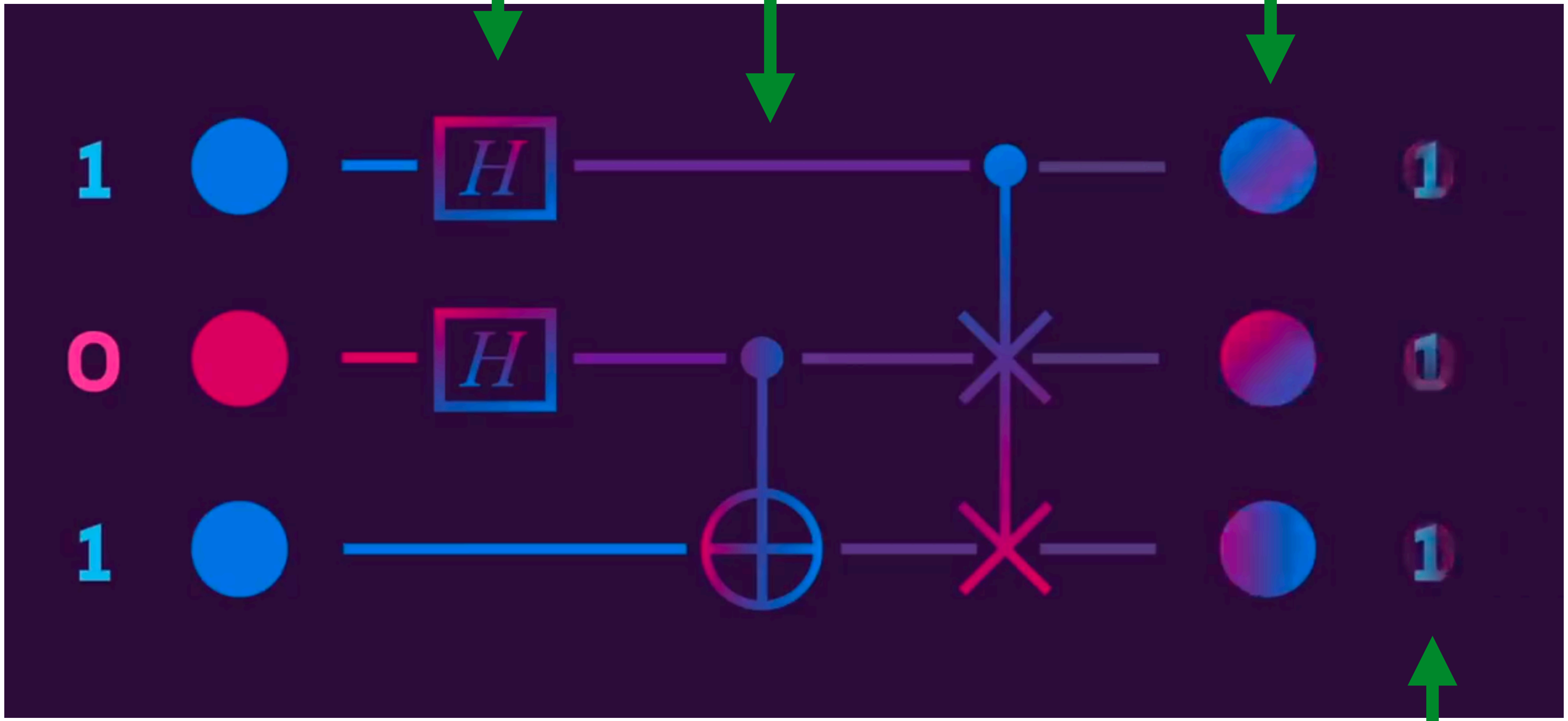
Extending this to a system of N qubits forms a 2^N-dimensional Hilbert Space

Quantum Gate

operations on qubits

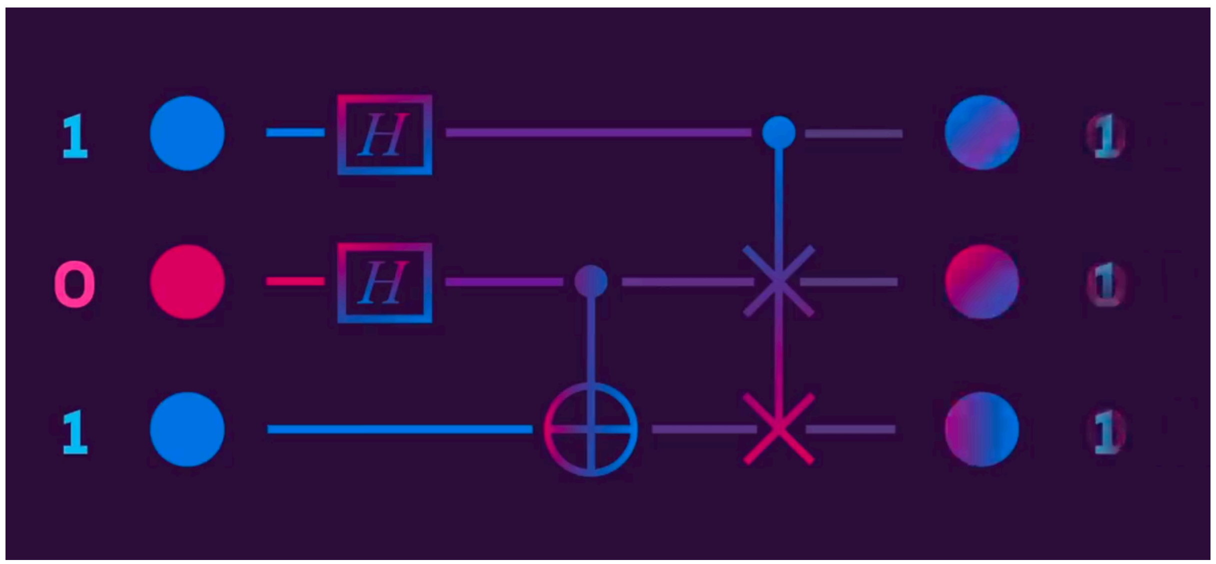
initialisation

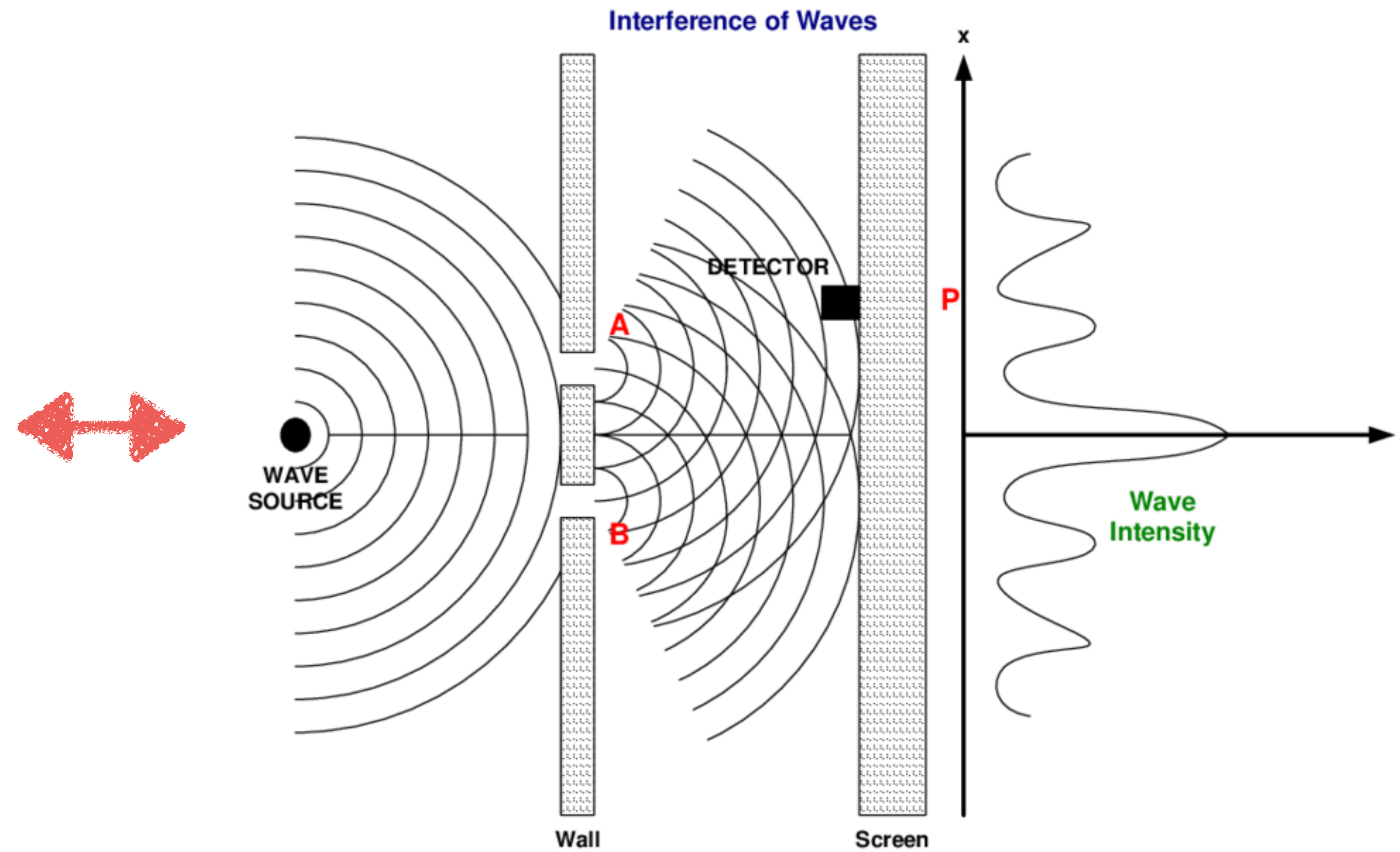
results in output of superpositions



We then measure one specific outcome. Have to repeat measurement to statistically evaluate how likely each outcome is (by calculating and measuring several times). Since we work only with probabilities, we measure only probabilities

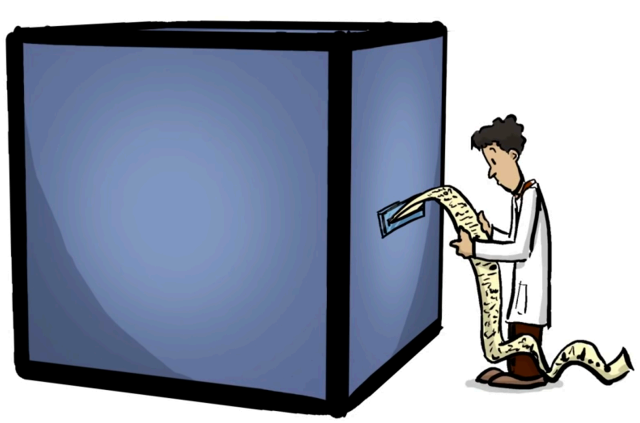
Quantum Gate





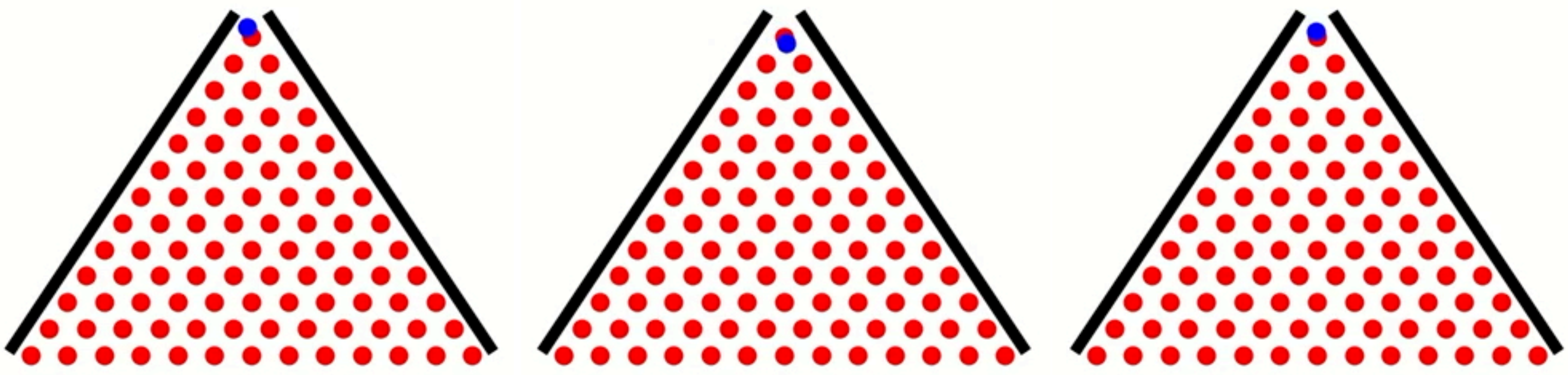
quantum gate and multi slit experiment are conceptually identical

It's a secret computation...



While operating one cannot see how the gate works. Only at the end one can measure the outcome
(box is closed during operations)

Galton Board as analogy for Quantum Computer

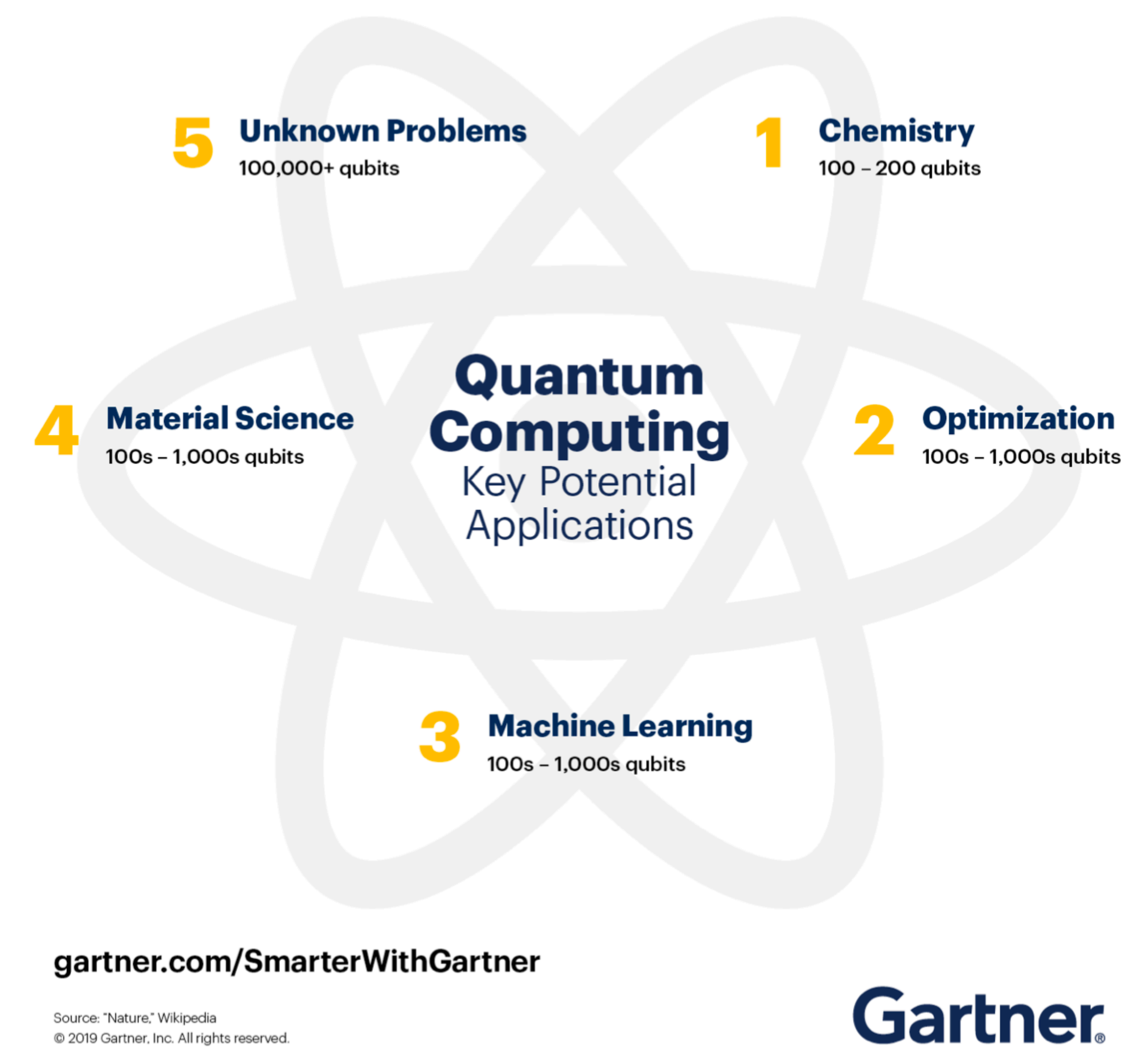


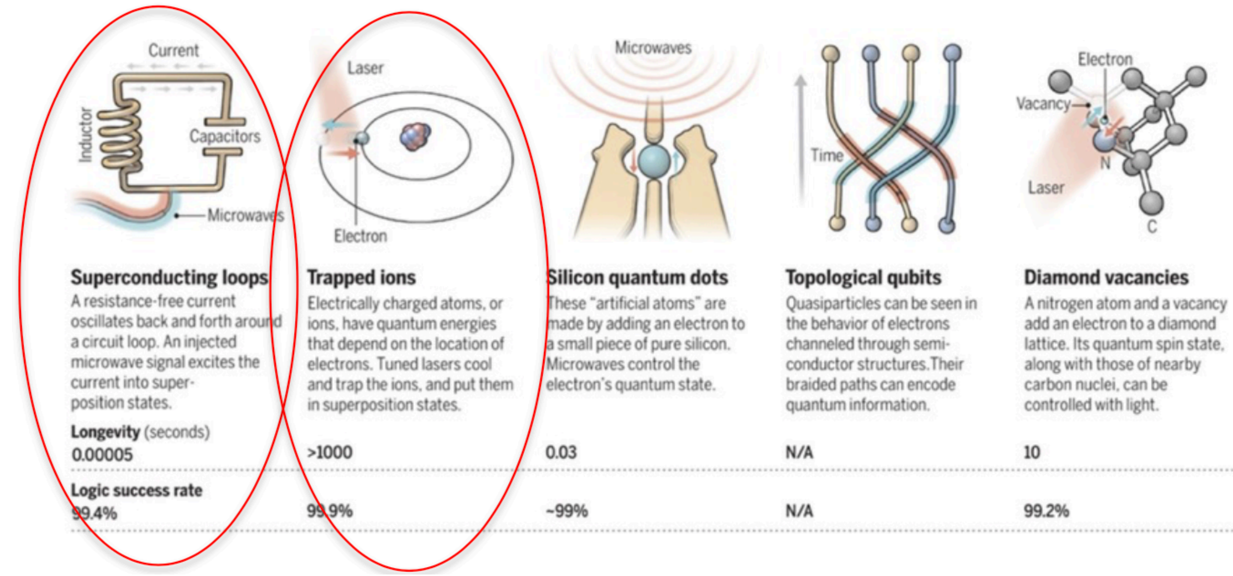
Technical challenges of a quantum computer

- Many quantum paradigms require system to be perfectly isolated (shielded from outside) to maintain coherence - for as long as the algorithm takes

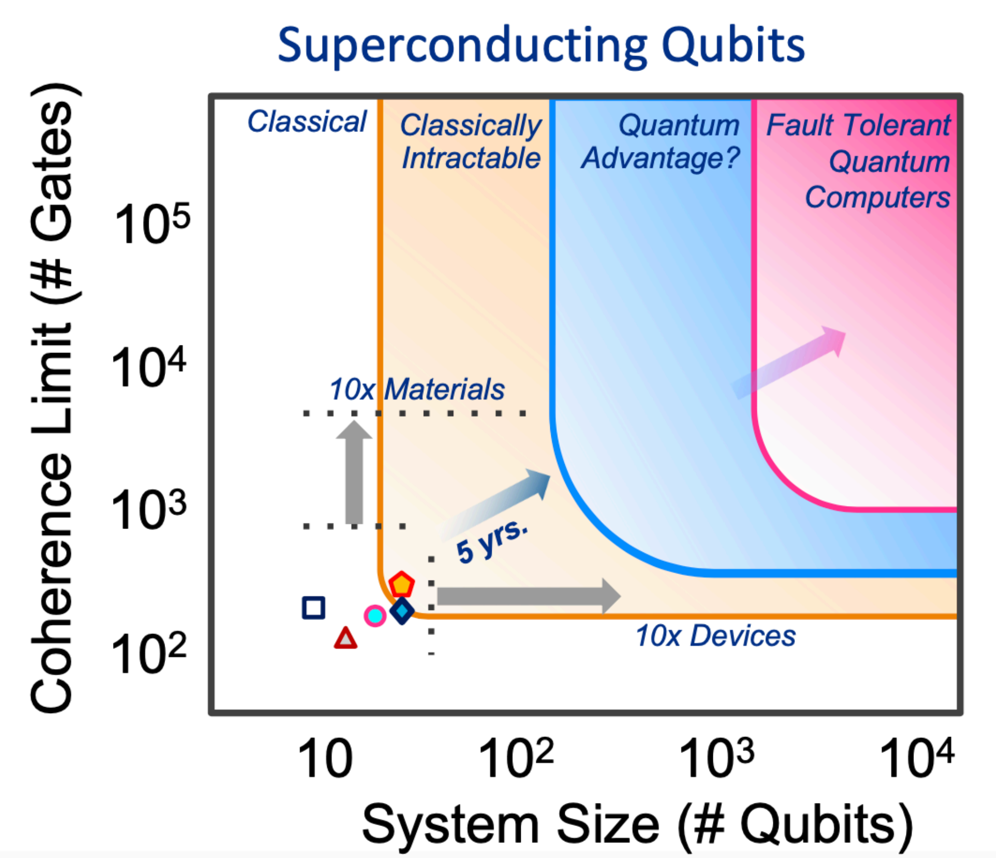
60

The road to Quantum Advantage





Qubit technologies overview. From: Forbes, *Quantum Computer Battle Royale: Upstart Ions Versus Old Guard Superconductors*

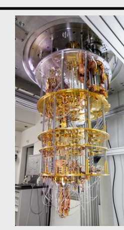
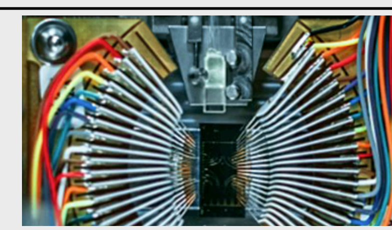
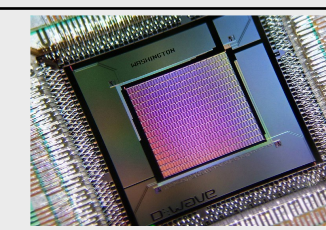
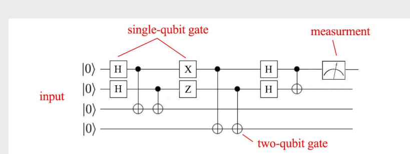
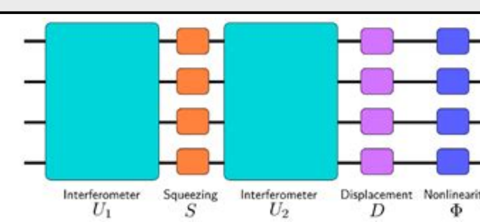
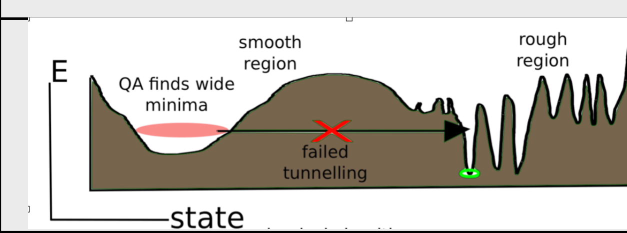


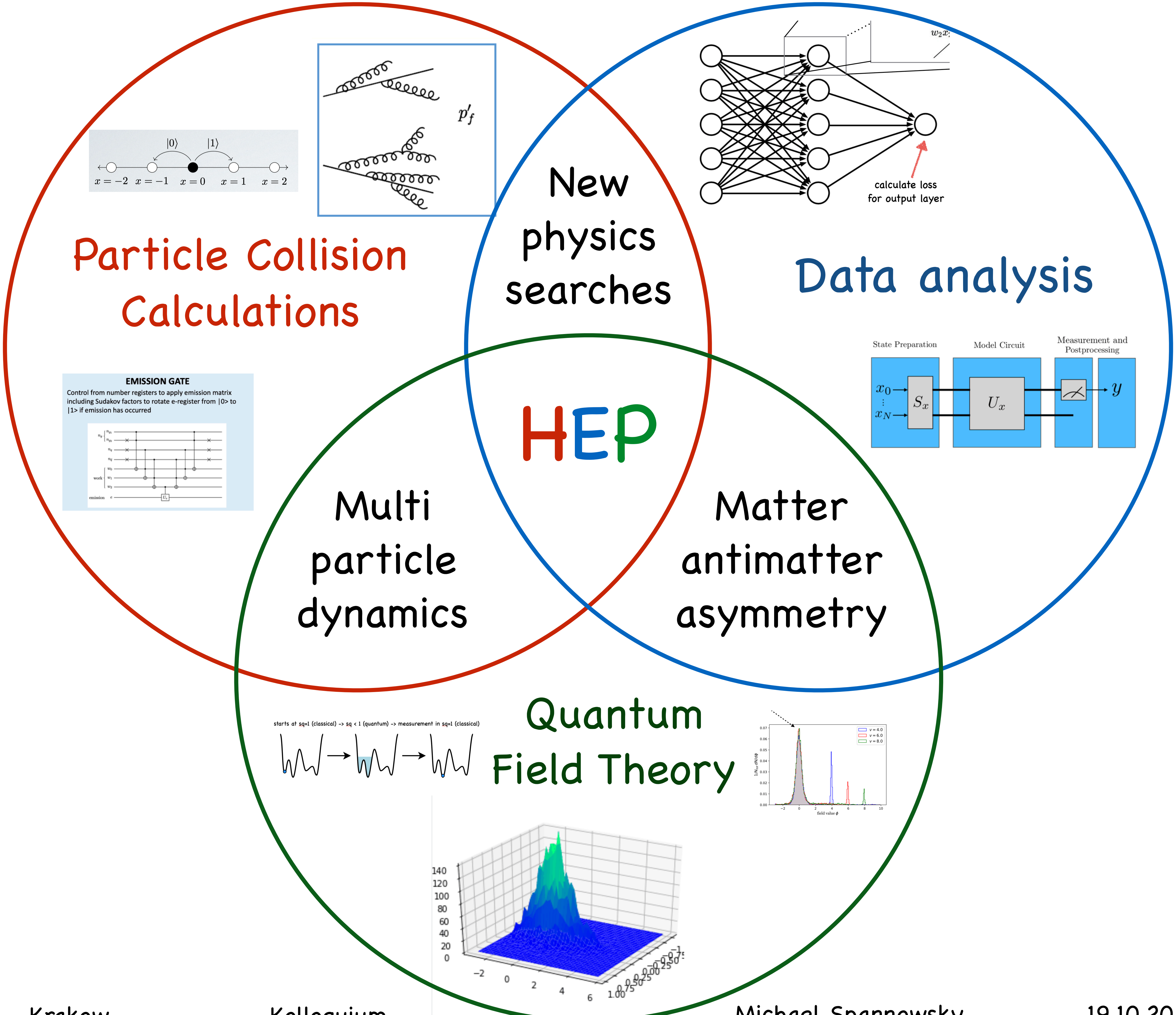
IBM 400 qubits in 2021

IBM 1000 qubits in 2022

Popular Quantum Computing paradigms

Quantum computing has long and distinguished history but is only now becoming practicable.

Type	Discrete Gate (DG)	Continuous Variable (CV)	Quantum Annealer (QA)
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 ~ 50 Qubits	Xanadu	DWave - LEAP ~5000 Qubits
What?			
			



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, ...

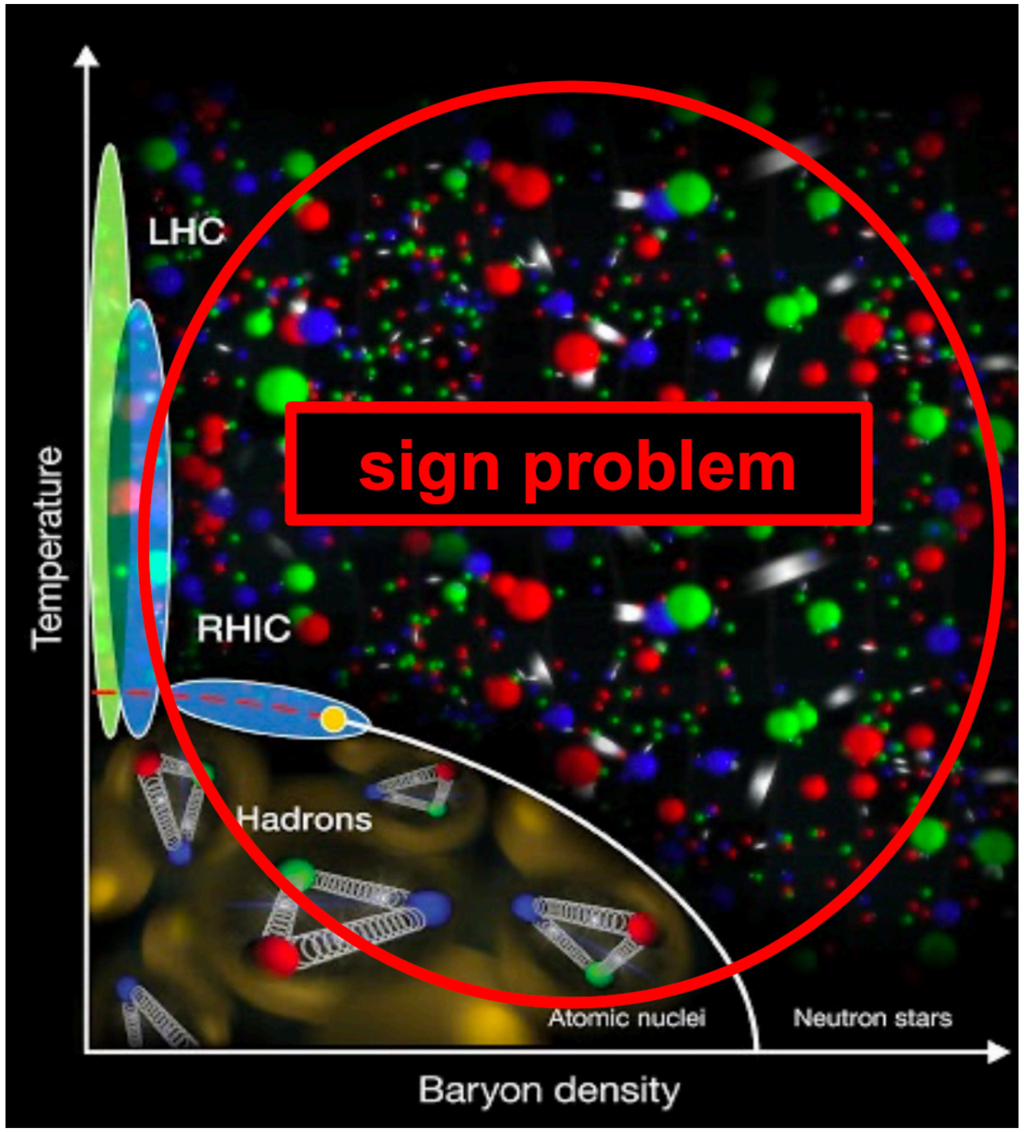
- Example chemical potential

Partition function

$$Z = \int DUD\bar{\psi}\,D\psi e^{-S} = \int DUe^{-S_g} \det M$$

For $\mu \neq 0$ complex determinant

$$[\det M(\mu)]^* = [\det M(-\mu^*)]$$



HEP application focused quantum simulations

- Importance sampling

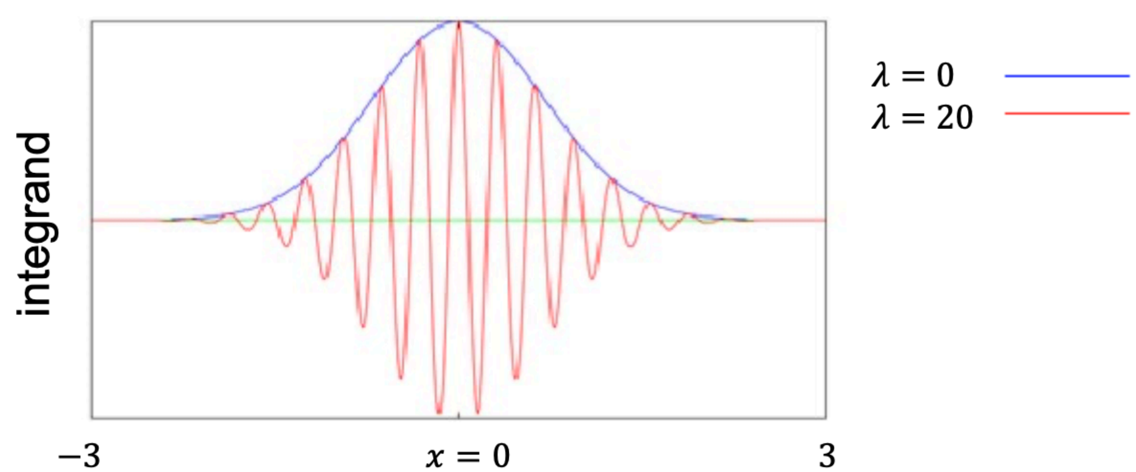
  Interpretation of $e^{-S_g} \det M$

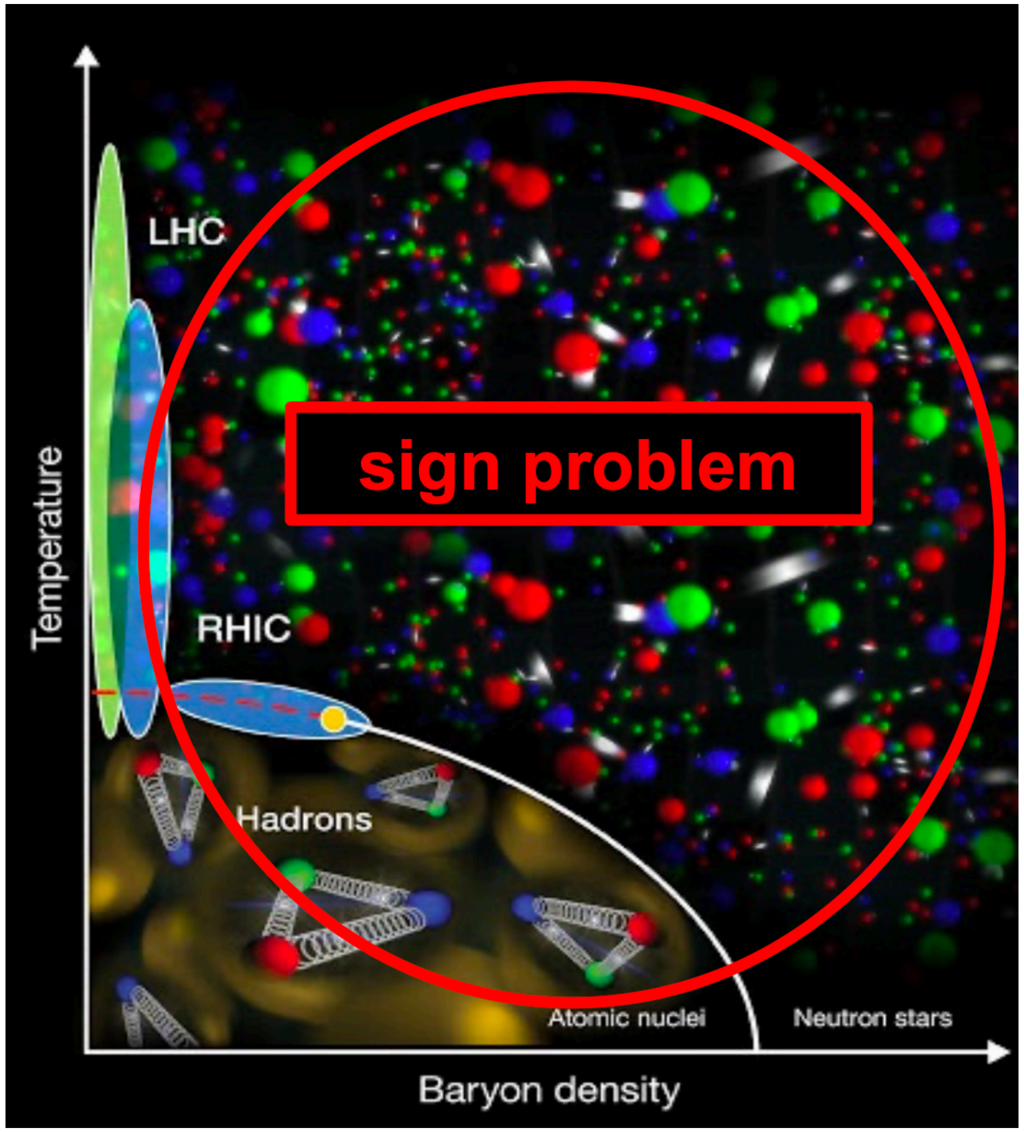
  as probability weight

- Highly oscillatory integrands

$$\langle O \rangle = \frac{\int DU e^{-S_g} |\det M| \, e^{i\phi} O}{\int DU e^{-S_g} |\det M| \, e^{i\phi}}$$

near cancellation of pos and neg contribs

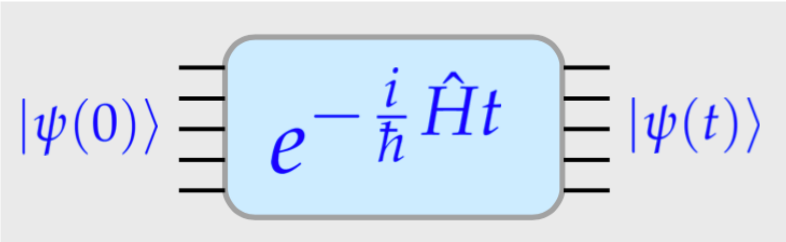




$$\int dx \exp(-x^2 + i\lambda x) \rightarrow \int dx \exp(-x^2)\cos(\lambda x)$$

HEP application focused quantum simulations

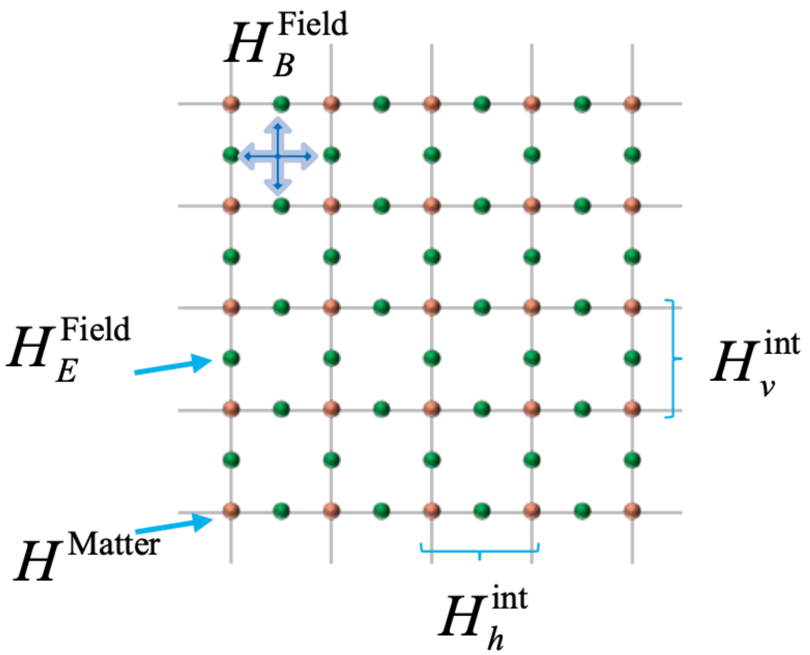
- Real-time evolution on quantum computer can avoid sign problem



Kogut-Susskind formulation

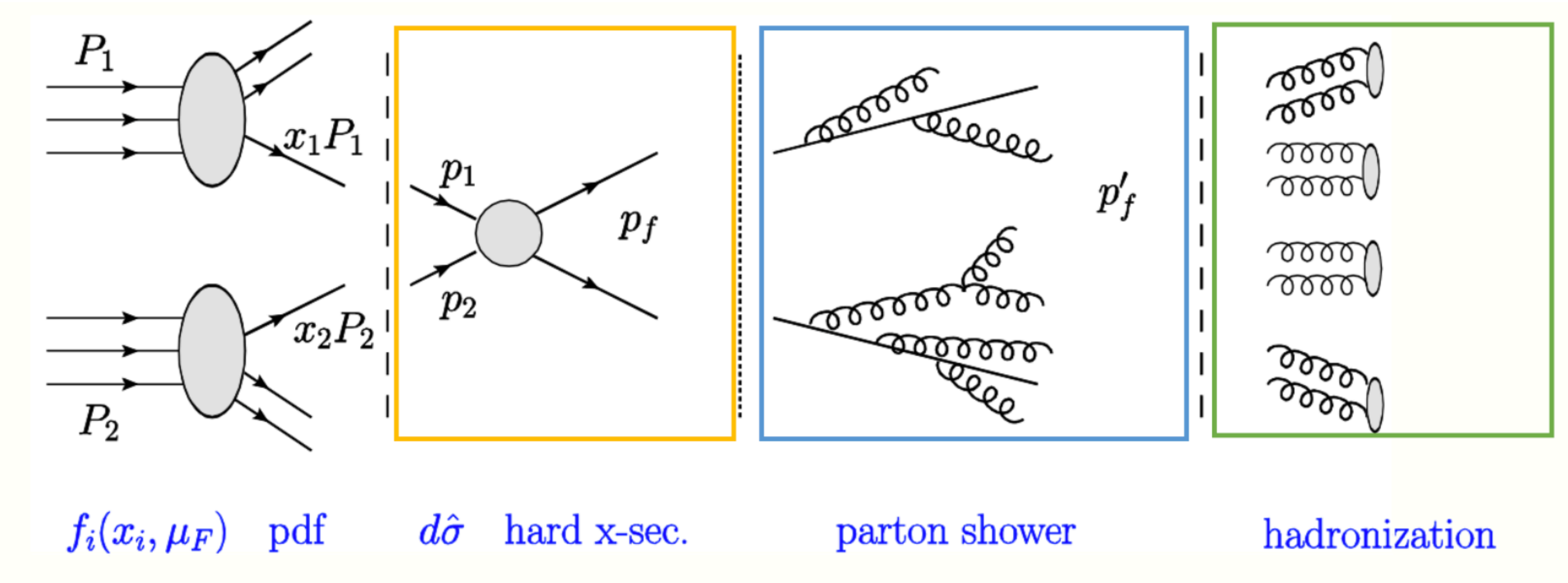
$$H = H^{\text{Matter}} + H^{\text{Field}} + H^{\text{int}}$$

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



- 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]

Calculation of particle collisions



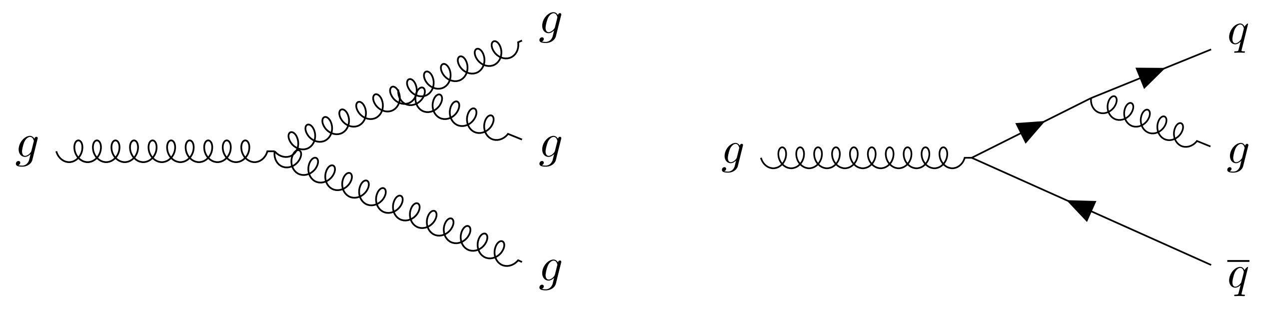
- hard process and parton shower most time consuming parts of event simulation - though carries most information!

- hard process calculated using modern helicity amplitude techniques and parton showers using perturbative QCD resummation techniques.

→ Event generators: Pythia, Herwig, Sherpa, ...

Parton shower

Particle cascade in collinear limit given by splitting functions and non-emission probabilities



(a) $g \to ggg$ (b) $g \to q\bar{q}g$ (c) $g \to q\bar{q}g$ (d) $q \to qgg$

Splitting functions:

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

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

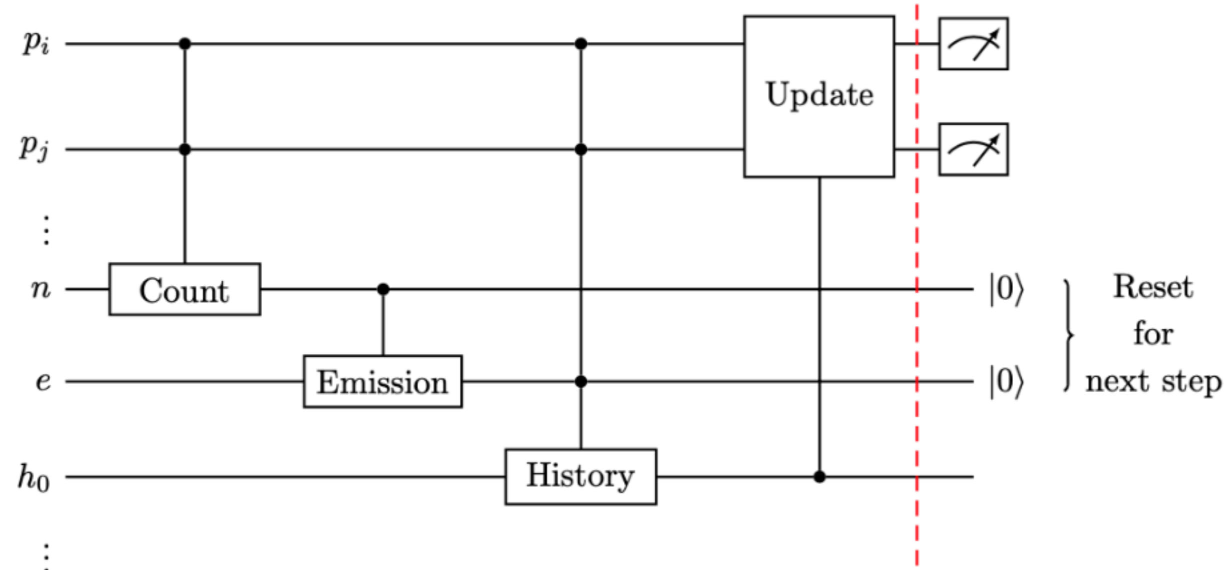
Sudakov factors for non-emission probability $\Delta_{i,k}(z_1,z_2) = \exp\left[-\alpha_s^2 \int_{z_1}^{z_2} P_k(z')dz'\right]$

Total Sudakov, i.e. non-emission prob $\Delta_{\text{tot}}(z_1,z_2) = \Delta_g^{n_g}(z_1,z_2)\Delta_q^{n_q}(z_1,z_2)\Delta_{\bar{q}}^{n_{\bar{q}}}(z_1,z_2)$

Circuit for parton shower algorithm

- Circuit consists of: particle registers, emission registers, and history registers and uses a total of 31 qubits

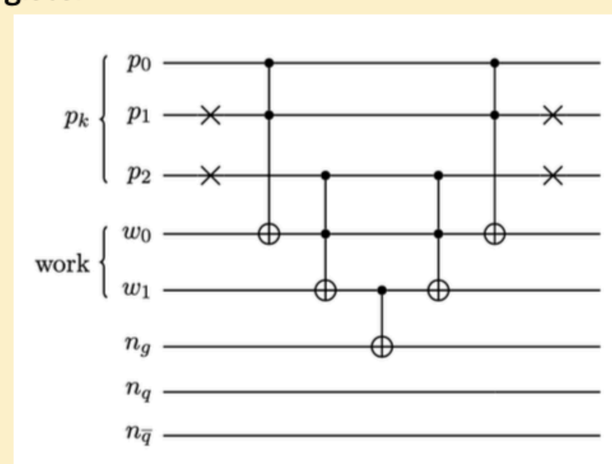
	gluon	quark	antiquark
p0	1	0	0
p1	0	0	1
p2	0	1	1



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

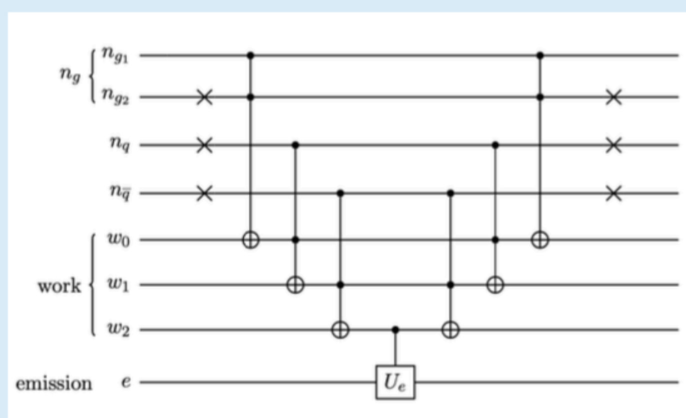
COUNT GATE

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



EMISSION GATE

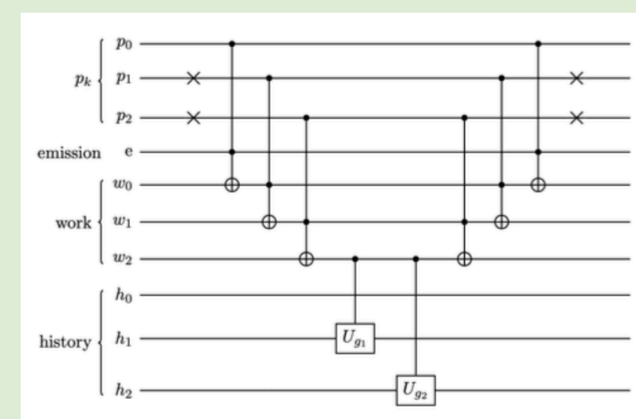
Control from number registers to apply emission matrix including Sudakov factors to rotate e-register from |0> to |1> if emission has occurred



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

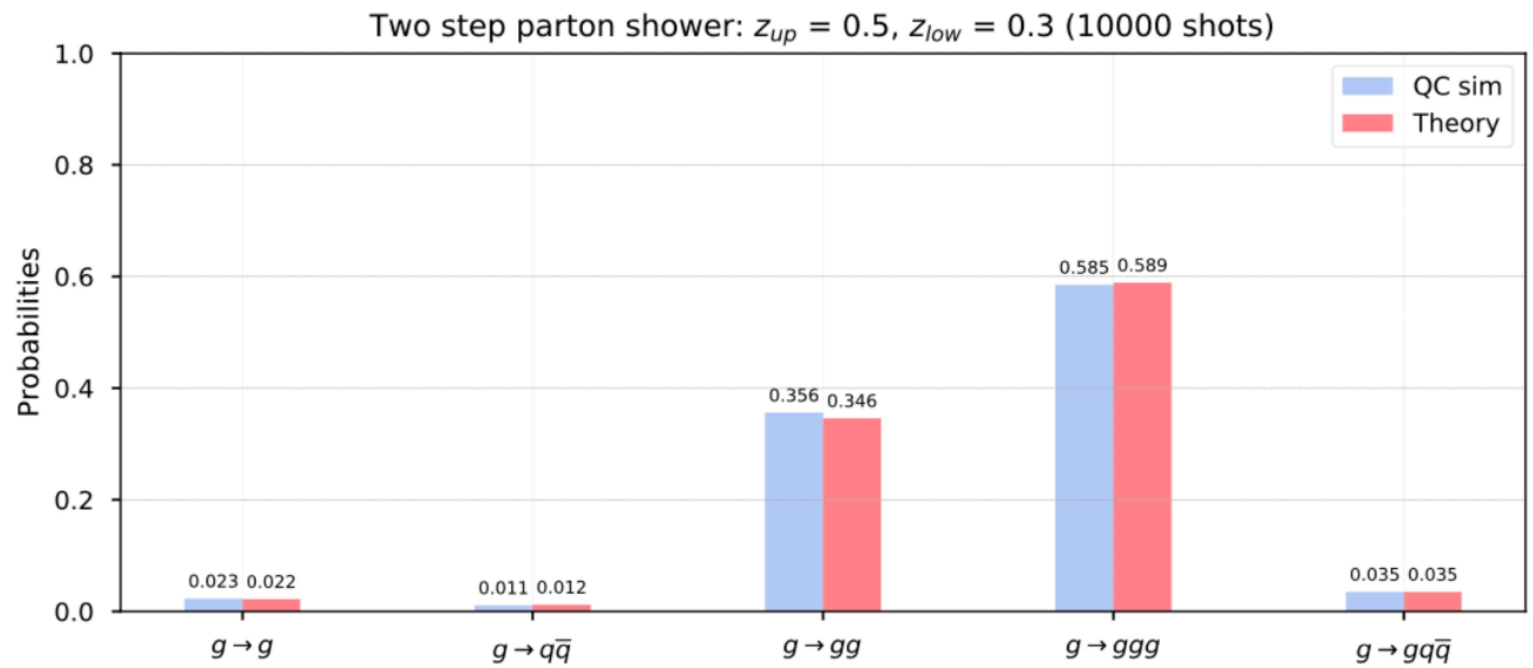
HISTORY GATE

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

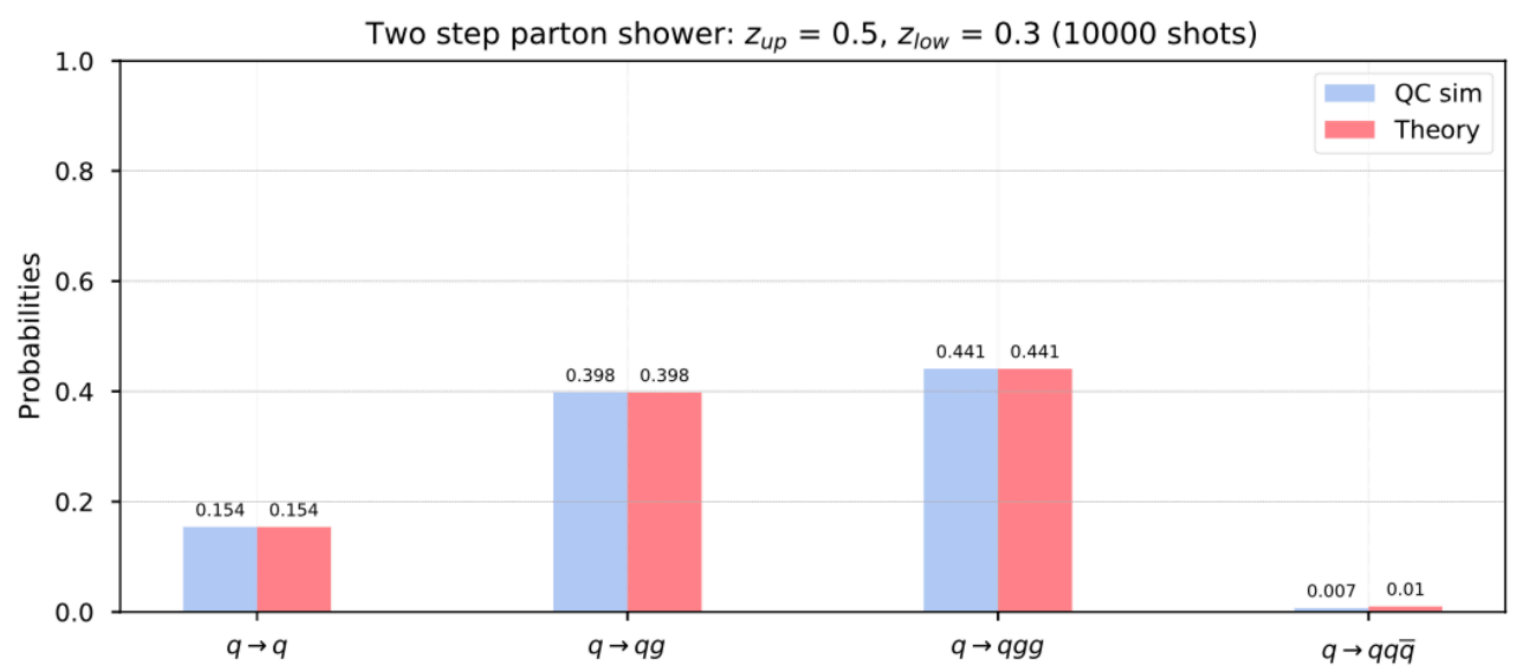


$$U_h = \begin{pmatrix} \sqrt{1 - \frac{P_{k \to ij}(z)}{P_{\text{tot}}(z)}} & -\sqrt{\frac{P_{k \to ij}(z)}{P_{\text{tot}}(z)}} \\ \sqrt{\frac{P_{k \to ij}(z)}{P_{\text{tot}}(z)}} & \sqrt{1 - \frac{P_{k \to ij}(z)}{P_{\text{tot}}(z)}} \end{pmatrix}$$

- **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:
    - $\to qgg$
    - $\to qq\bar{q}$

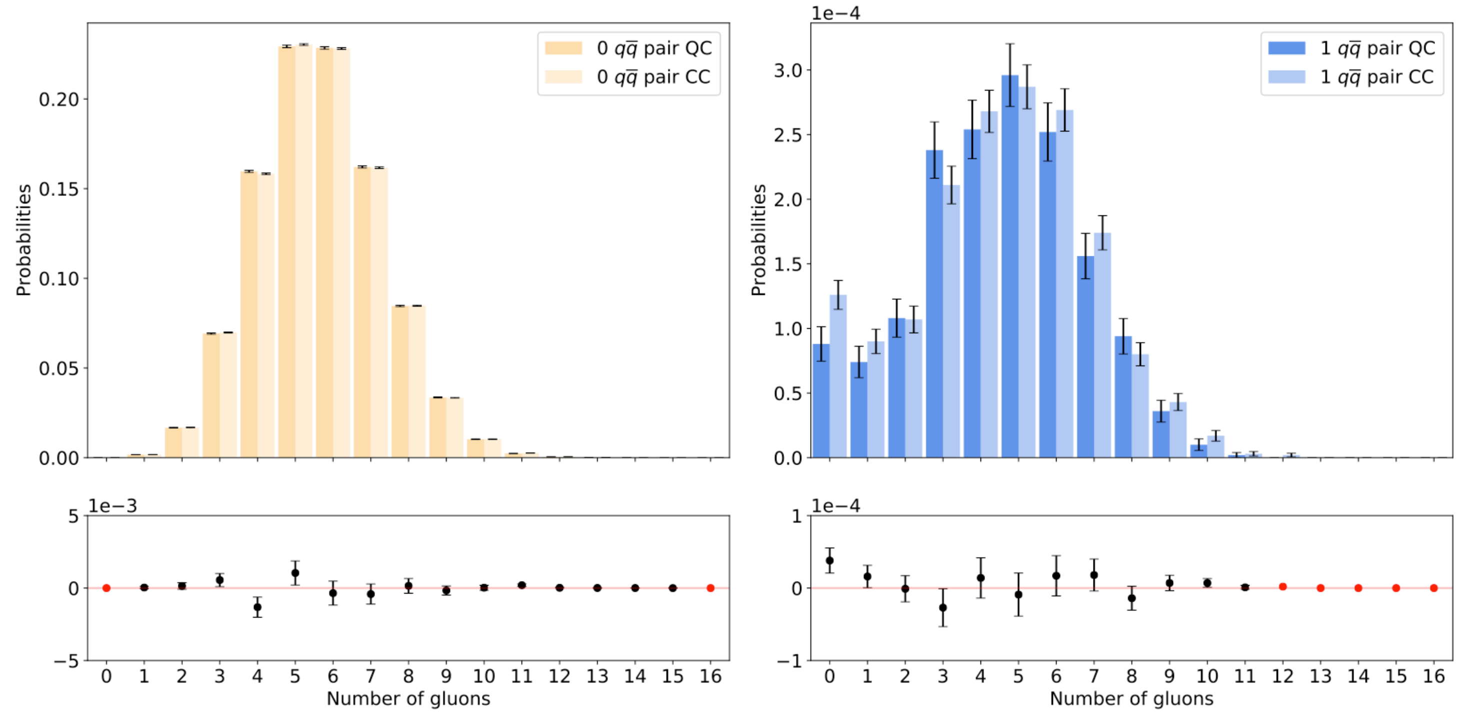


- More powerful algorithms using Quantum Walks

[Bepari, Malik, MS, Williams '21]

#steps grows exponentially with #qubits

Circuit depth grows linearly with #steps



Here, up to 16 emissions

But practically not limited

- Scales as $q = 2\log_2(N+1) + 6$
- Including kinematics see [Gustafson, Prestel, MS, Williams '22]
- Conversely to classical algorithm, quantum algorithm keeps the entire shower history in wave function

→ measurement by projecting onto specific state

→ whether quantum algorithm advantageous over classical depends on technical factors and hardware specs

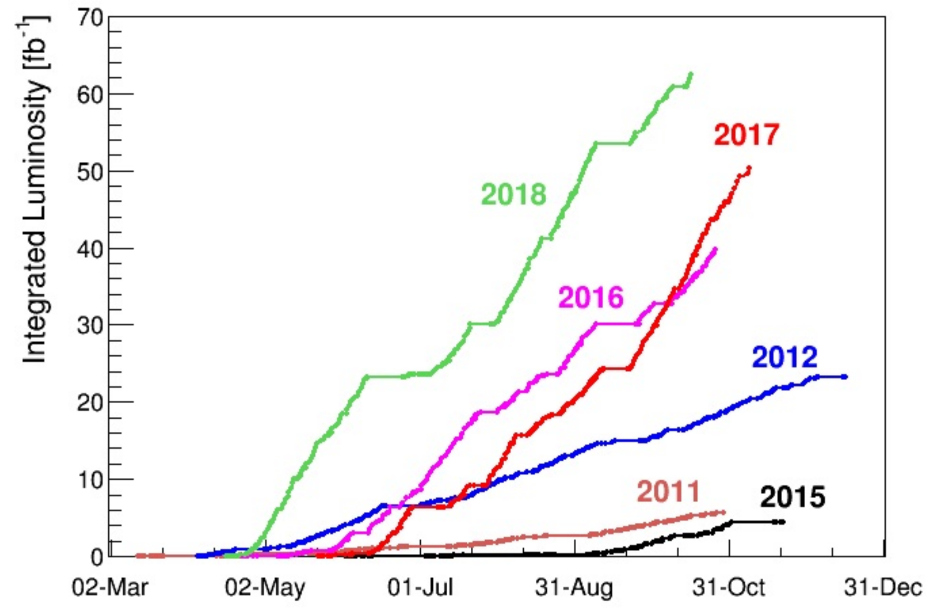
- Helicity amplitudes formalism and simplified parton shower algorithm covered in [Bepari, Malik, MS, Williams '20]

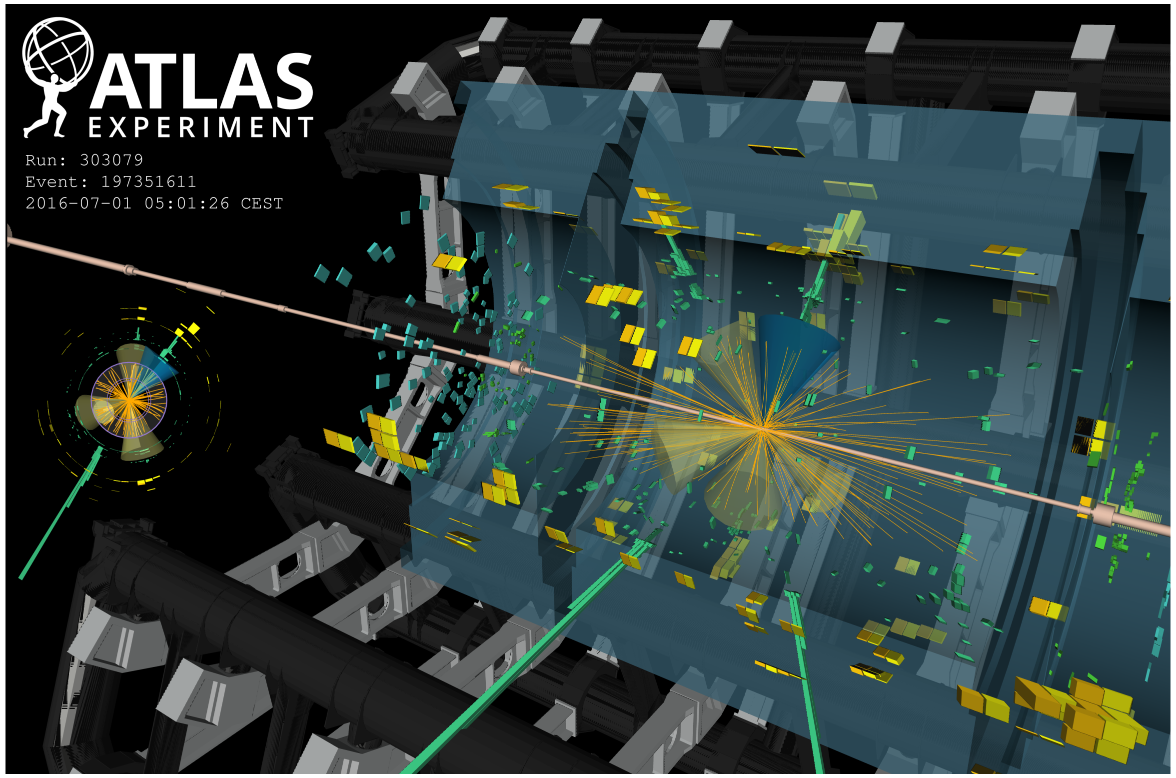
Data analysis for high-energy physics

Big Data at the LHC

→ ATLAS/CMS 200 events/s passing triggers

→ ATLAS/CMS 2 PB/year of data



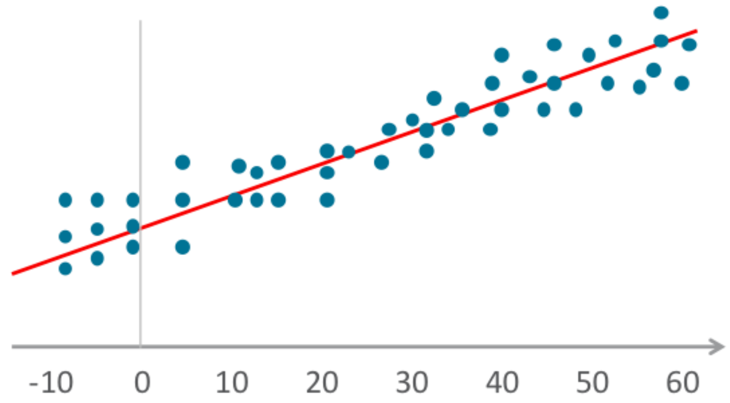


Candidate event tth ATLAS

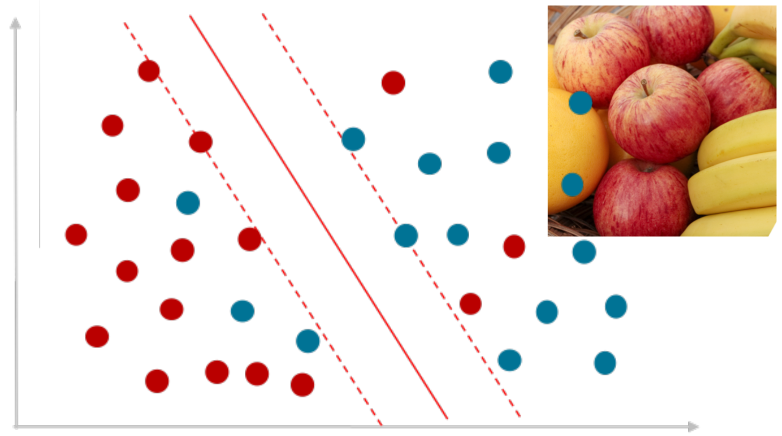
- Highly complex data
- Need sophisticated automated data analysis methods to discriminate signal from backgrounds

Supervised

Regression



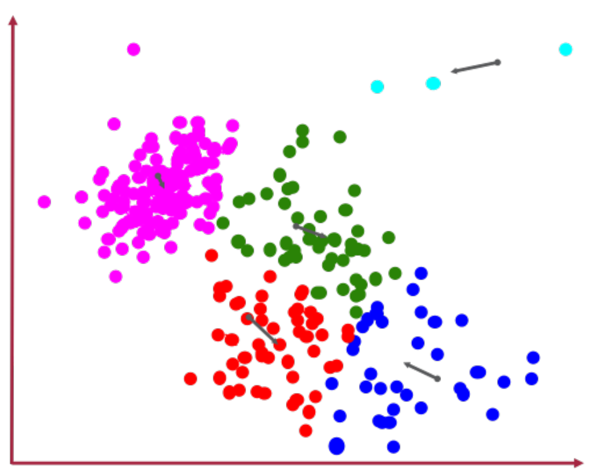
Classification



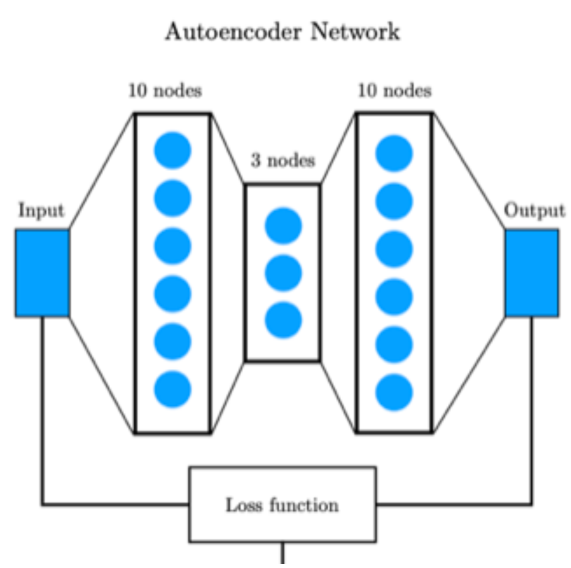
Fine-grained small net

Unsupervised

Clustering

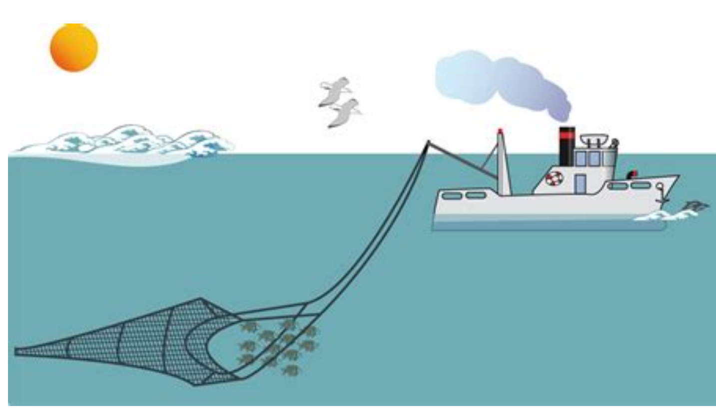


Autoencoder



for quantum continuous variable algorithm see [Blance, MS '21]

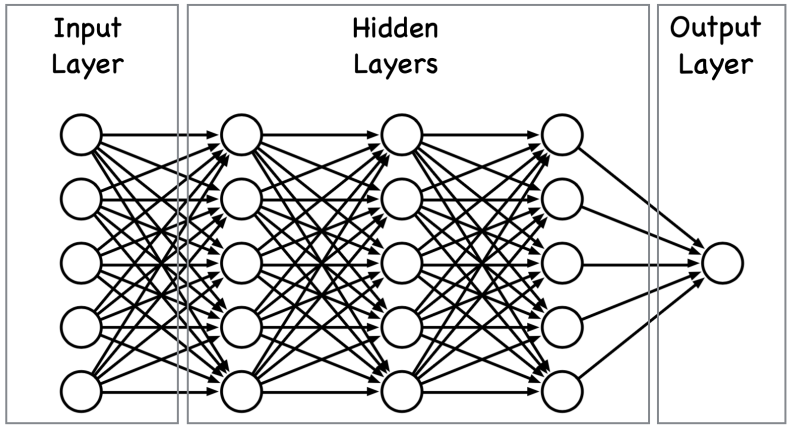
Large net



Classical Neural Network recap

Very powerful principle which NNs are designed to exploit

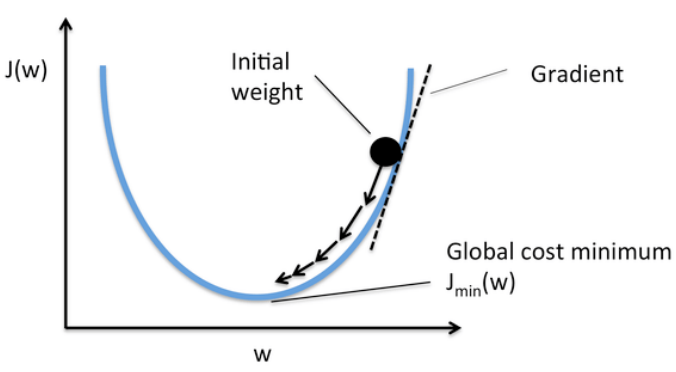
1. an adaptable complex system that allows approximating a complicated function



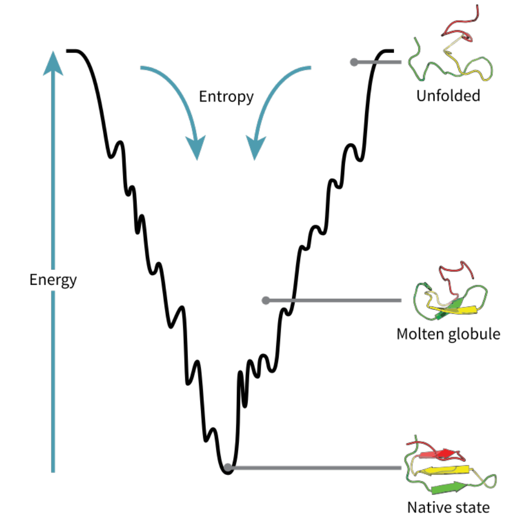
2. the calculation of a loss function in the output layer which is used to define the task the NN algorithm should perform by minimising this function

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

3. a way to update the network continuously while minimising the loss function, e.g. backpropagation



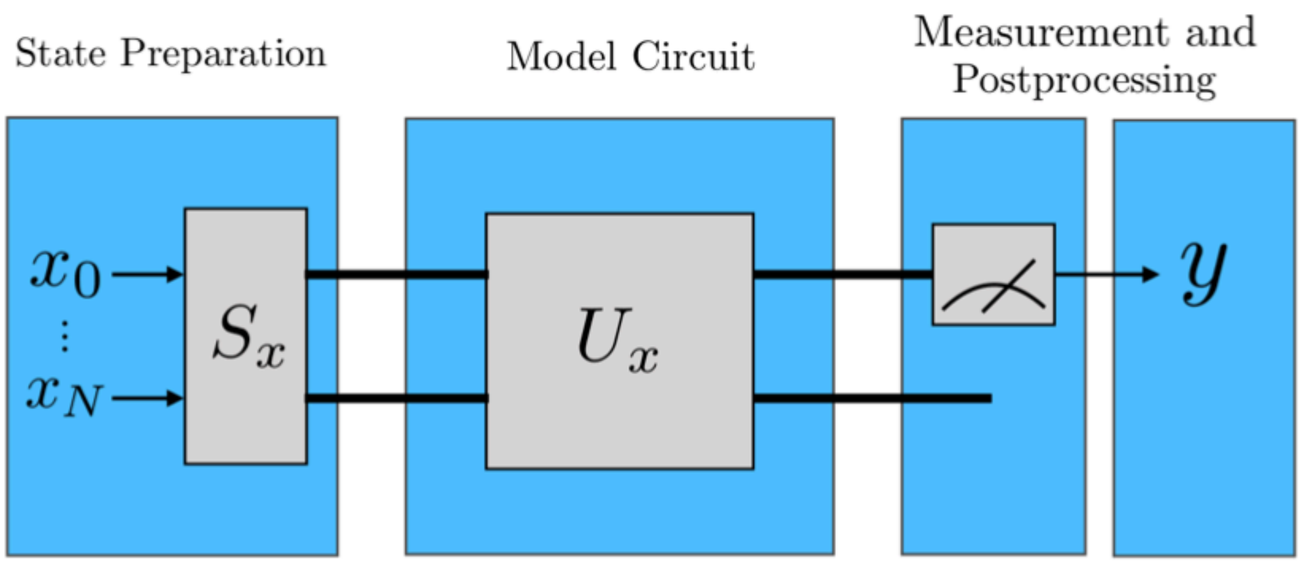
=



Difficult to keep all in quantum system - but not impossible? stay tuned!

Quantum Machine Learning with a Variational Quantum Circuit

[Blance, MS '20]



state preparation

n corresponds to # features

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

angle encoding

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

→ angles define Hilbert space

for single qubit $\alpha,\ \beta,$ and γ

model circuit / trainable parameters / prepared state

$$|\psi\rangle = U(w)|x\rangle$$

with

$$U(w) = U_{l_{\max}}(w_{l_{\max}})...U_l(w_l)...U_1(w_1)$$

single qubit gate

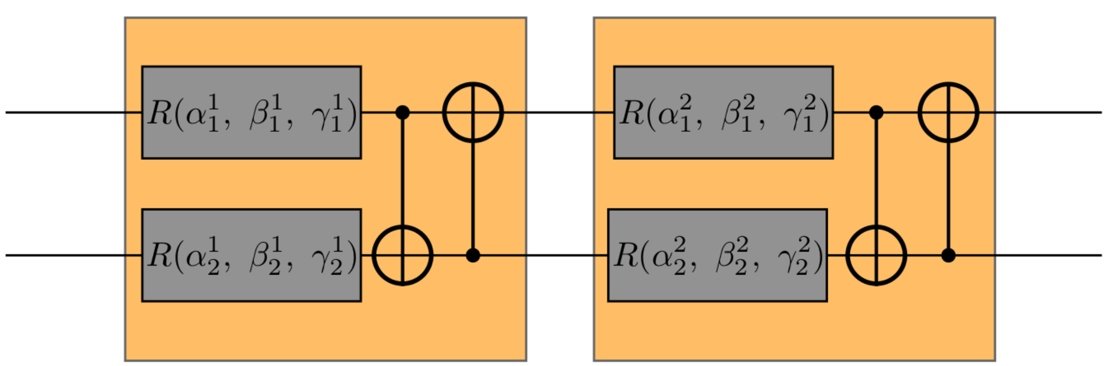
$$G(\alpha,\beta,\gamma,\phi) = e^{i\phi}\begin{pmatrix} e^{i\beta}\cos(\alpha) & e^{i\gamma}\sin(\alpha) \\ -e^{-i\gamma}\sin(\alpha) & e^{-i\beta}\cos(\alpha) \end{pmatrix}$$

CNOT gate

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

to entangle/ disentangle states

2-layer Variational Quantum Circuit

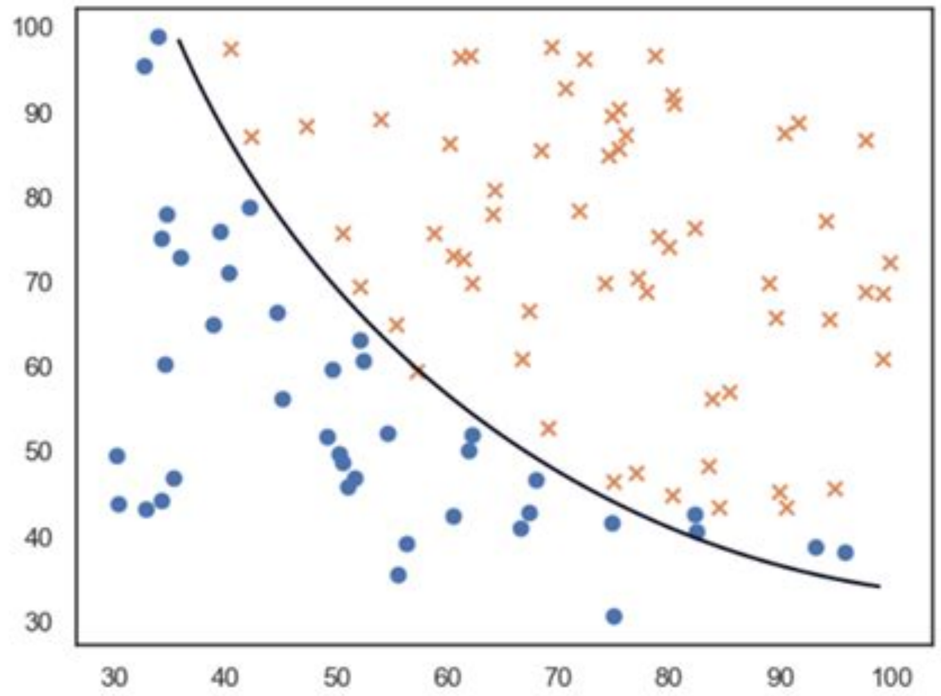


Gate quantum machine learning in action

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

Quantum network output:

$$f(w,b,x) = \pi(w,x) + b$$



Classification loss

$$L = \frac{1}{n}\sum_{i=1}^{n}\left[y_i^{\text{truth}} - f(w,b,x_i)\right]^2$$

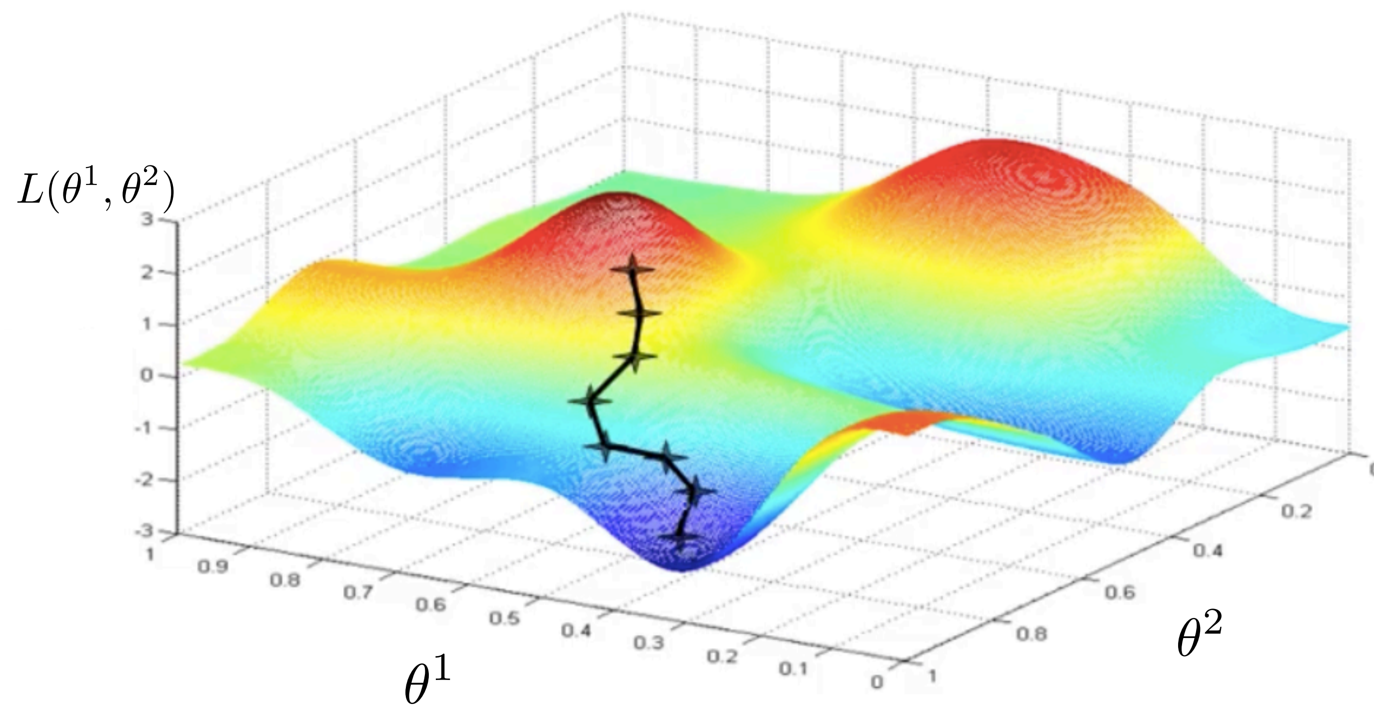
label (signal, bkg)
supervised learning

could be RMSE, binary cross entropy or etc

Gate quantum machine learning in action

classical gradient descent (GD):

$$\theta_{t+1} = \theta_t - \eta \nabla L(\theta)$$



quantum gradient descent (QDC):

Fisher Information Matrix F promotes
gradient descent to natural gradient descent (Riemannian geometry):

$$\theta_{t+1} = \theta_t - \eta F^{-1} \nabla L(\theta)$$

Fubiny-Study metric underlies
geometric structure of VQC
parameter space:

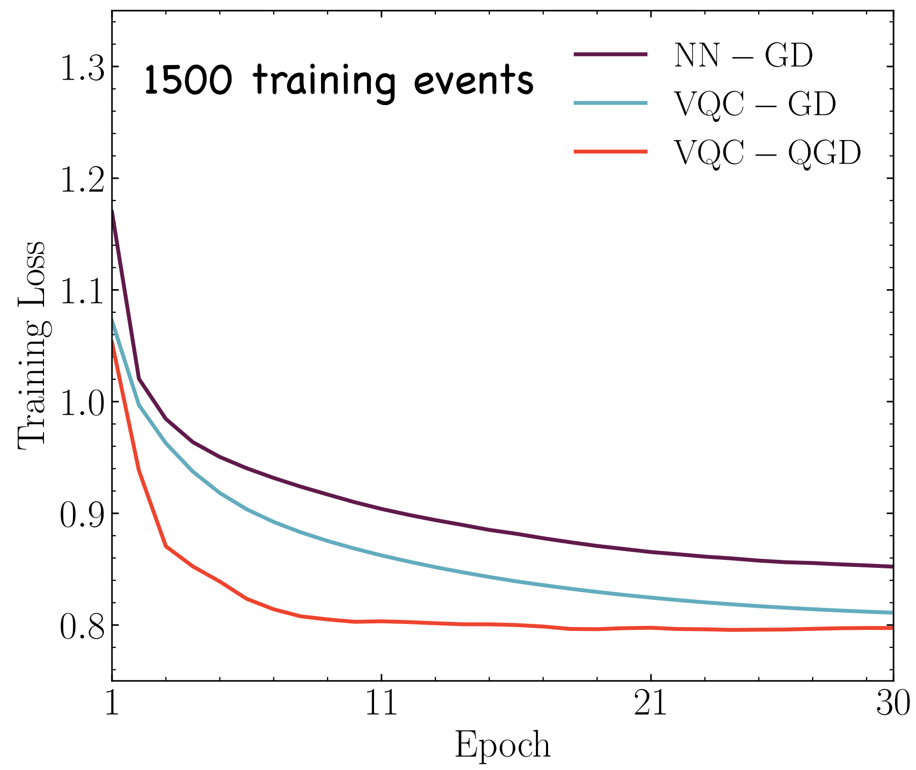
$$\theta_{t+1} = \theta_t - \eta g^{+} \nabla L(\theta)$$

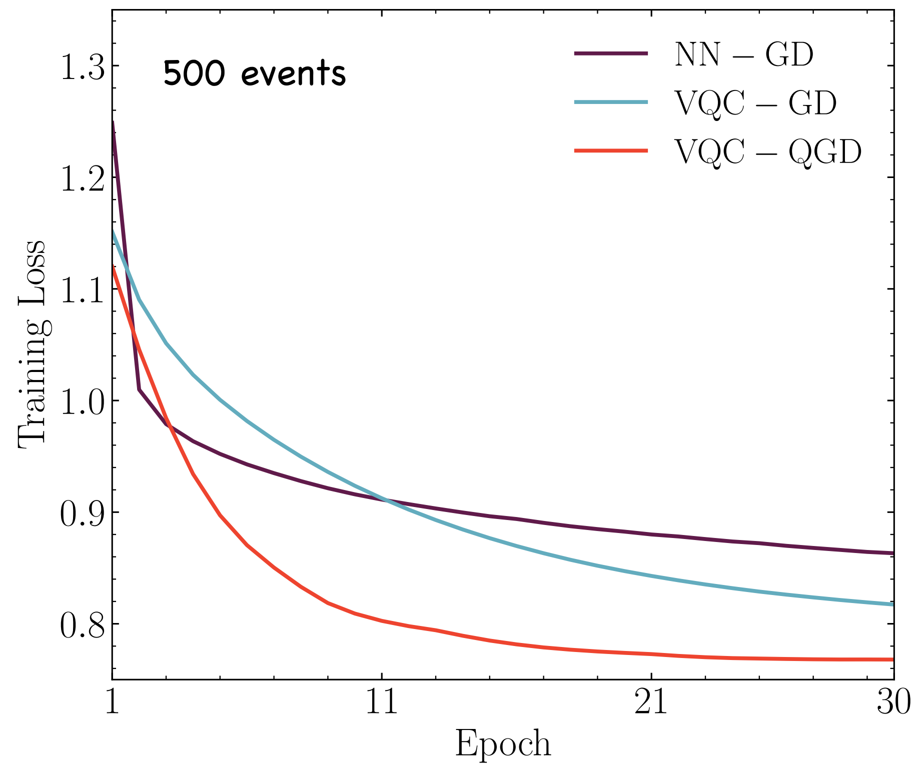
VQC parameters

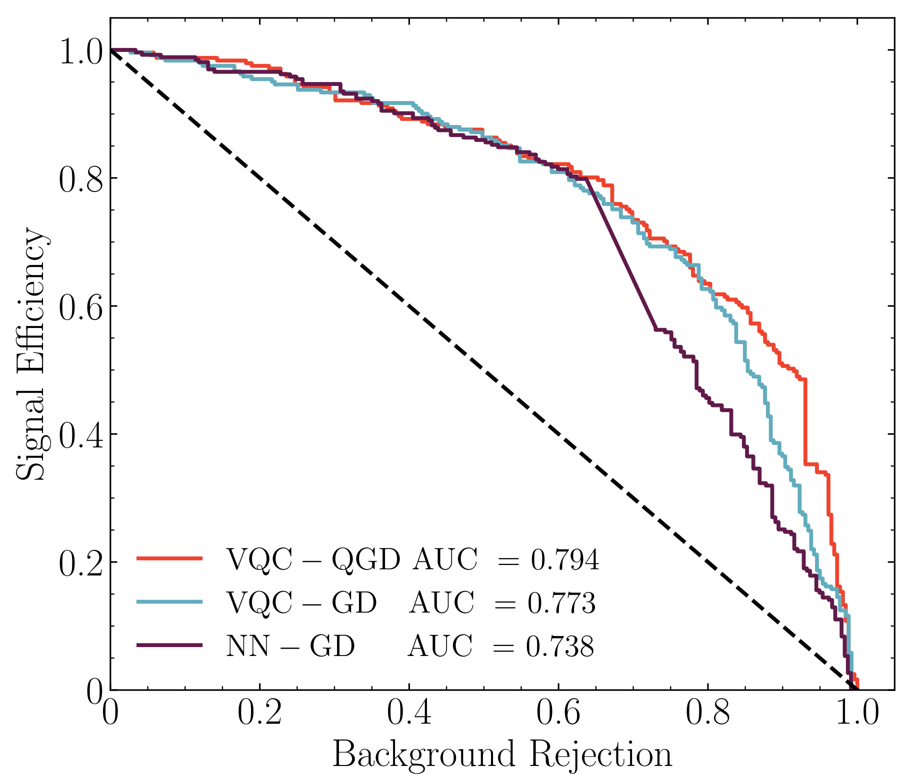
weights $\theta^w_{t+1} = \theta^w_t - \eta g^{+} \nabla^w L(\theta)$,

bias $\theta^b_{t+1} = \theta^b_t - \eta \nabla^b L(\theta)$,

Gate quantum machine learning in action







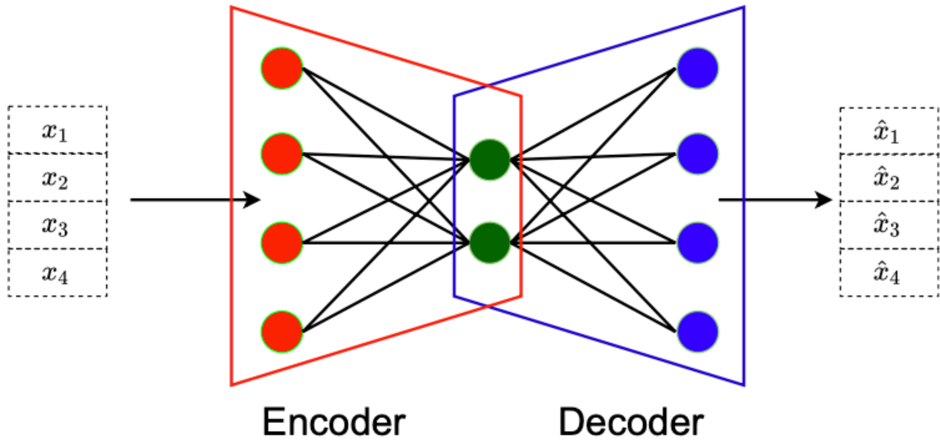
performance
QC device vs simulator

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

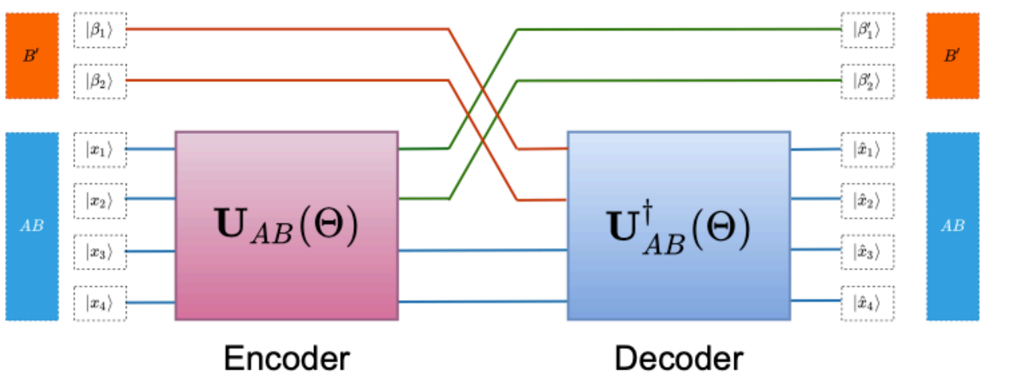
Anomaly detection

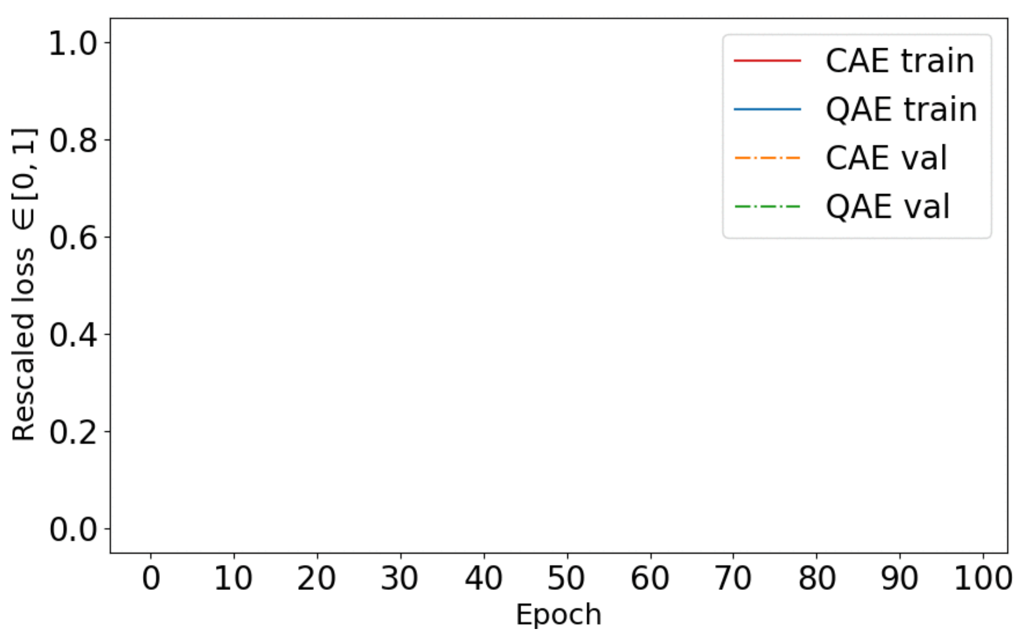
[Ngairangbam, MS, Takeuchi '21]

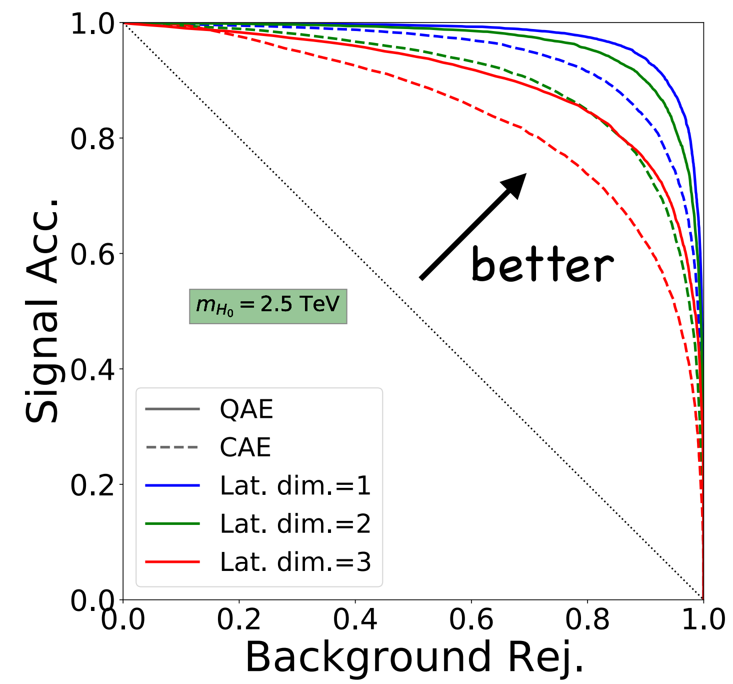
Classical autoencoder



Quantum autoencoder

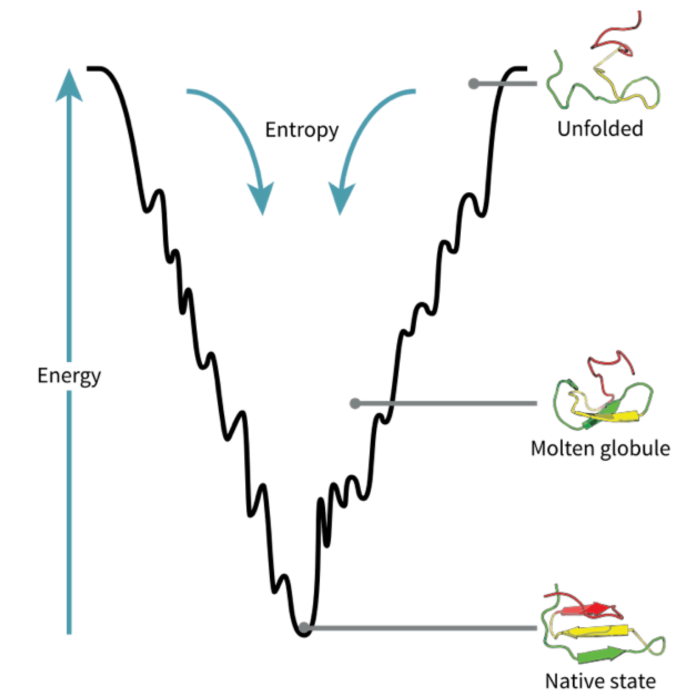






Much faster training and better performance for Quantum autoencoder

Quantum annealing:
Non-universal but universally powerful?



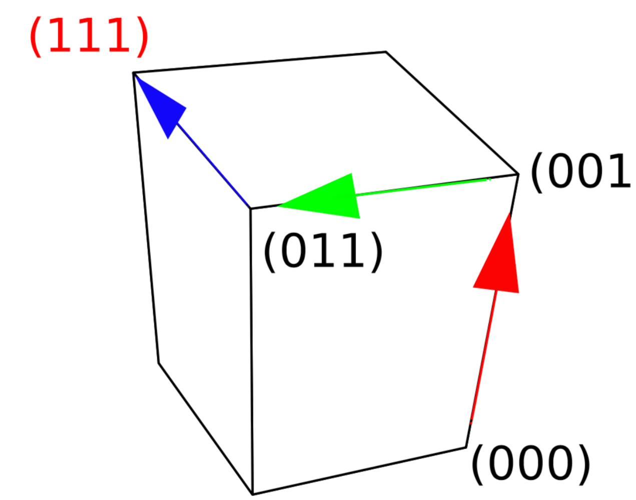
- Specific Hamiltonian. What does the "anneal" mean?

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

final Hamiltonian (encodes actual problem)

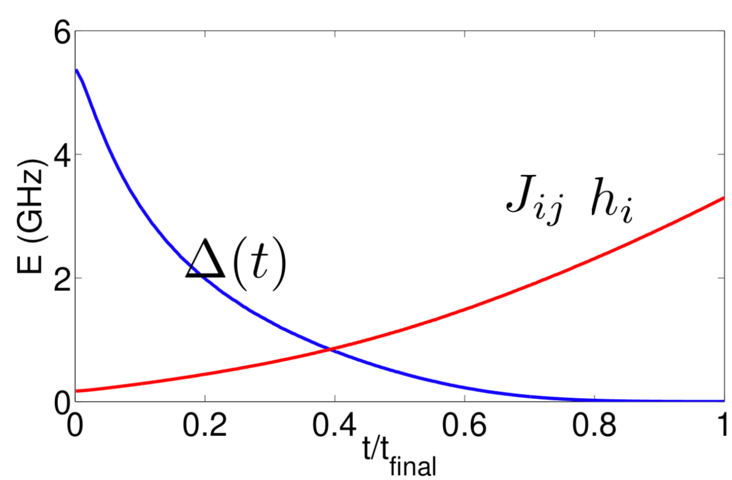
initial Hamiltonian (ground state = superposition of qubits with 0 and 1)

$\Delta(t)$ 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:

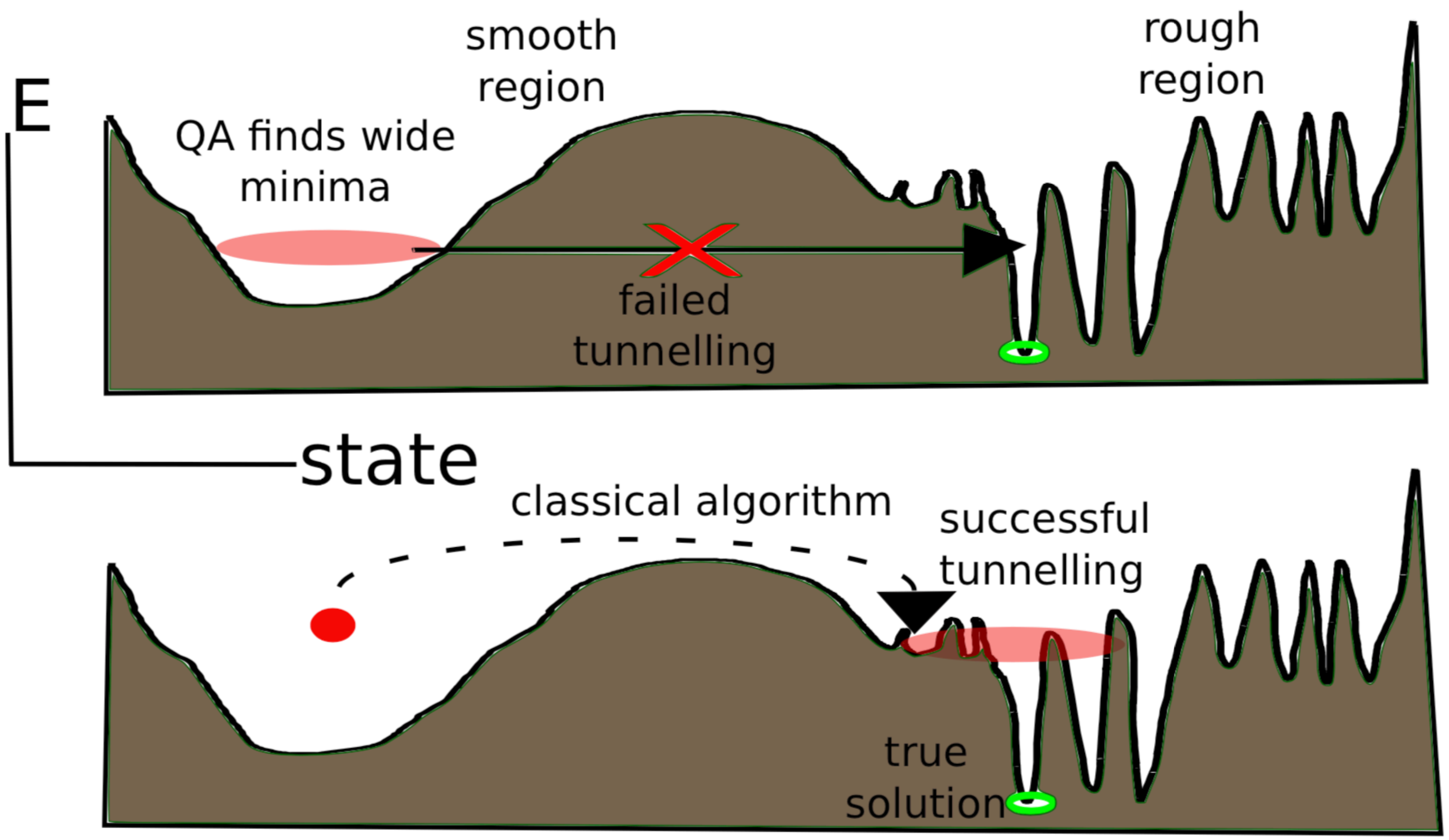


Thermal (classical) and Quantum Annealing are complementary:

- Thermal tunnelling is fast over broad shallow potentials (Quantum "tunnelling" is exponentially slow)

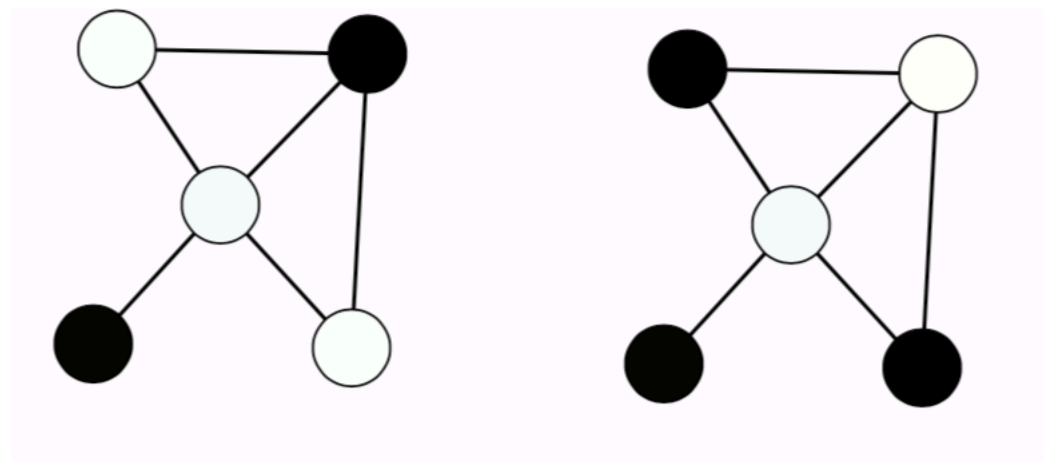
- Quantum tunnelling is fast through tall thin potentials (Thermal "tunnelling" is exponentially slow - Boltzmann suppression)

- 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 are to sit an 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?

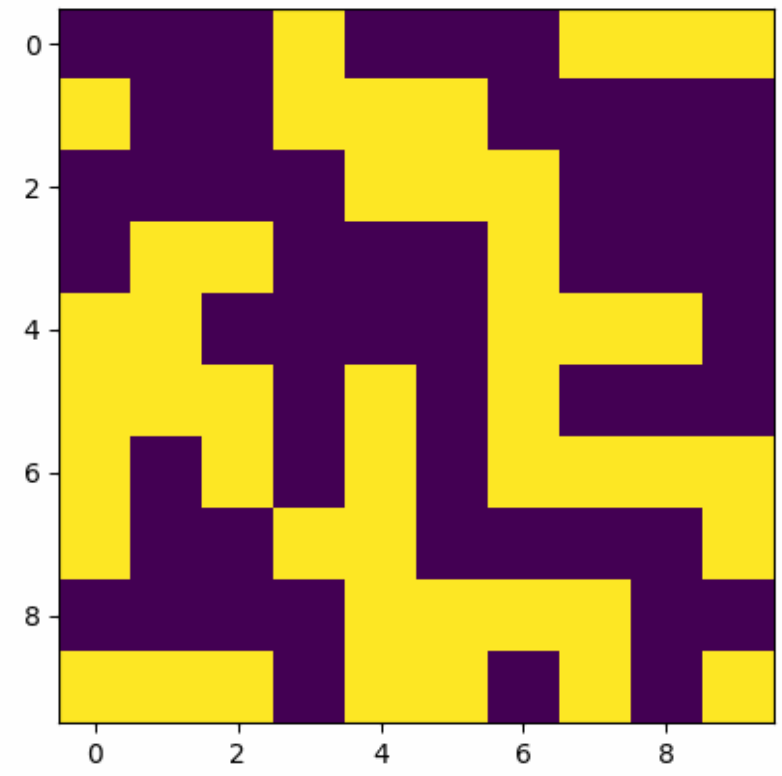
There are N^2 spins σ^Z_{lN+j} arranged in rows and columns. We do not care if A>=<A or B>=<B, but if A>=<B then we put a penalty of 2+ on the Hamiltonian (ferromagnetic coupling)

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

Finally we need to apply constraint that #A=#B:

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

- Example 2 done with classical thermal annealing using the Metropolis algorithm. Note this represents a search over solution space of 2^100 configurations



- Importantly the constraint hamiltonian cannot be too big otherwise the hills are too high and it freezes too early. This makes the process require a (polynomial sized) bit of "thermal tuning".

- Could be done more easily on quantum annealers as constraints could be high and it would still work, e.g. D-Wave quantum annealer. However, architecture (connectivity of J, h) is limited.

Encoding a field theory

[Chancellor '19] [Abel, Chancellor, MS '20]

Consider encoding a continuous filed value $\phi(\rho)$ at some point, and discretise into N

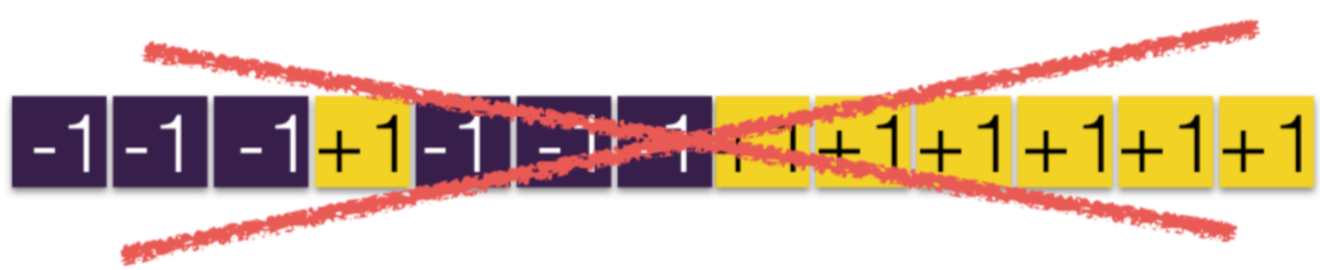
$$\phi(\rho_l) \;=\; \phi_0 + \alpha_l \xi \;=\; \phi_0 + \xi \, \ldots \, \phi_0 + N\xi$$

Wish to represent it as a point on a spin chain == domain wall encoding:

We translate this to a field value using $\phi(\rho_\ell) = \frac{1}{2} \sum_{j=1}^{N-1} (\phi_0 + j\xi) \, \langle \sigma^Z_{\ell N+j+1} - \sigma^Z_{\ell N+j} \rangle$

receiving only contribution from frustration at $j = \alpha_\ell$

For this domain wall encoding to work we have to avoid mult. frustrations e.g.

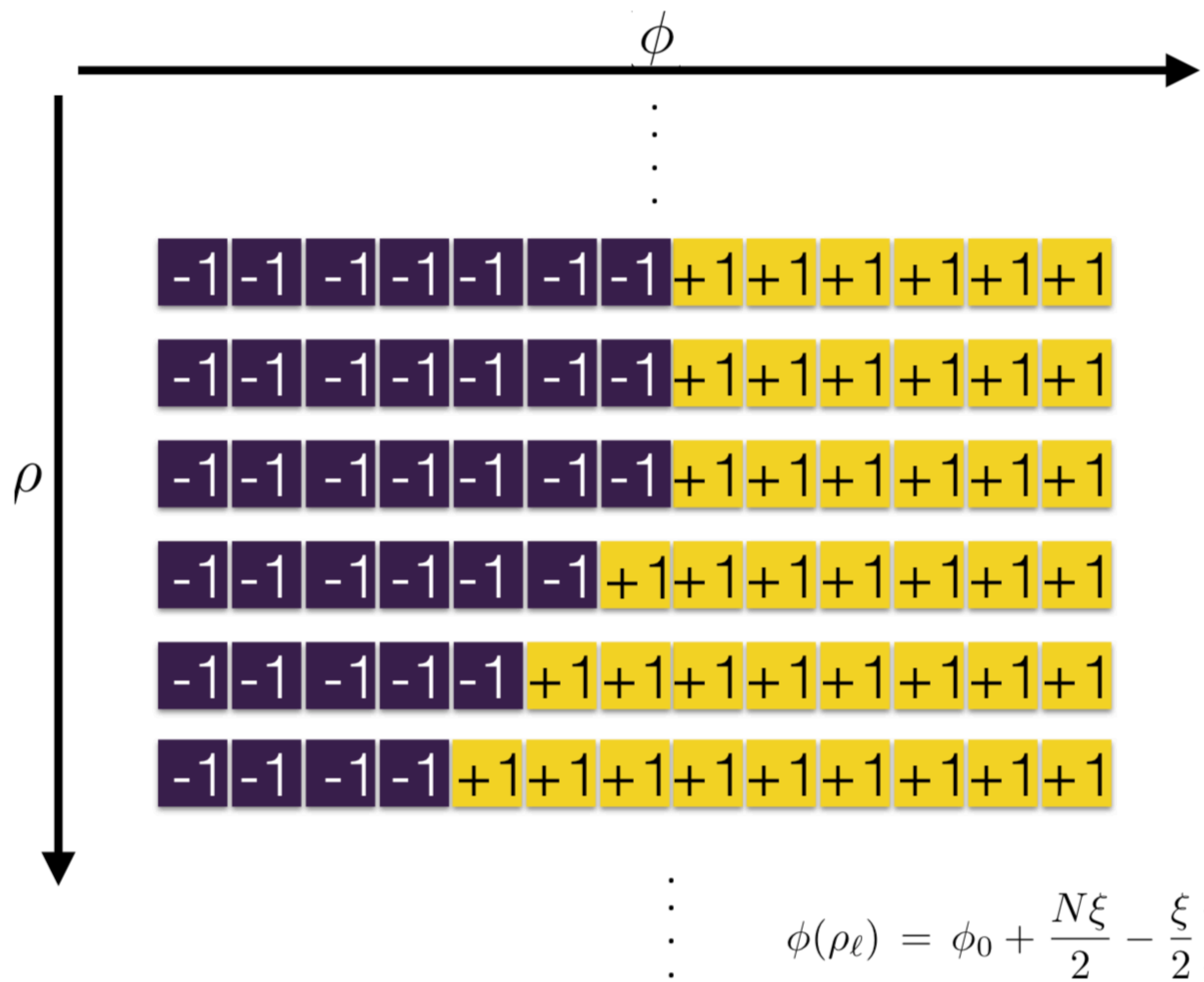


include $\mathcal{H}^{(\mathrm{chain})}_\ell = -\Lambda \left(\sum_{j=1}^{N-1} \sigma^Z_{\ell N+j} \sigma^Z_{\ell N+j+1} - \sigma^Z_{\ell N+1} + \sigma^Z_{\ell N+N} \right)$

Pictorial representation of a solution

spacetime discretised

$$\rho_\ell \;=\; \ell\nu \;=\; \nu \ldots M\nu$$

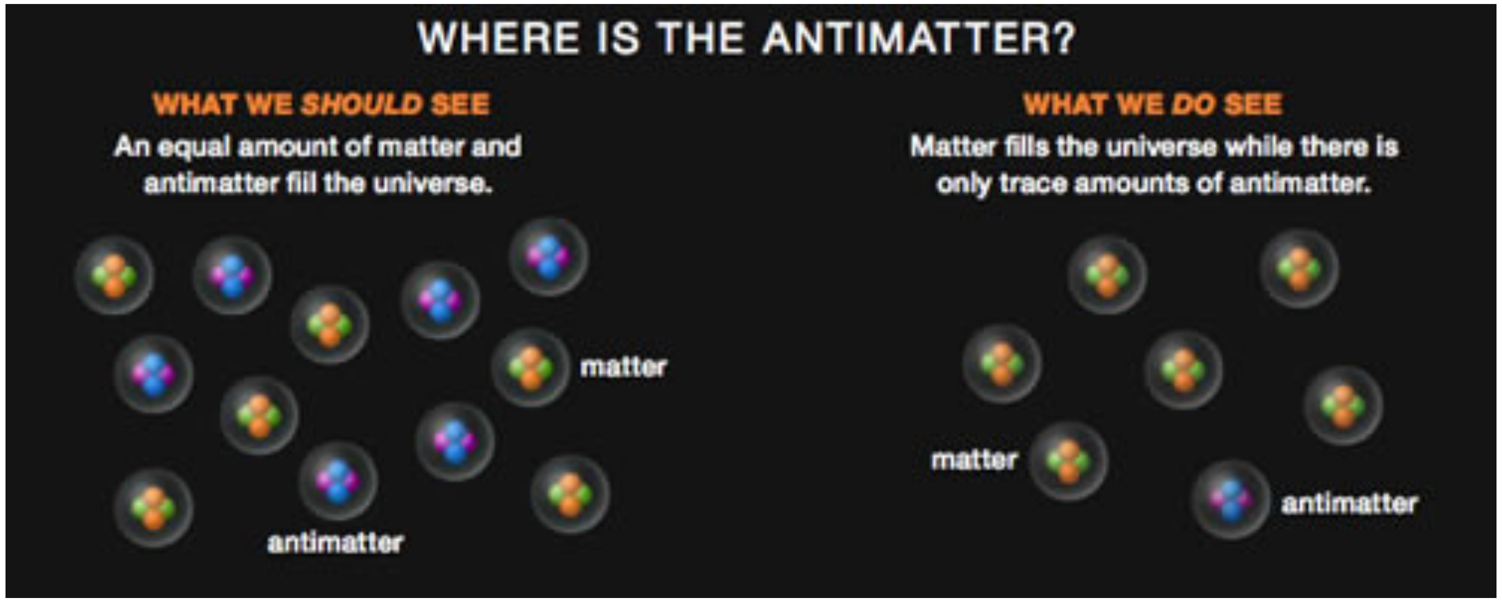


$$\phi(\rho_\ell) = \phi_0 + \frac{N\xi}{2} - \frac{\xi}{2}\sum_{j=1}^{N} \langle \sigma^Z_{\ell N+j} \rangle$$

→ Can be extended to multi-dim (2D) examples/functions/field theories

[Abel, Blance, MS '21]

Example 1: Matter-Antimatter asymmetry



<u>Sakharov conditions:</u> (for dynamical generation of Baryon asymmetry)

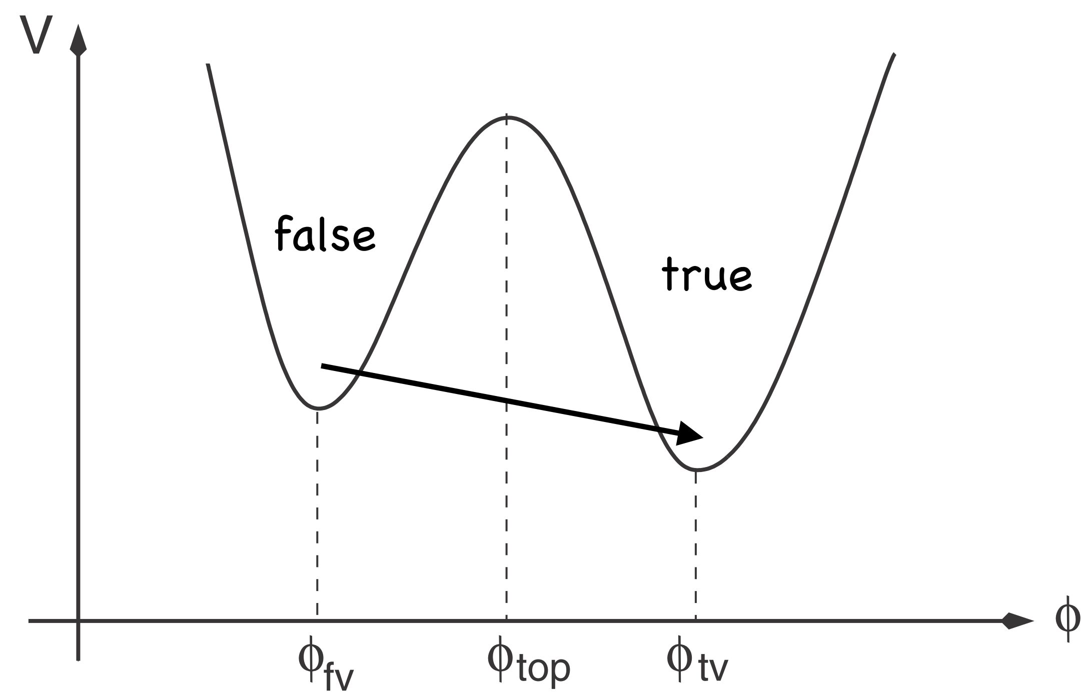
- B violation ✓ **Sphaleron**
- CP violation ⚡✓ enough? -> flavour physics
- Departure from thermal equilibrium ⚡ not enough

Semiclassical calculations for bubbles and phase transitions

Need to find stationary points of Euclidean action:

Potential energy

$$S = \int d\tau\, d^3x \left[\frac{1}{2}\left(\frac{\partial\phi}{\partial\tau}\right)^2 + \frac{1}{2}(\boldsymbol{\nabla}\phi)^2 + V(\phi) \right]$$

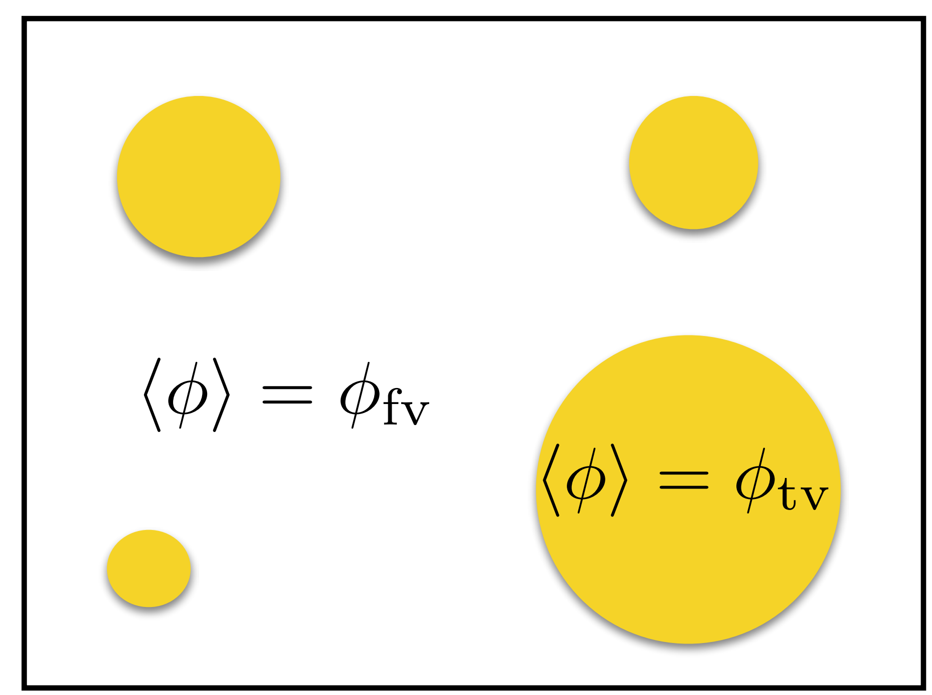


Transition from false to true via tunnelling. Bubble can nucleate anywhere, with nucleation rate per unit volume:

$$\frac{\Gamma}{\mathcal{V}} = Ae^{-B} \qquad B = S(\phi_b) - S(\phi_{\rm fv})$$

Growth of bubble via classical equation of motion

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2\right)\phi = \frac{\partial}{\partial\phi}V(\phi)$$



Methods to calculate bubble nucleation:

- Thin-wall approximation
- Polygon approximation
- over/undershoot method
- **Neural-Net approach** [Piscopo, MS, Waite '19]

[Guada, Maiezza, Nemevsek '18]

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.

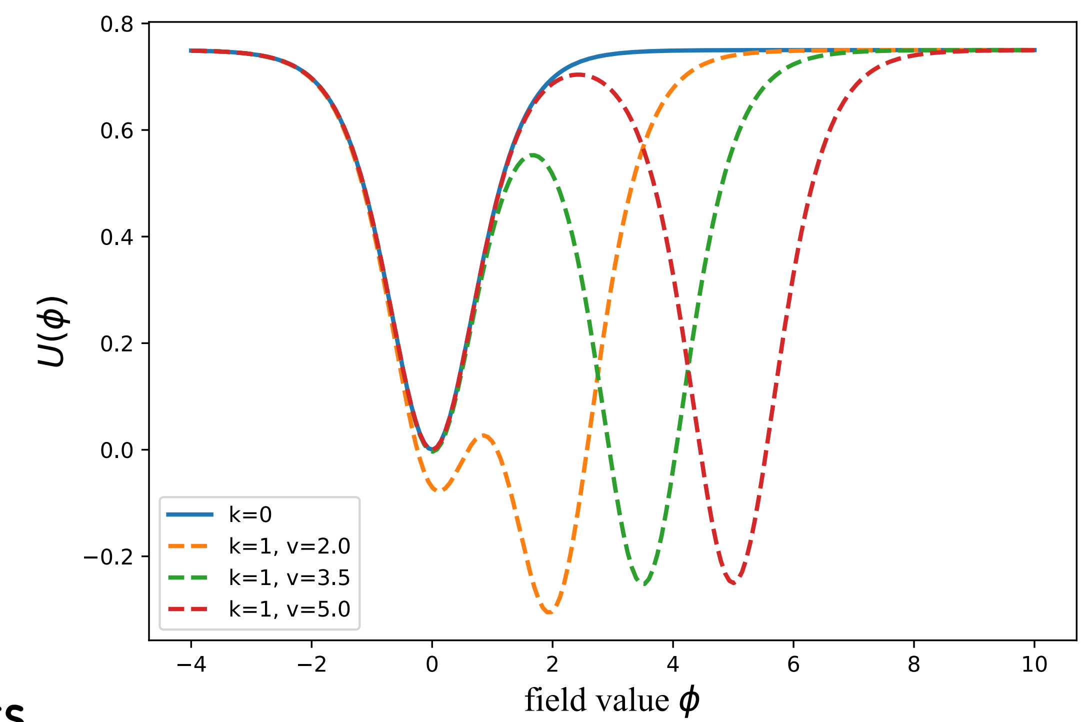
- Choose a potential of interest:

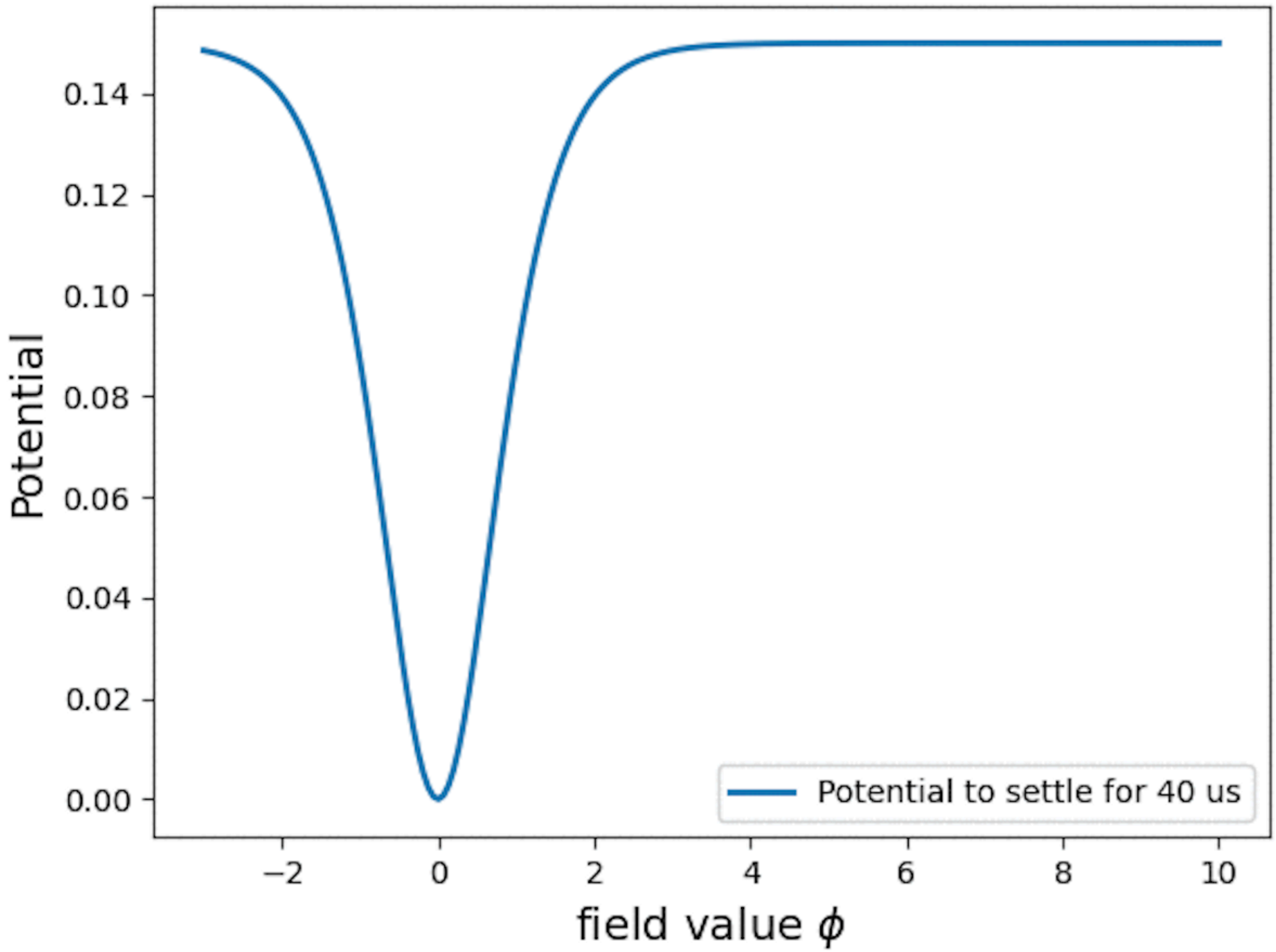
$$U(\phi) = \frac{3}{4}\tanh^2\phi - k(t)\,\text{sech}^2\left(c(\phi - v)\right)$$

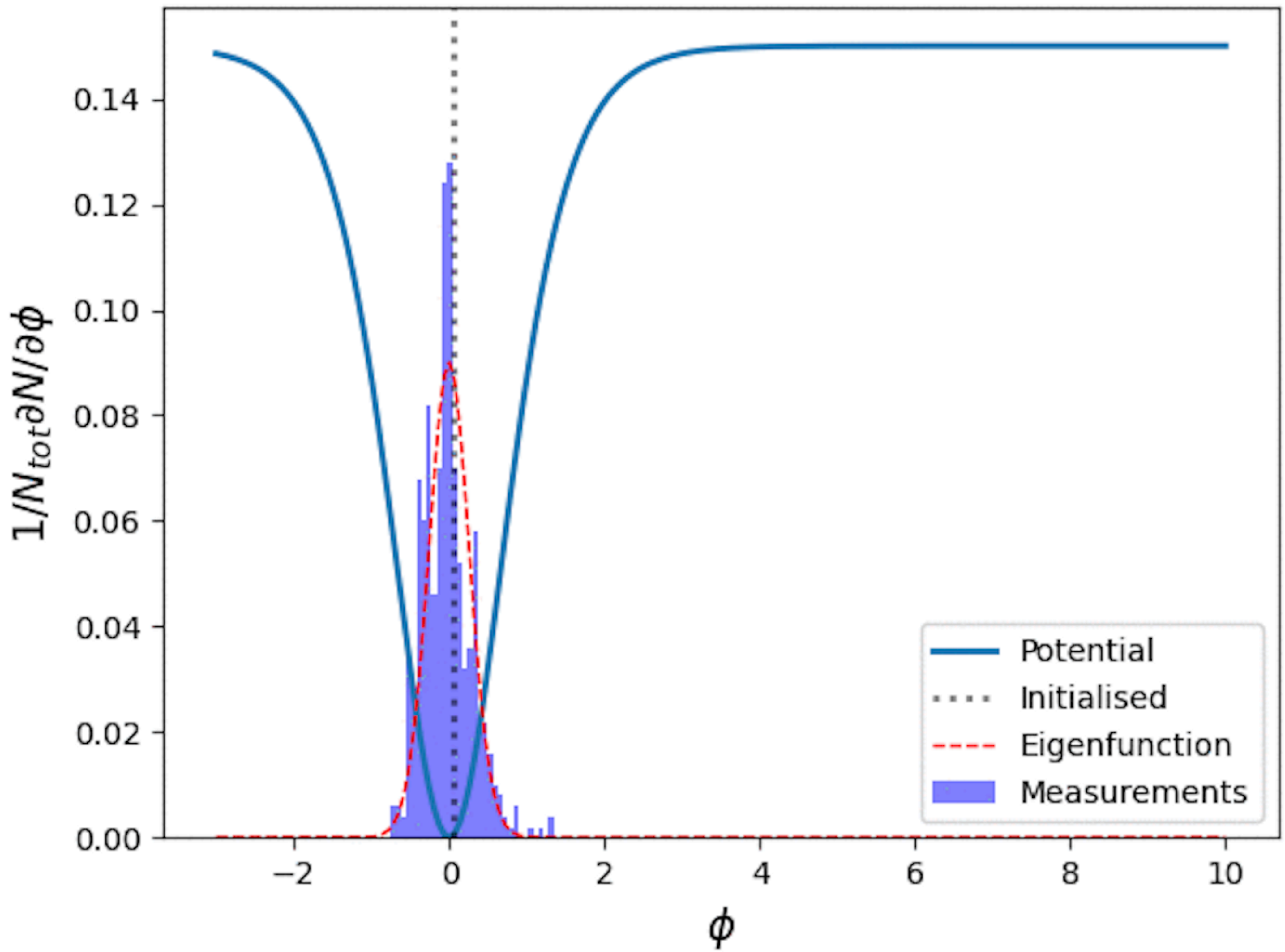
time dependent

where $\phi = \eta/\eta_0$

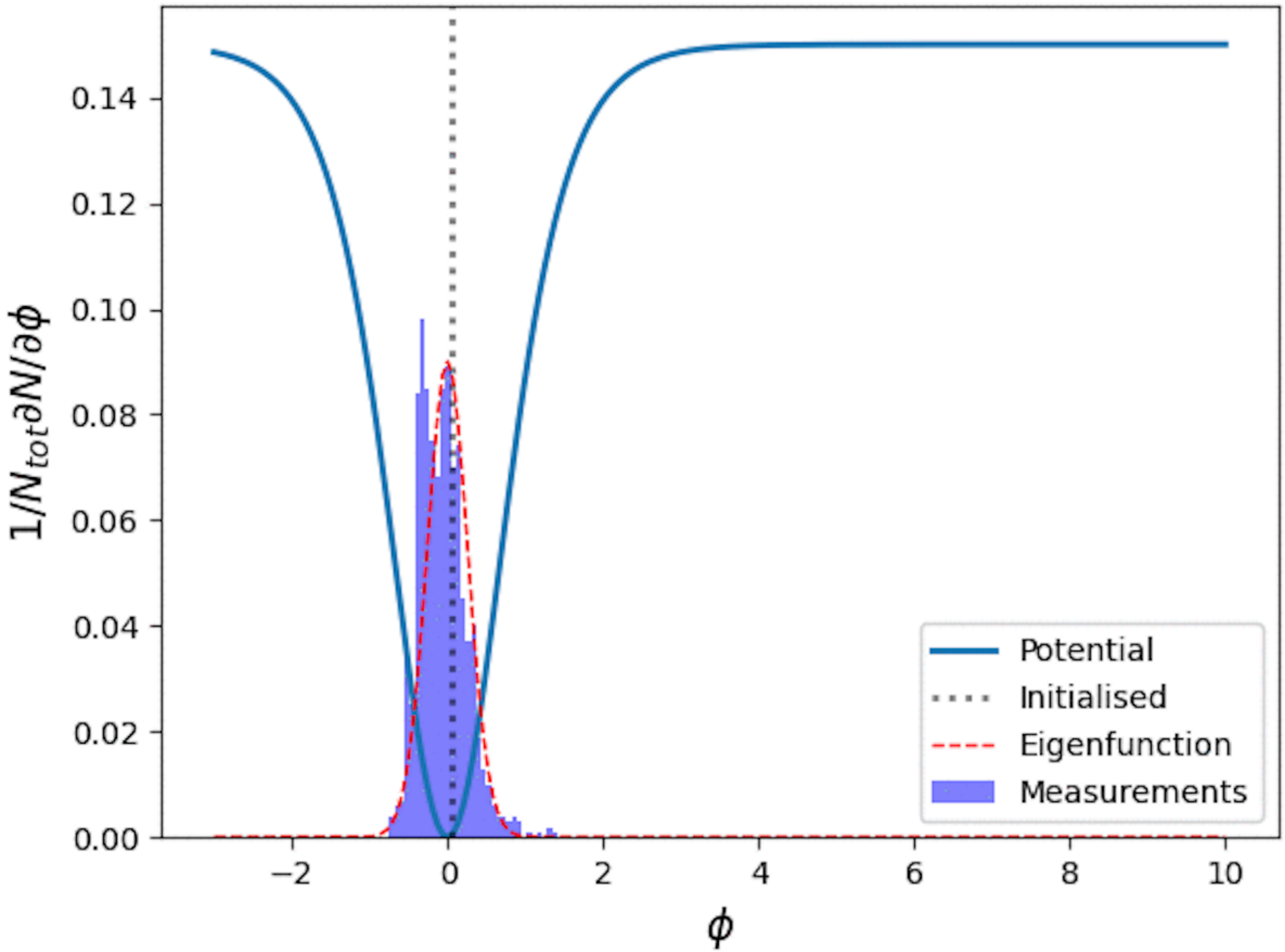
$\phi(t)$ is the field and c, v are dimless constants



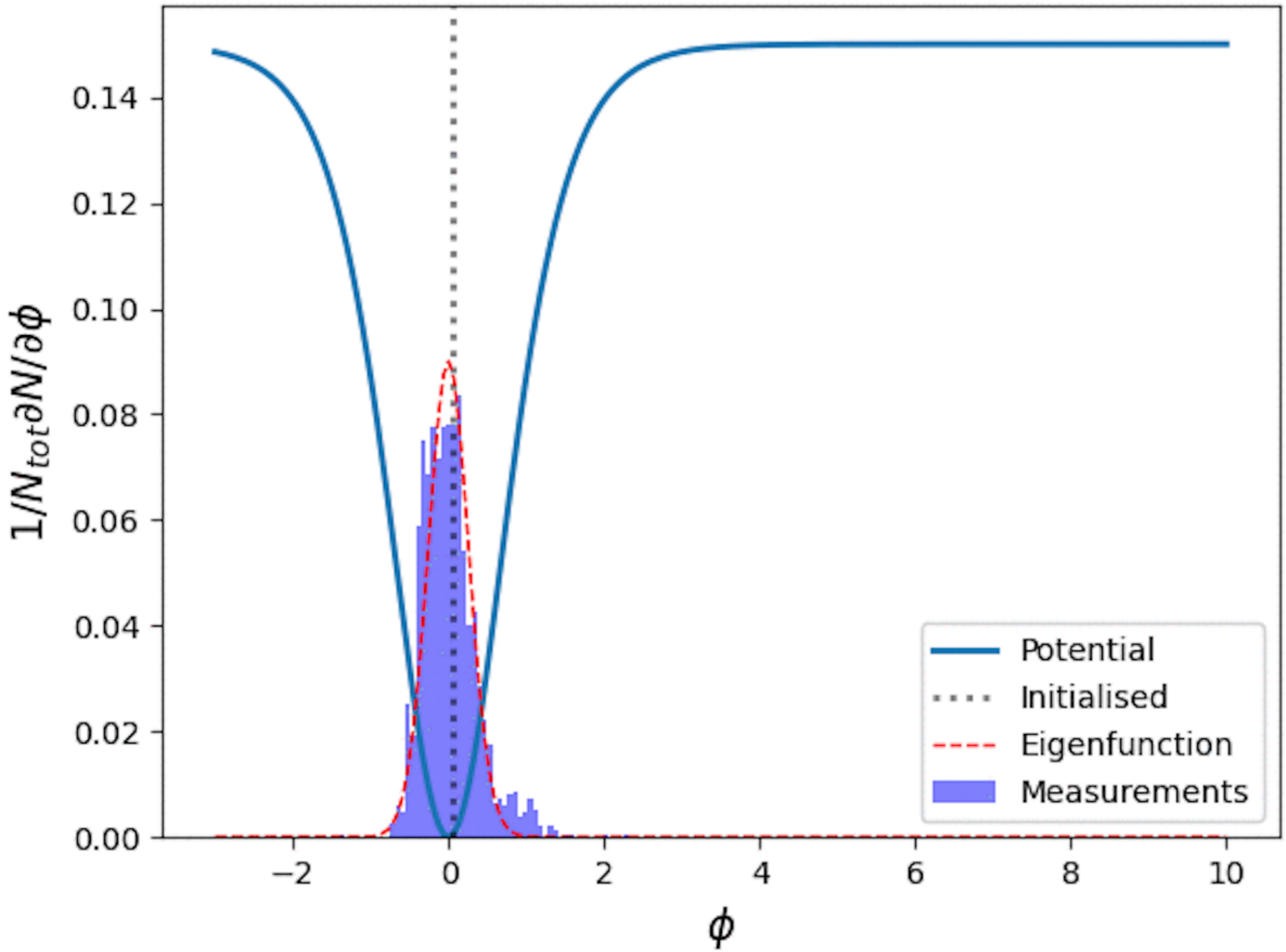

0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Potential
−2
0
2
4
6
8
10
field value ϕ
Potential to settle for 40 us



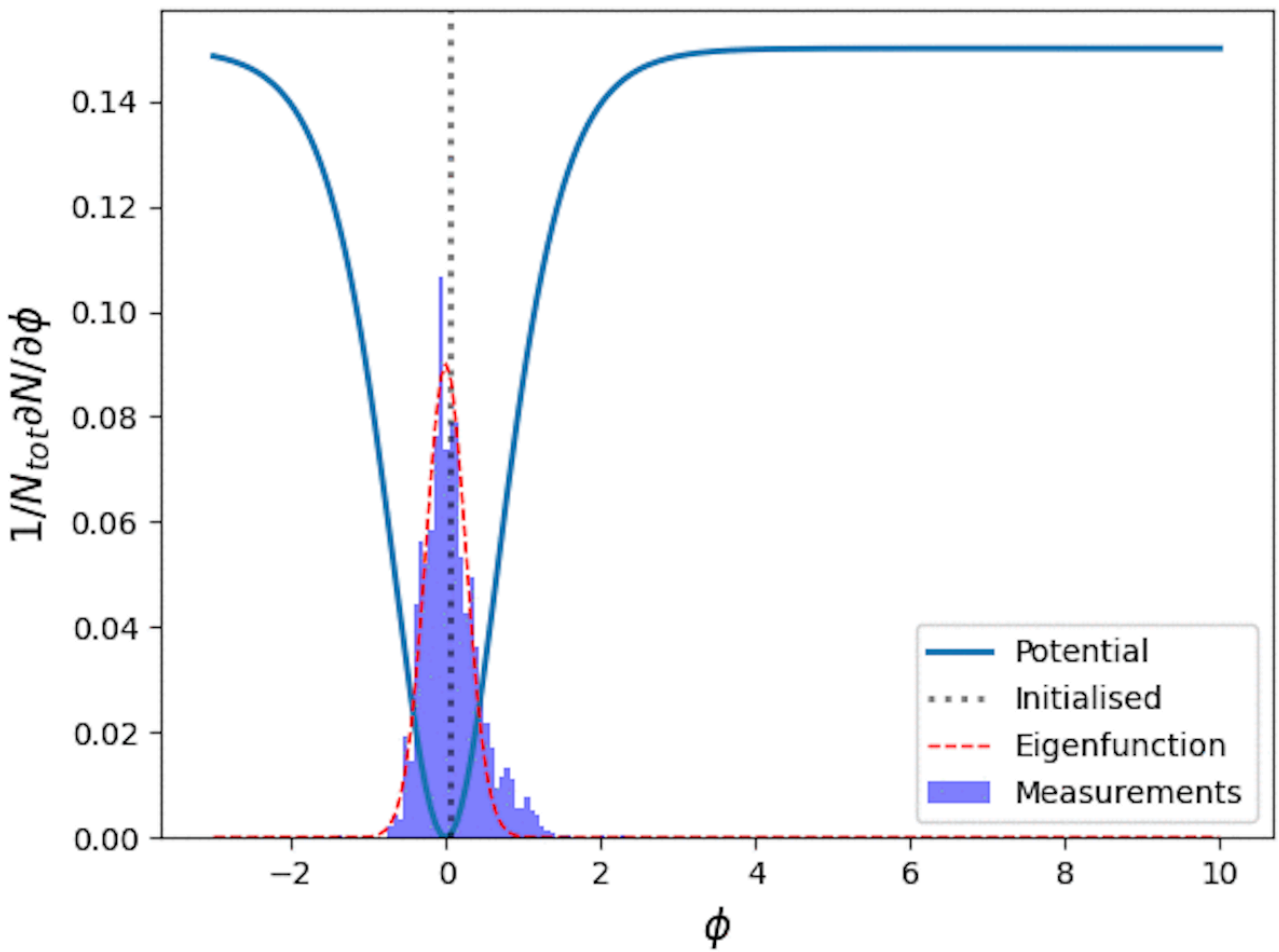
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$1/N_{tot} \partial N/\partial \phi$
−2
0
2
4
6
8
10
ϕ
Potential
Initialised
Eigenfunction
Measurements



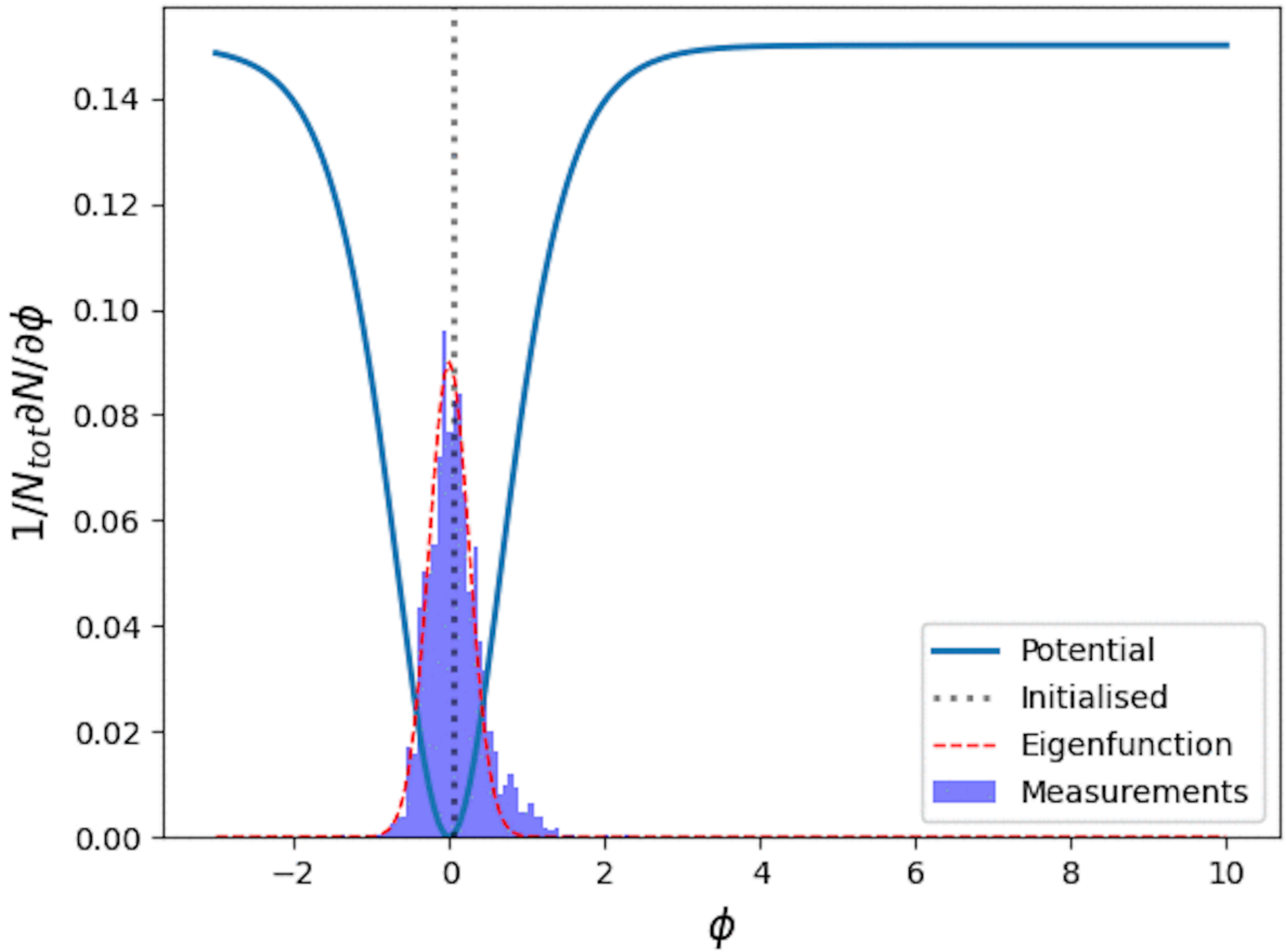
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$1/N_{tot}\partial N/\partial\phi$
−2
0
2
4
6
8
10
ϕ
Potential
Initialised
Eigenfunction
Measurements



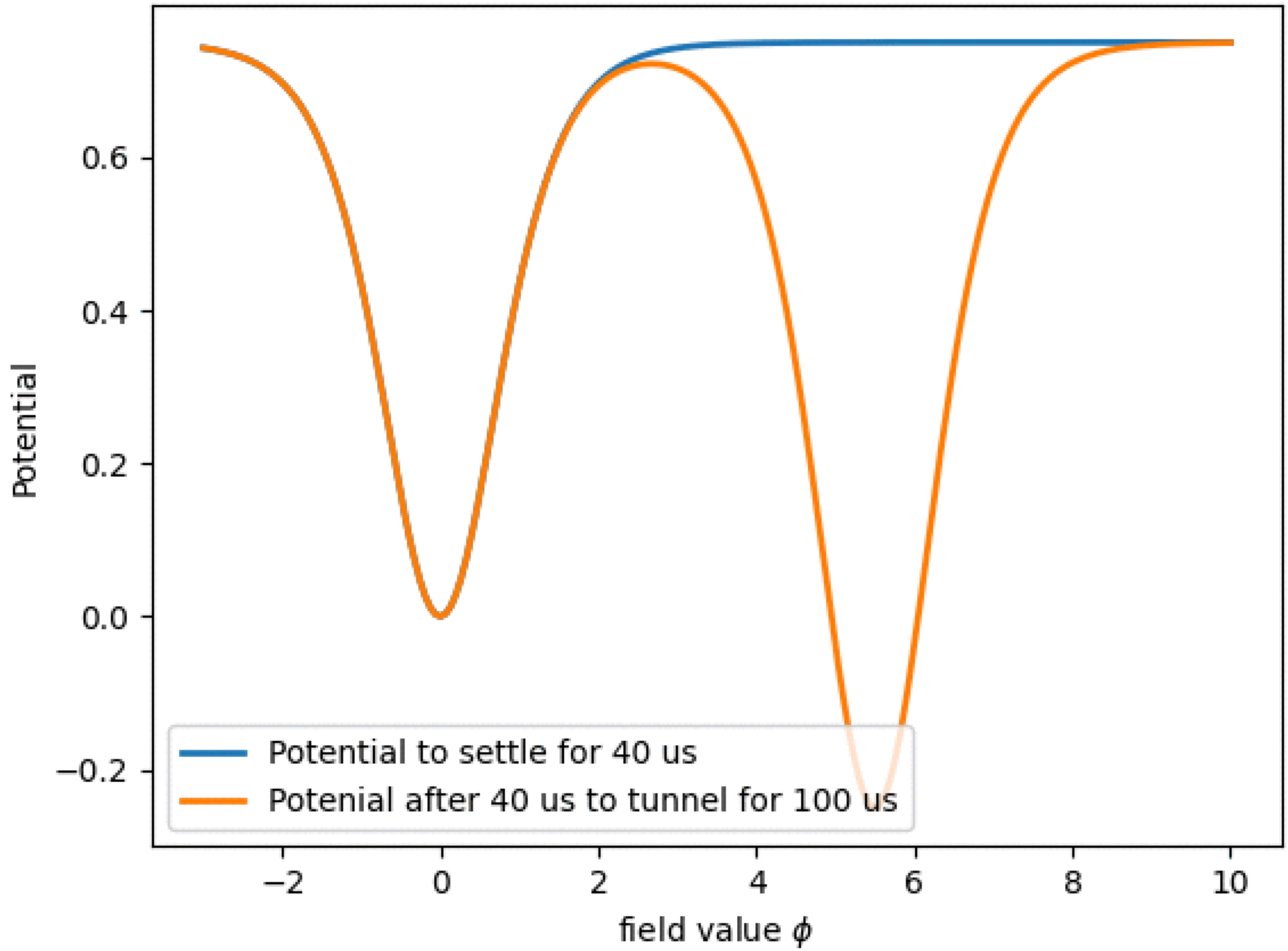
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$1/N_{tot}\partial N/\partial\phi$
−2
0
2
4
6
8
10
ϕ
Potential
Initialised
Eigenfunction
Measurements



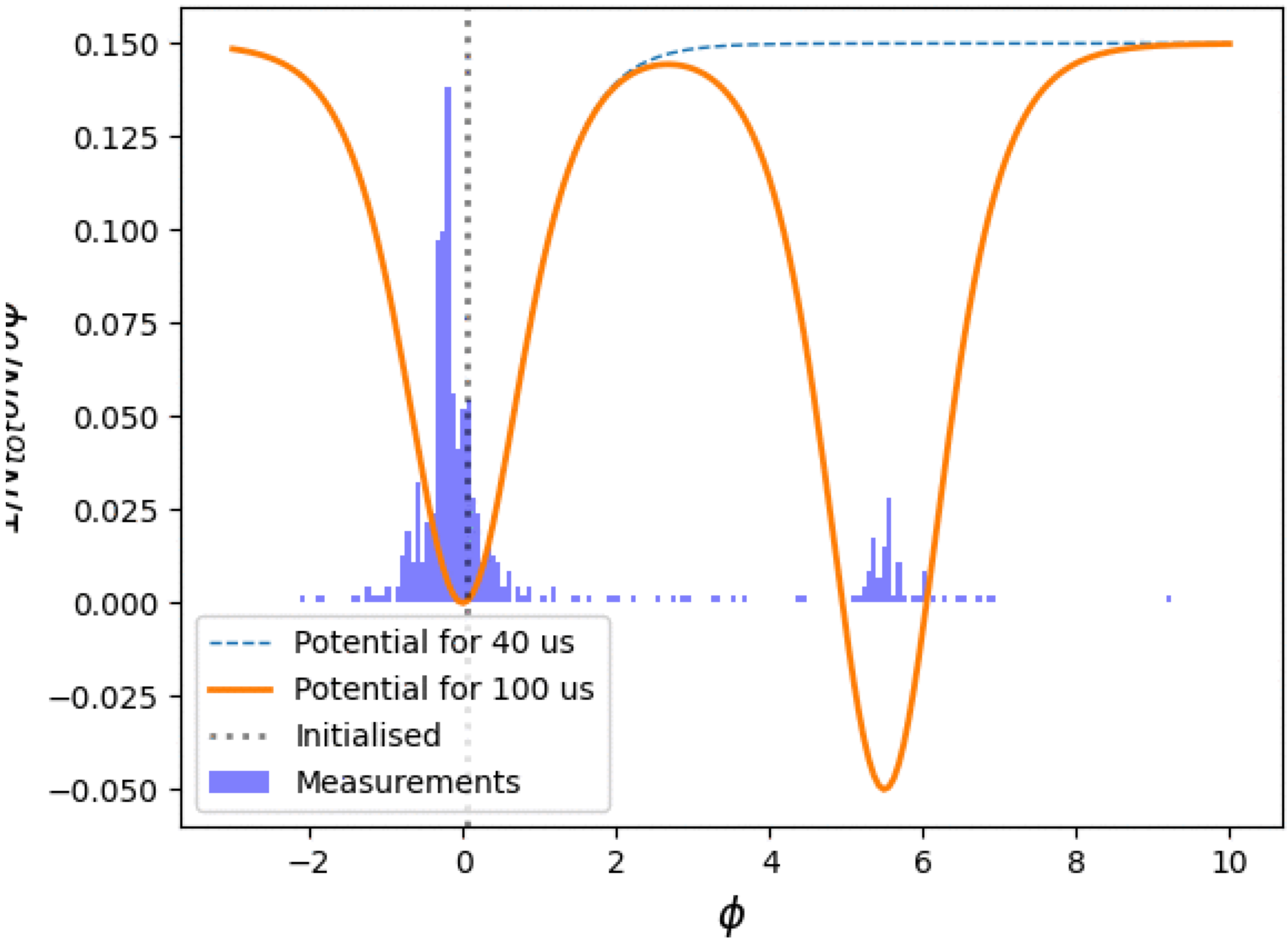
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$1/N_{tot}\partial N/\partial\phi$
−2
0
2
4
6
8
10
ϕ
Potential
Initialised
Eigenfunction
Measurements

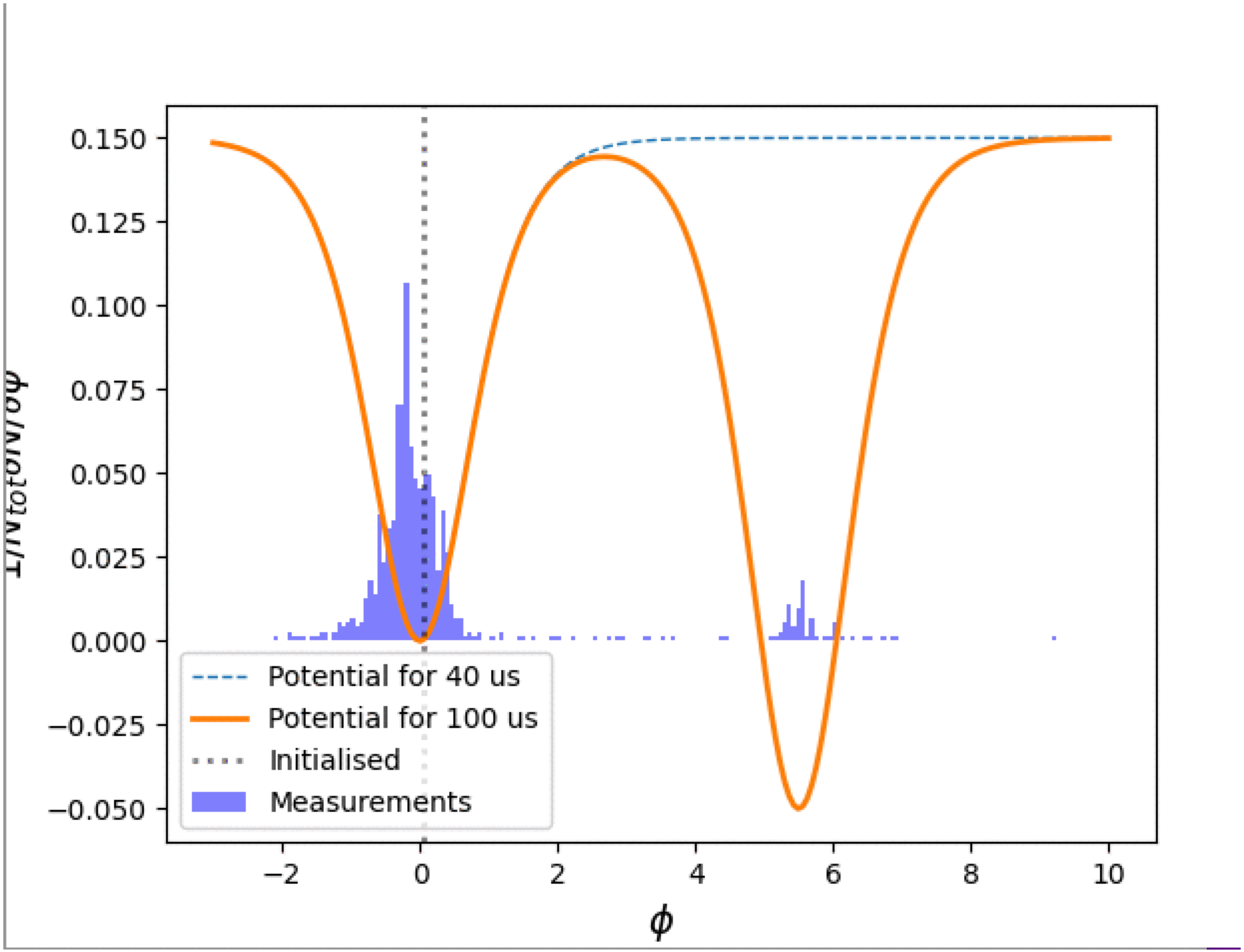


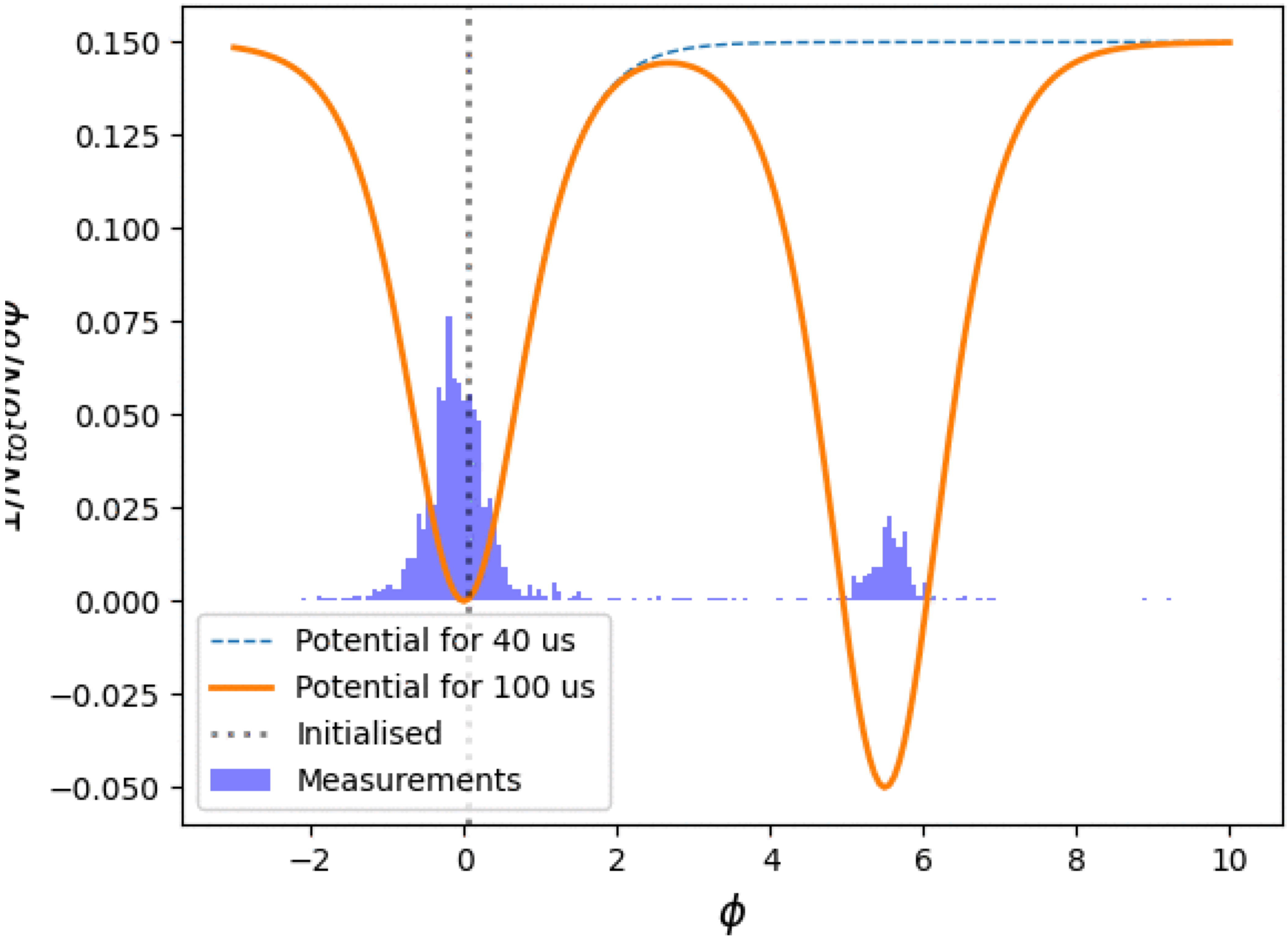
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$1/N_{tot}\partial N/\partial\phi$
−2
0
2
4
6
8
10
ϕ
Potential
Initialised
Eigenfunction
Measurements



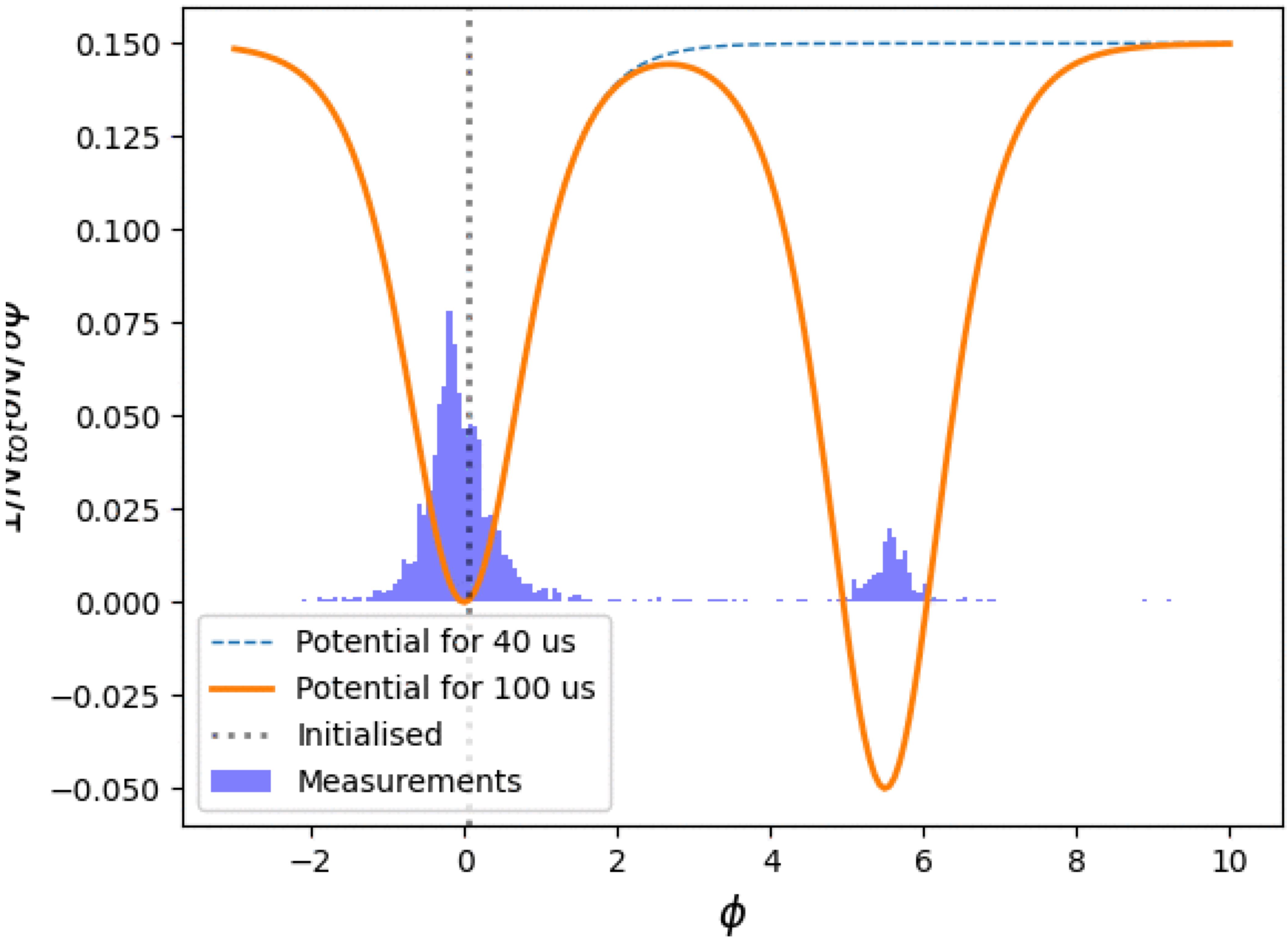
Potential
0.6
0.4
0.2
0.0
−0.2
Potential to settle for 40 us
Potenial after 40 us to tunnel for 100 us
−2
0
2
4
6
8
10
field value ϕ


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
Potential for 40 us
Potential for 100 us
Initialised
Measurements

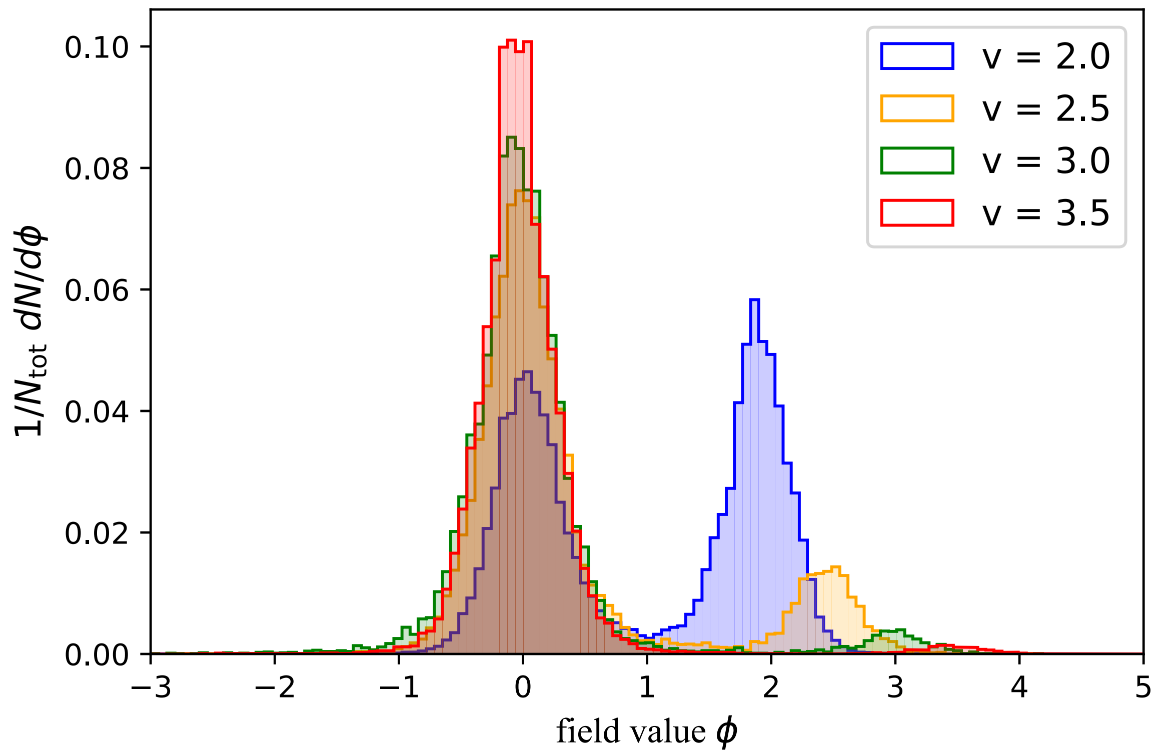

0.150
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
−0.050
−2
0
2
4
6
8
10
ϕ
Potential for 40 us
Potential for 100 us
Initialised
Measurements



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
Potential for 40 us
Potential for 100 us
Initialised
Measurements


0.150
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
−0.050
Potential for 40 us
Potential for 100 us
Initialised
Measurements
−2
0
2
4
6
8
10
ϕ

Results: it decays with v as expected

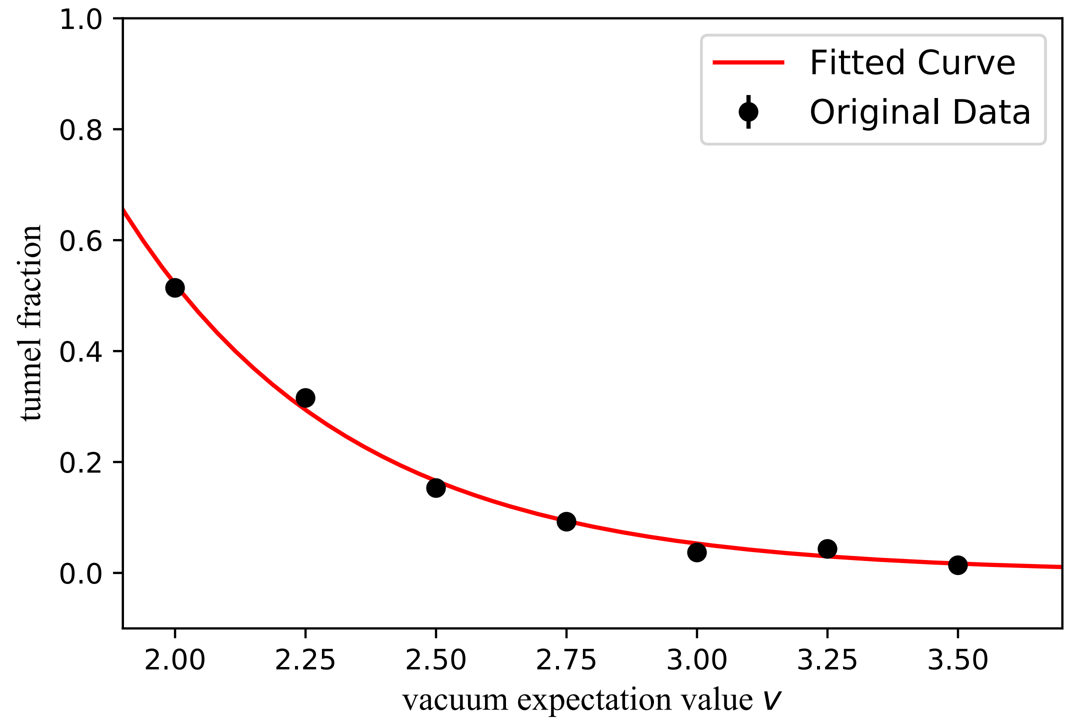


Perform tunnelling for

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

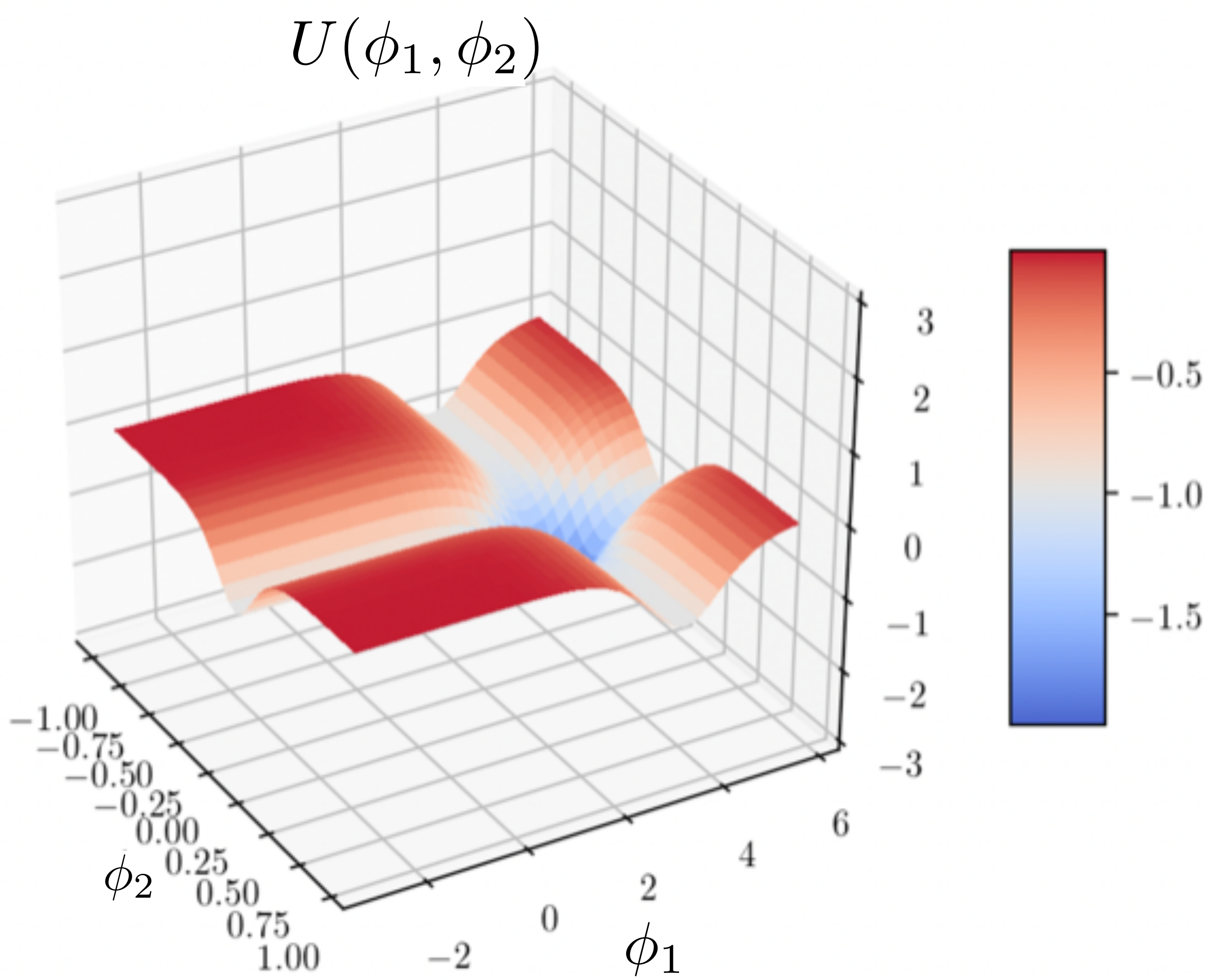
Theory: $\log\Gamma = 3.0 \times (1.66 - v)$

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



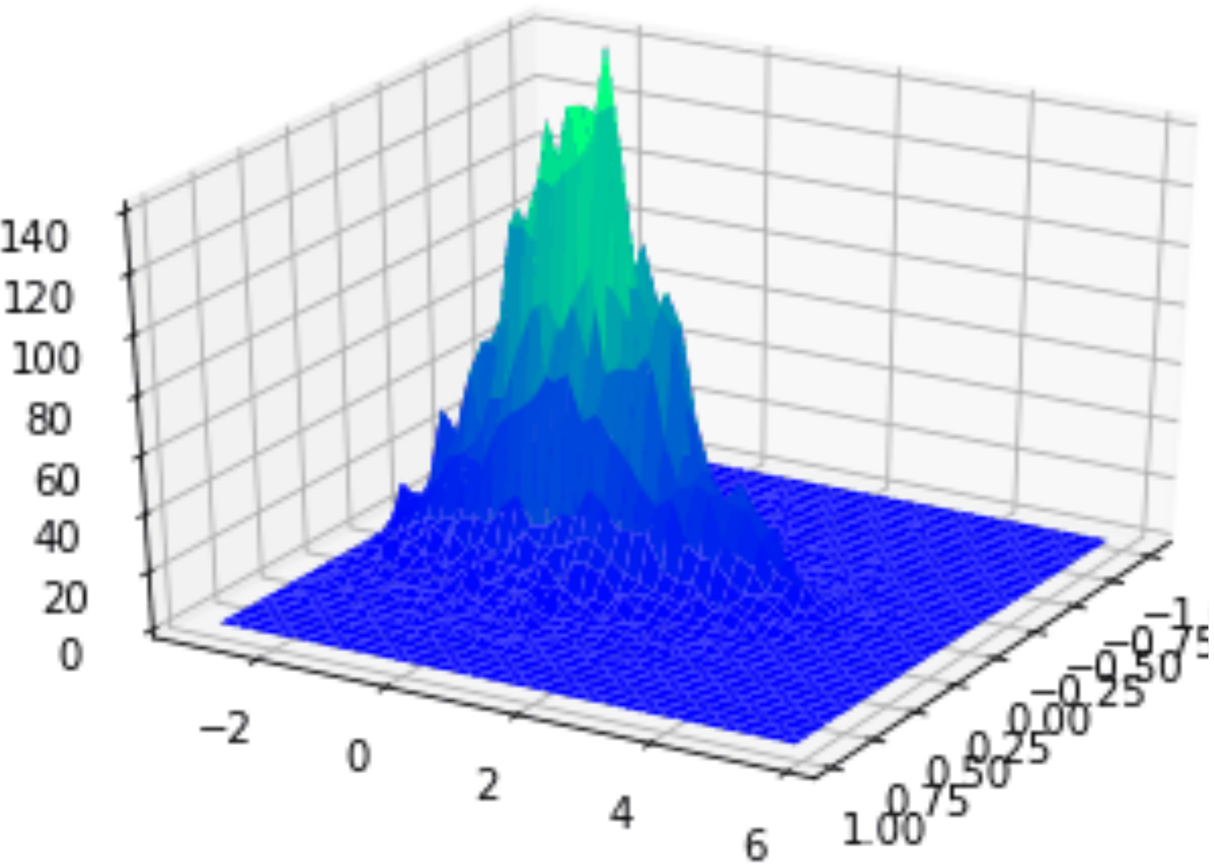
Also dynamics has characteristic behaviour. For example it still “tunnels” to the bottom of a potential even if there is no barrier: i.e. the wave function leaks across, rather than rolling as a lump —

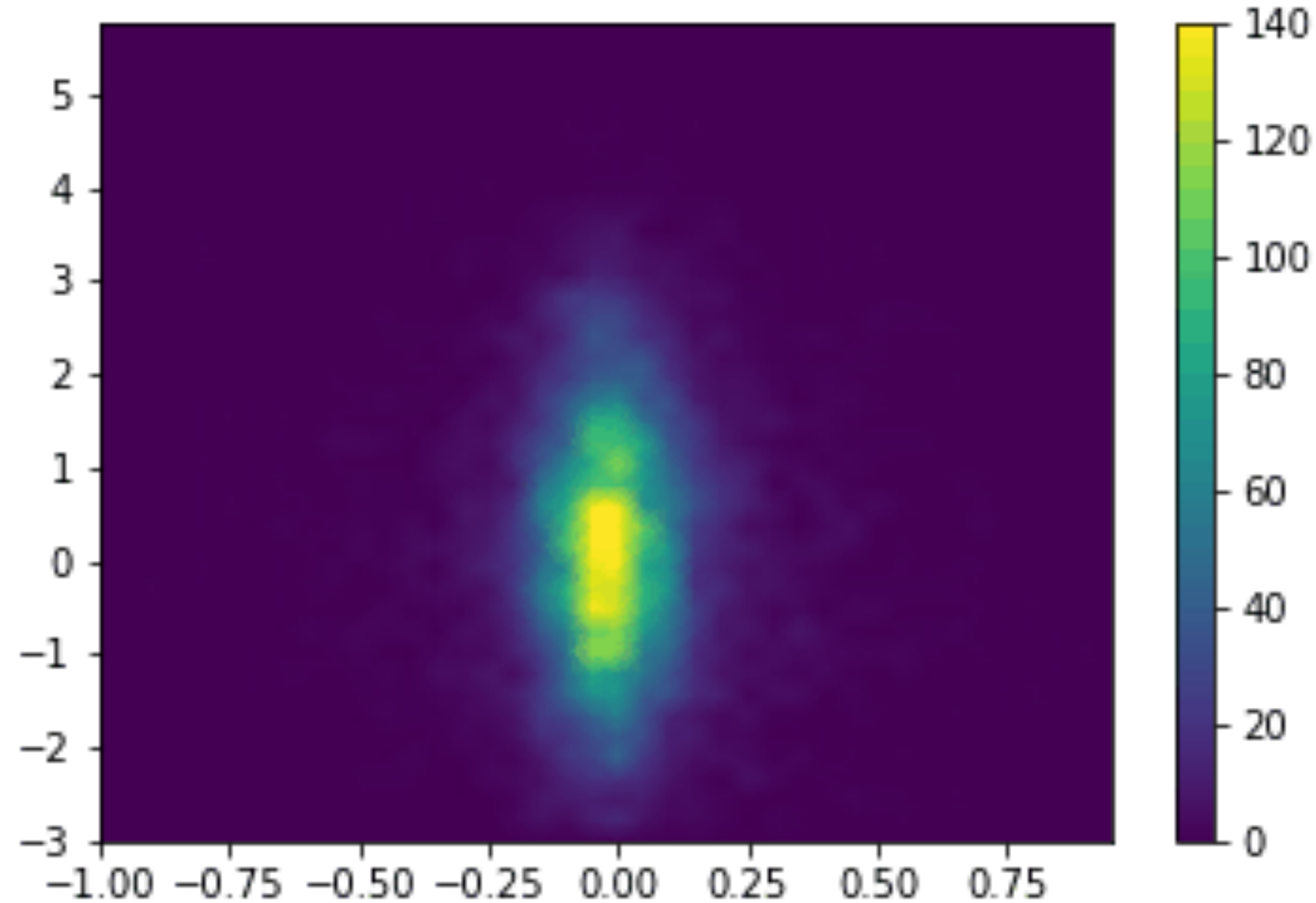
Multiple measurements on the quantum annealer:



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 —

Multiple measurements on the quantum annealer:



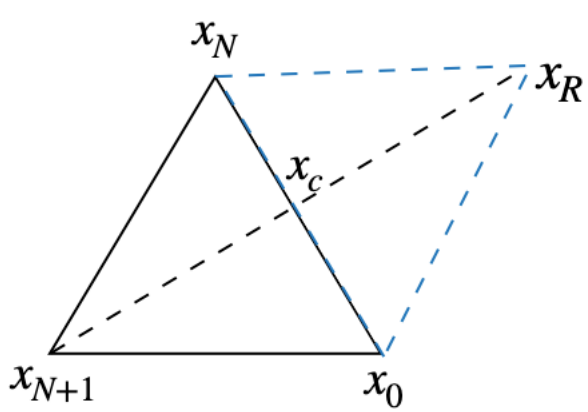


Example 2: Optimisation comparison quantum vs classical

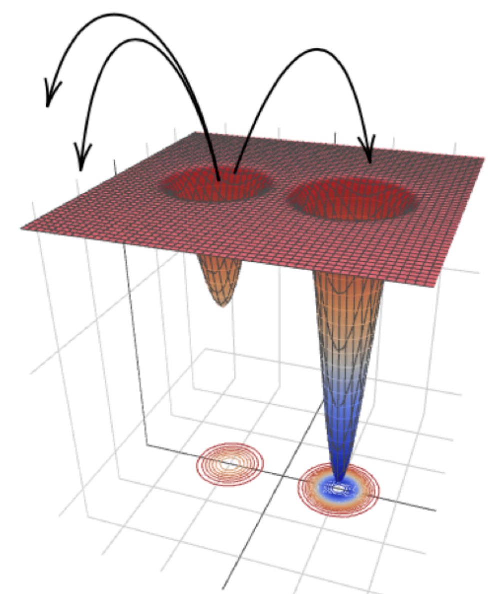
gradient descent

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

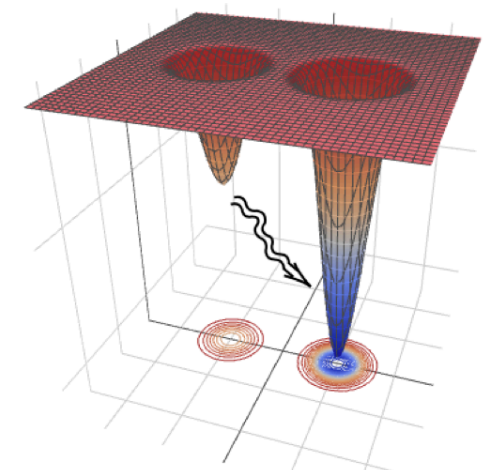
Nelder-Mead



Thermal Annealing

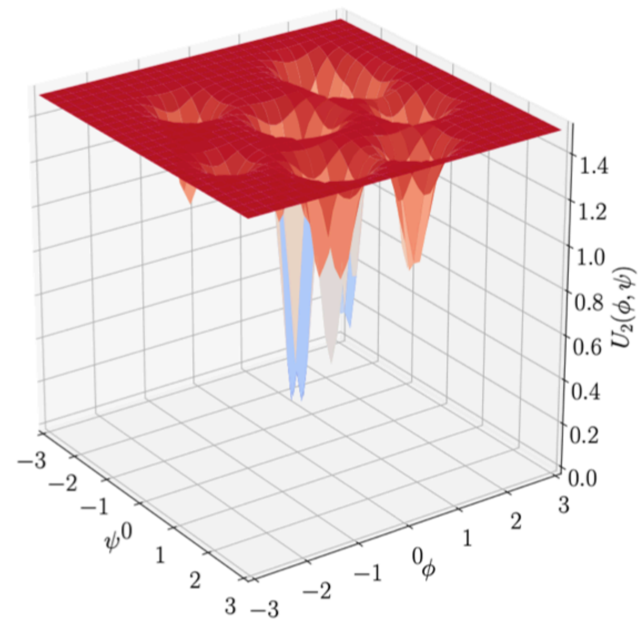


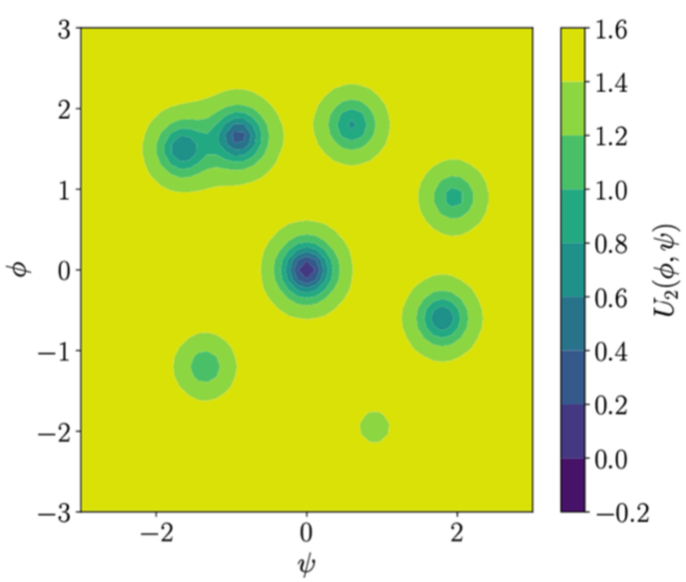
Quantum Annealing



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

Multi-well potential



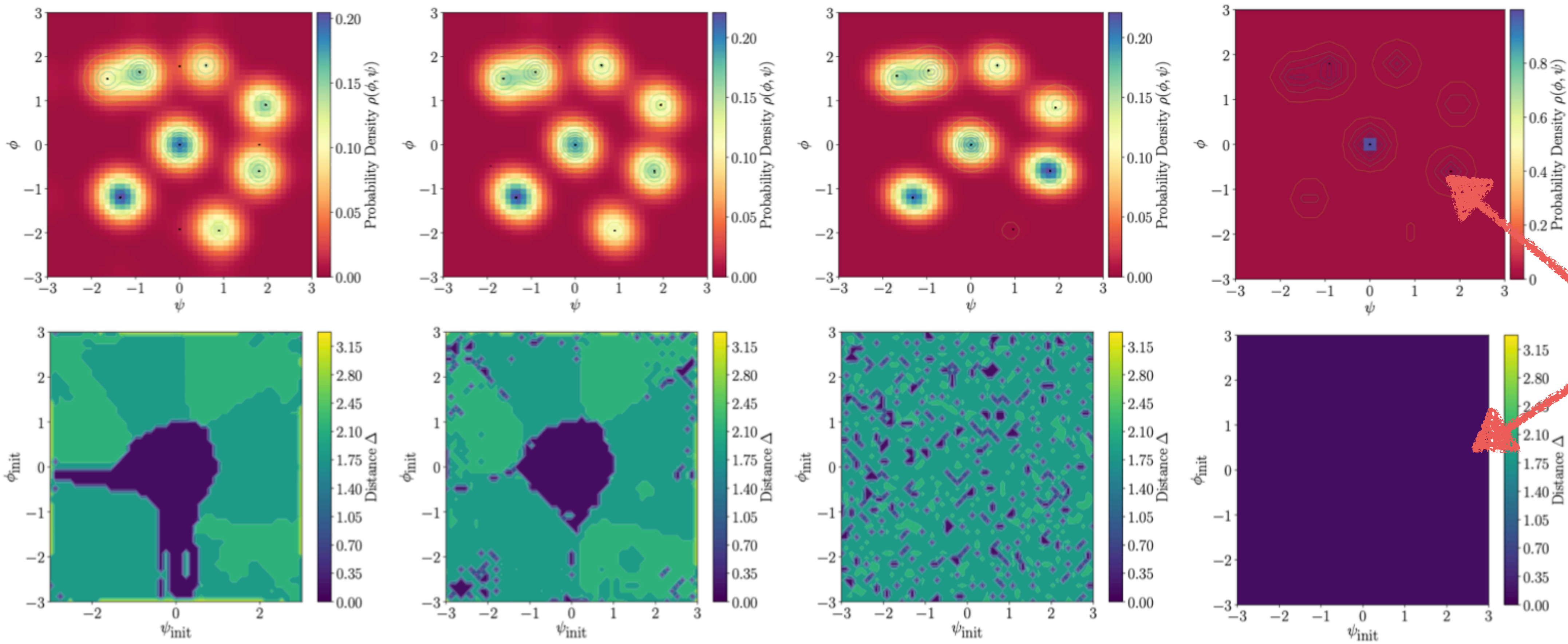


Results for Multi-well potential

[Abel, Blance, MS '21]

- 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



(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 significant quantum advantage

Completely Quantum Neural Networks

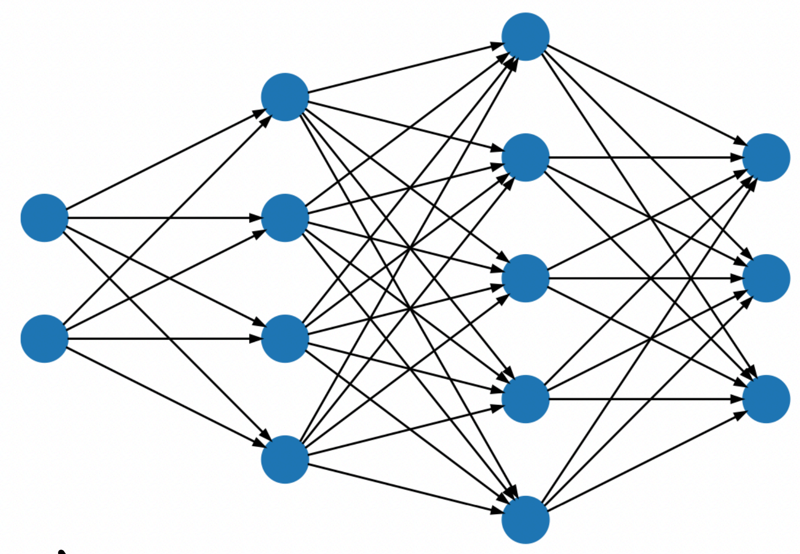
Structure of node i, in layer L $$L_i(x) = g\left(\sum_i w_{ij} x_i + b_i\right)$$

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)

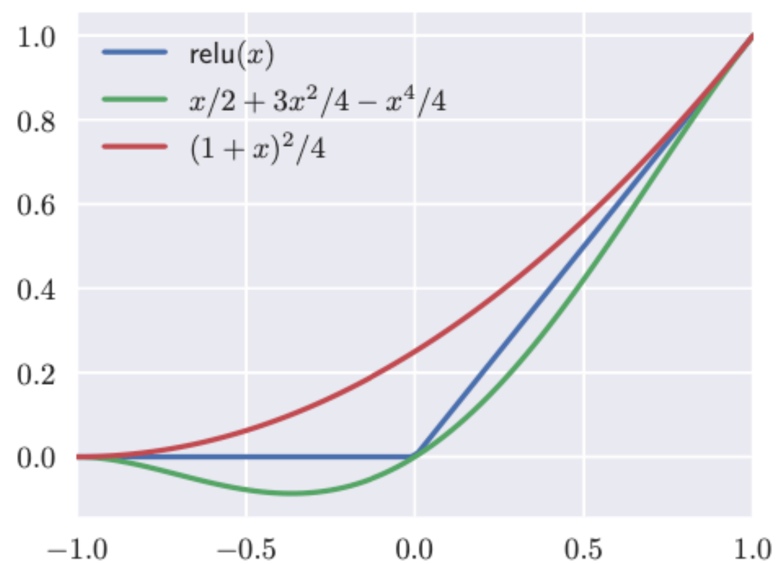


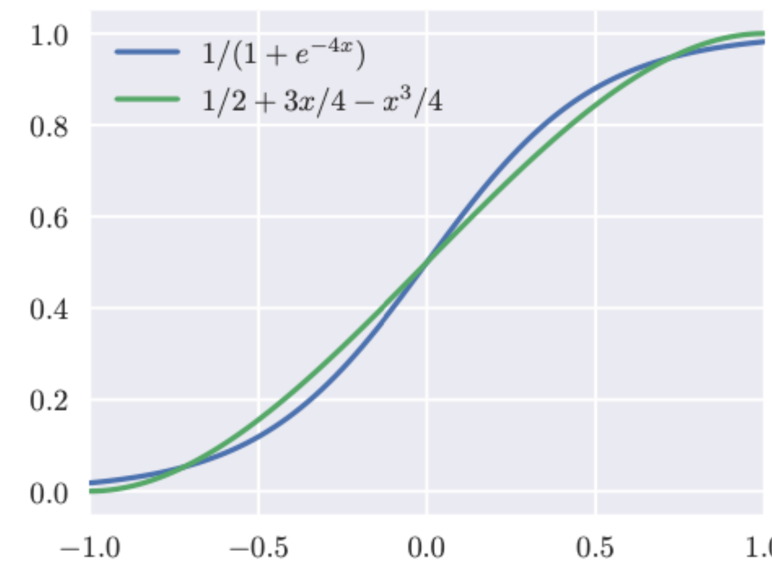
Details about encoding - our approach

Use QUBO encoding to write $\tau_\ell = \frac{1}{2}(\sigma_\ell + 1) \longrightarrow \tau_\ell = 0, 1$

encode weights of NN $p \sim w_{ij}^{(k)},\ b_i^{(k)}$ as binary $p = -1 + \frac{1}{1-2^{-N_b}} \sum_{\alpha=0}^{N_b-1} 2^{-\alpha} \tau_\alpha^p$

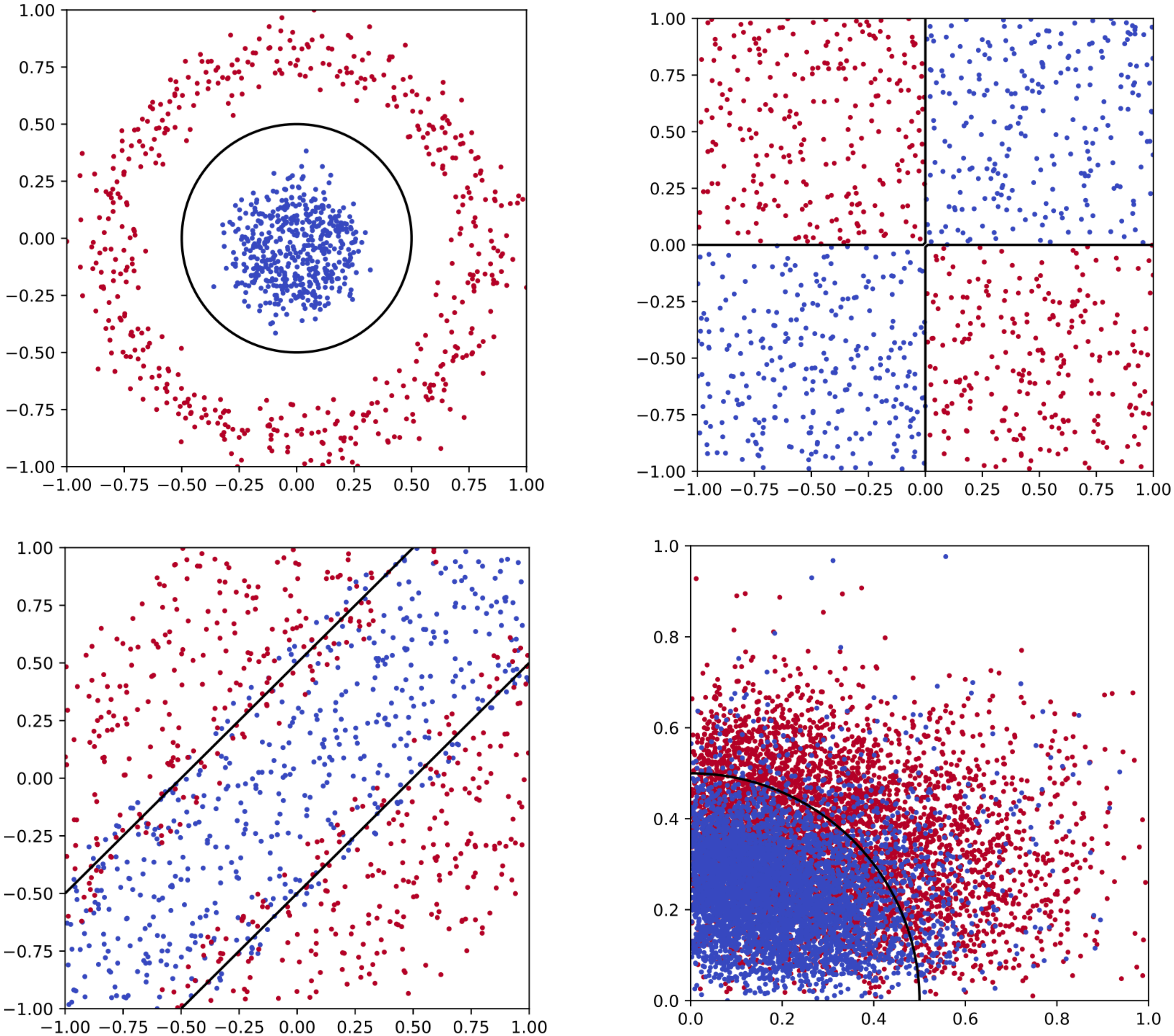
Express activation function as a polynomial:



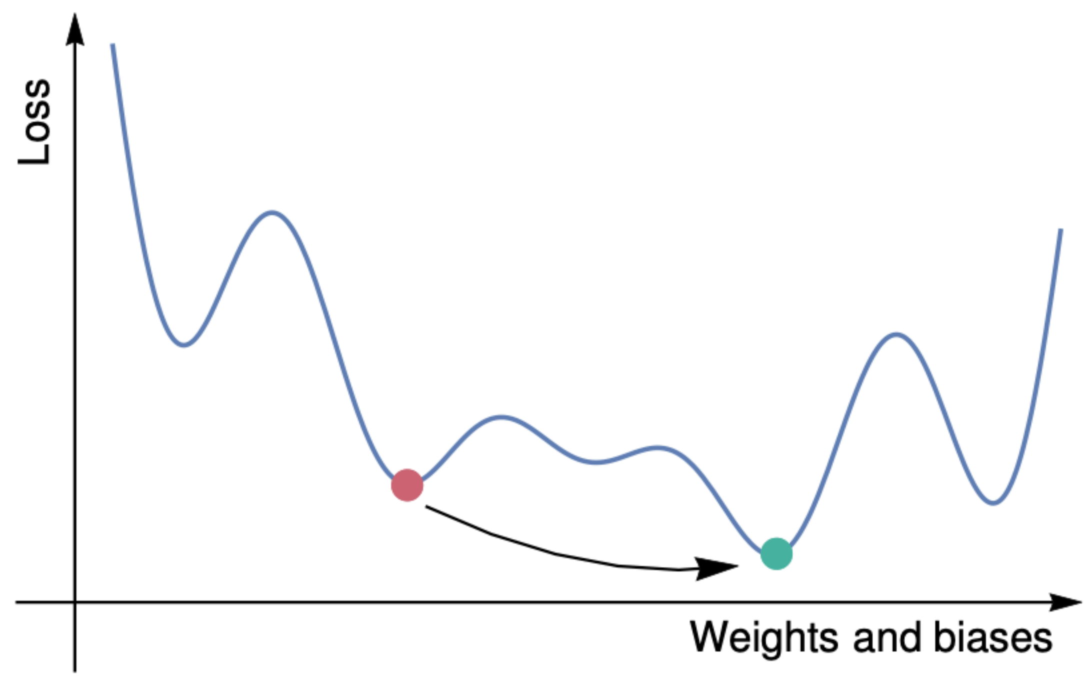


Express loss function using binary-form weights.

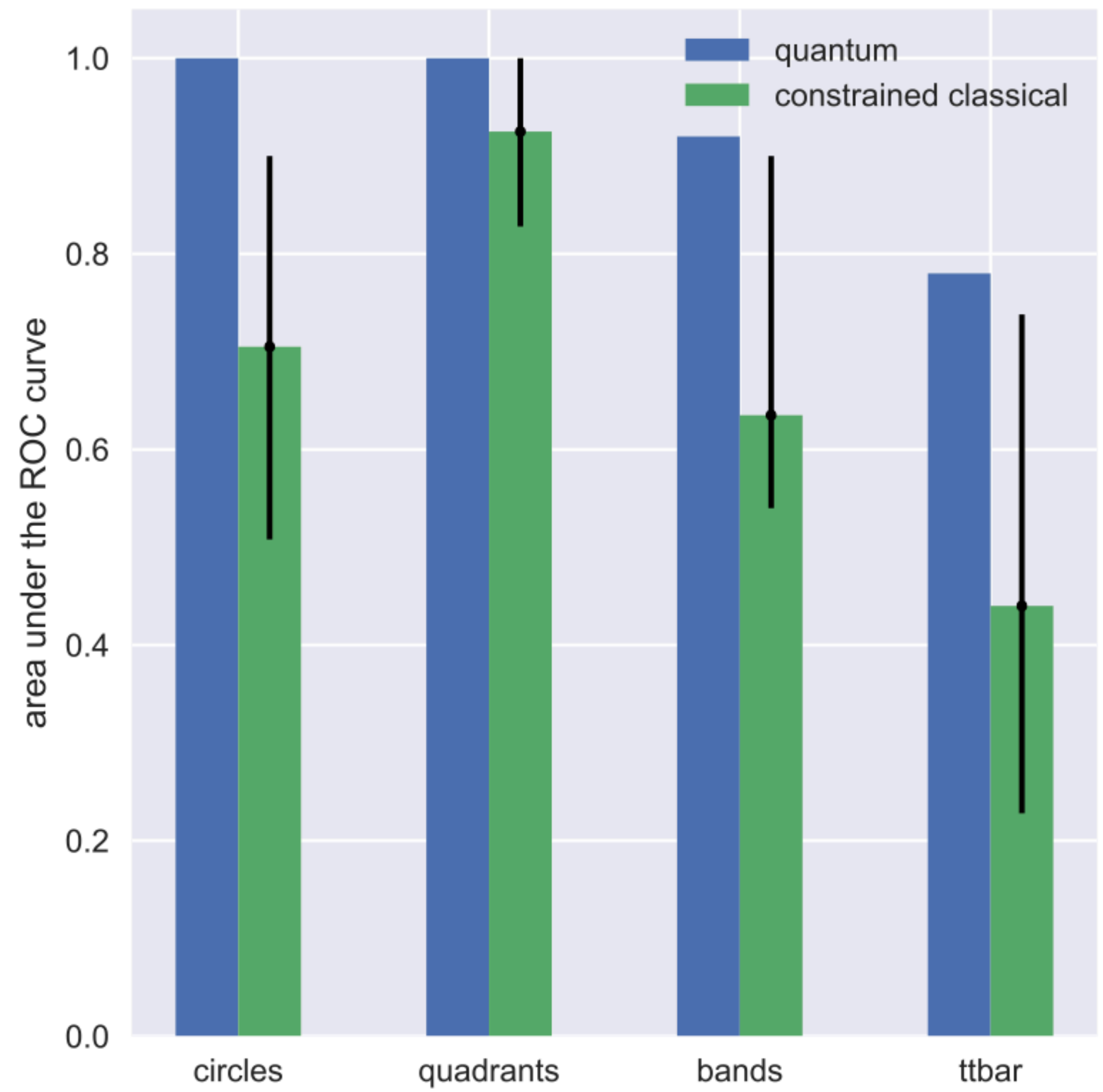
Problem: need to convert to Ising model → quadrature procedure


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−1.00 −0.75 −0.50 −0.25 0.00 0.25 0.50 0.75 1.00
1.0
0.8
0.6
0.4
0.2
0.0
0.0 0.2 0.4 0.6 0.8 1.0

Completely Quantum Neural Networks



Reliable and very fast ground-state finder of loss function



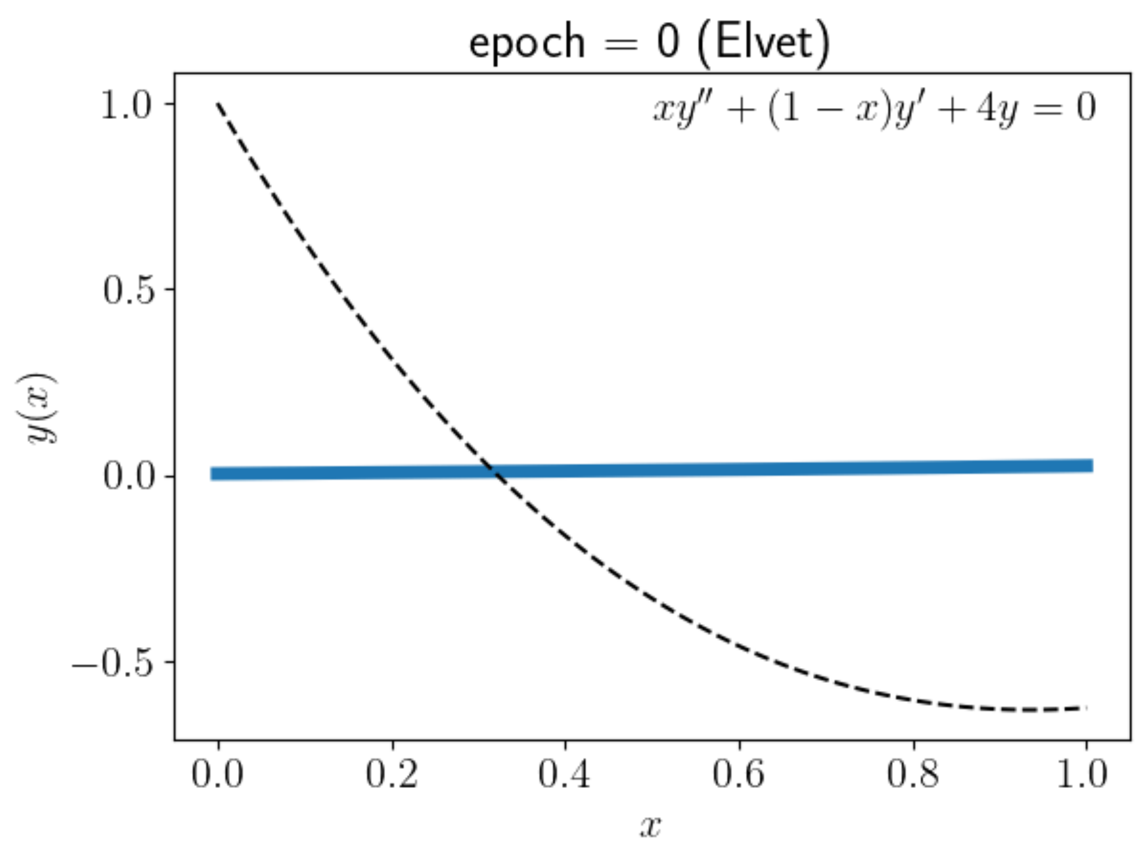
Optimal network training

QADE: Solving differential equations with a quantum annealer

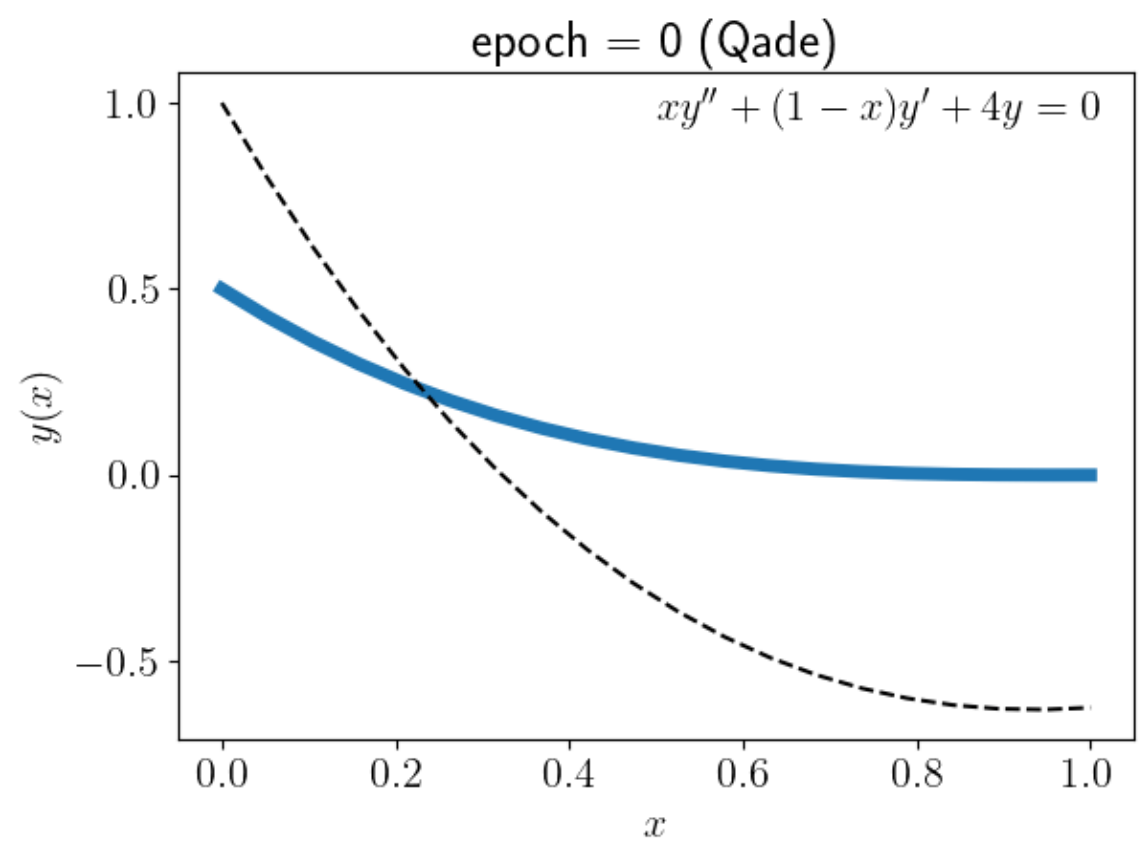
[Criado, MS '22]

Example Laguerre differential equation:

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

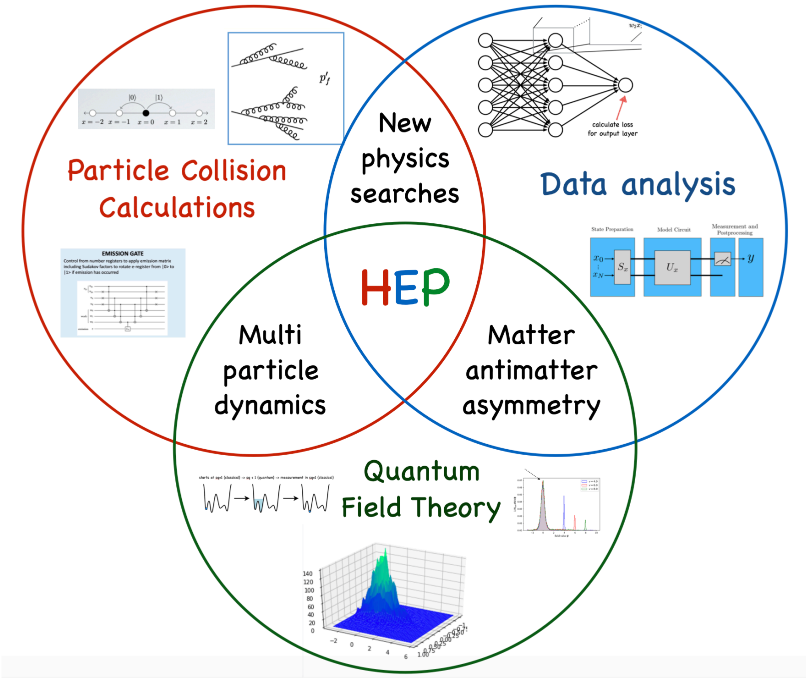


Classical Neural Network

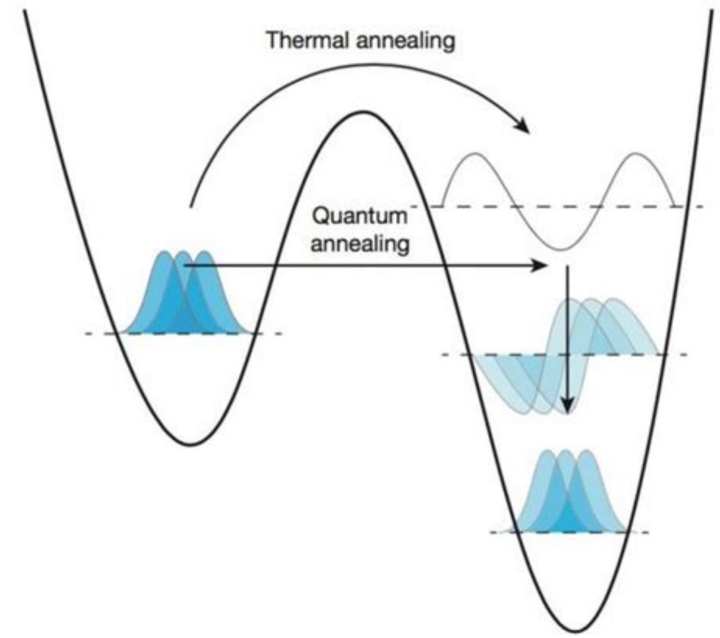


Quantum algorithm

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



Summary



- **Quantum computers** are near-to-midterm future experiments that can be used to **address problems in high-energy physics**, shown here particle collisions, data analysis and quantum field theory

- Exciting research area that rapidly expands, supported through private and public sector. Many algorithms to be invented.

- For many more exciting applications, need development of technical realisation of quantum computers (fault tolerance, coherence, operations,…)