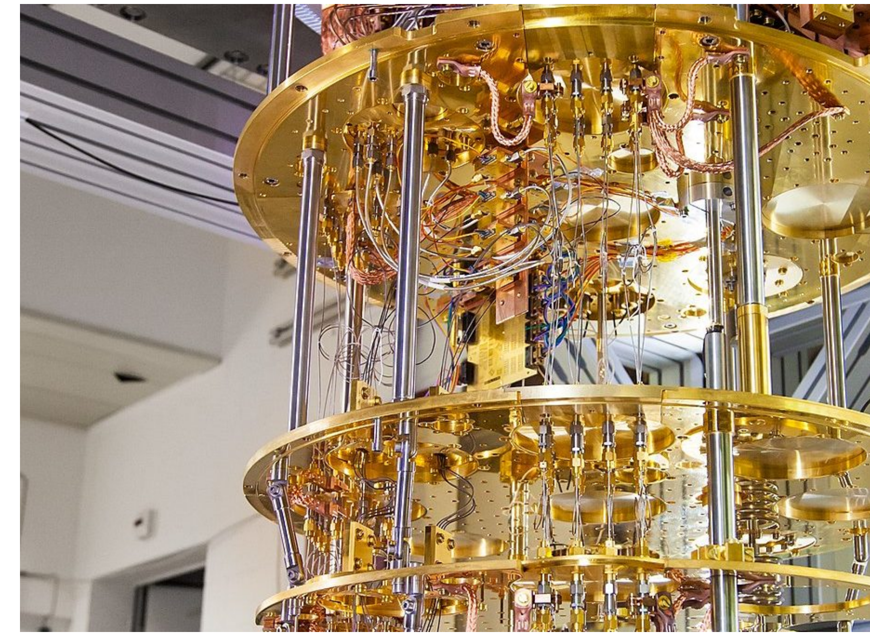
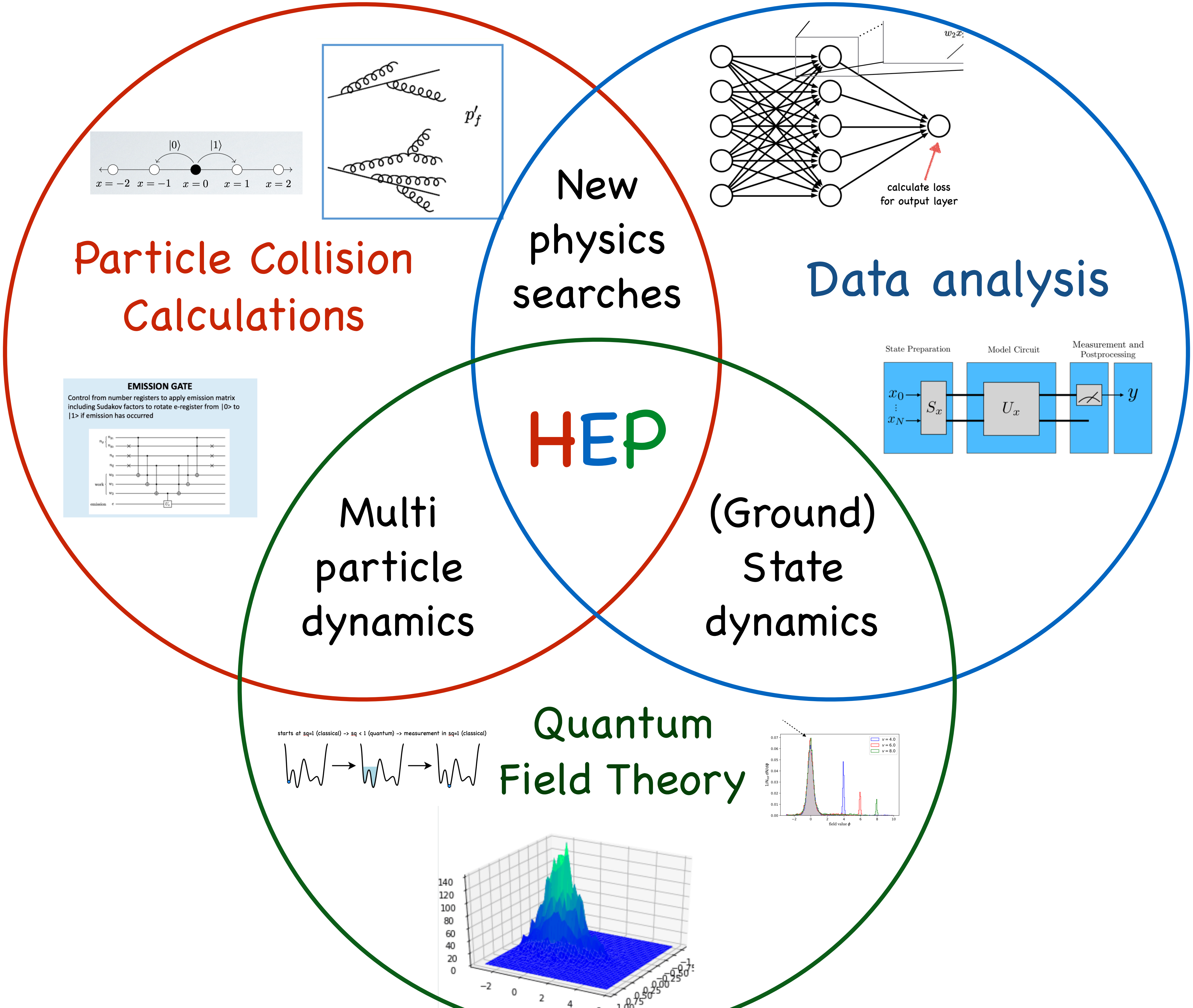


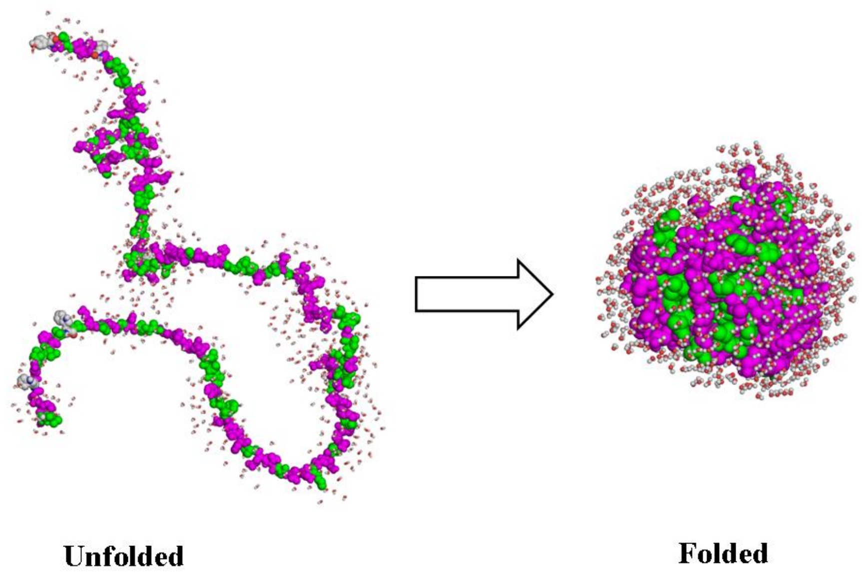
Quantum Algorithms for High-Energy Physics and Data Analysis

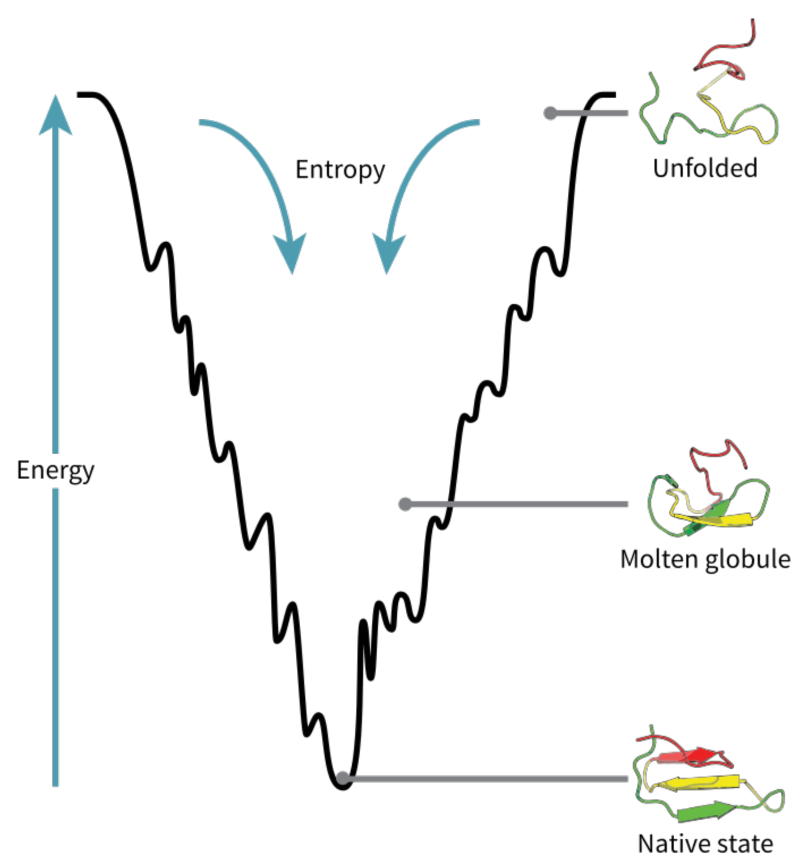
Michael Spannowsky

IPPP, Durham University


Particle Collision Calculations
New physics searches
Data analysis
HEP
Multi particle dynamics
(Ground) State dynamics
Quantum Field Theory
$|0\rangle$ $|1\rangle$
$x=-2$ $x=-1$ $x=0$ $x=1$ $x=2$
p'_f
calculate loss for output layer
State Preparation
Model Circuit
Measurement and Postprocessing
x_0 x_N S_x U_x y
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
starts at sq=1 (classical) -> sq < 1 (quantum) -> measurement in sq=1 (classical)

Protein-folding and Levinthal's Paradox





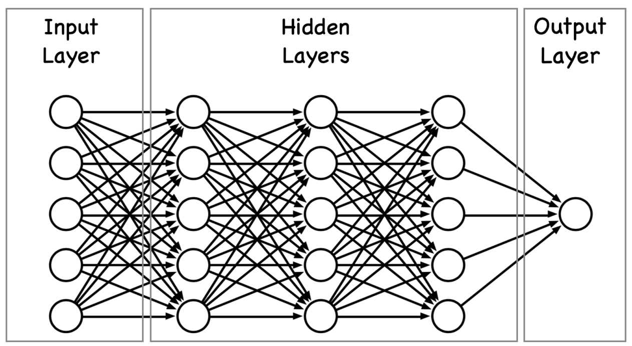
- Elongated proteins fold to same state within microseconds
- Some proteins have 3^{300} conformations
- Levinthal's Paradox (1969):
  Sequential sampling of states would take longer than lifetime of Universe (even if only nanoseconds per state spent)
- Solution: No sequential sampling, but rapid descend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

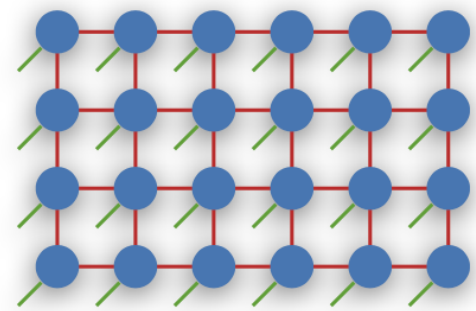
Optimisation is Life

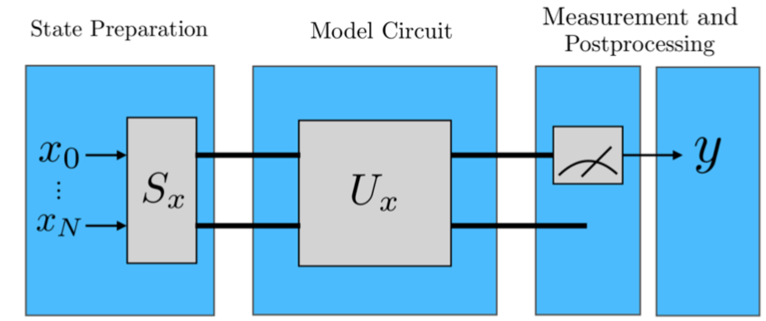
Solution of mathematical problem can be found quickly if encoded in ground state of complex system

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

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

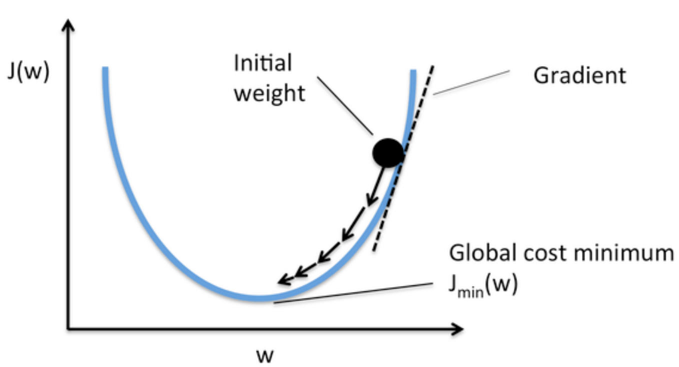
$$B^{s_2}{}_{p_1p_2}\Gamma^{lp_1p_2}{}_{s_2} = f^l(\mathbf{x}^{(\mathbf{n})})$$

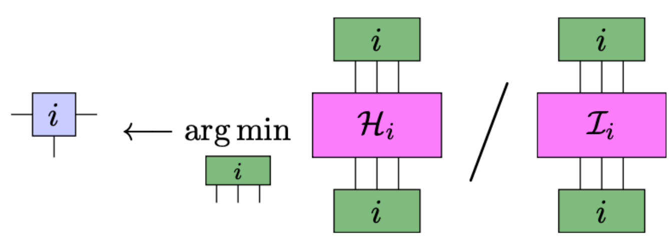
$$\mathcal{L} = L\left(p(l,\mathbf{x}),\ l^{truth}\right)$$

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

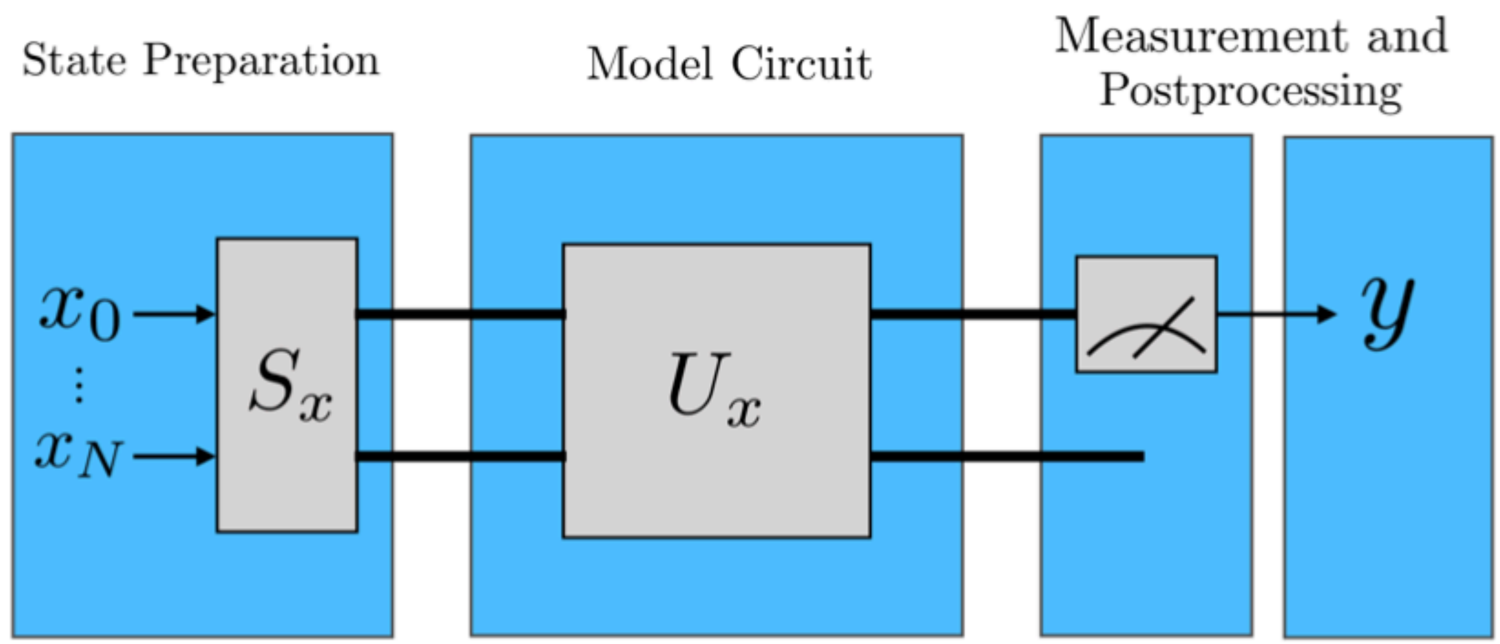
Quantum Machine Learning
with a Variational Quantum Circuit

[McClean et al '16]

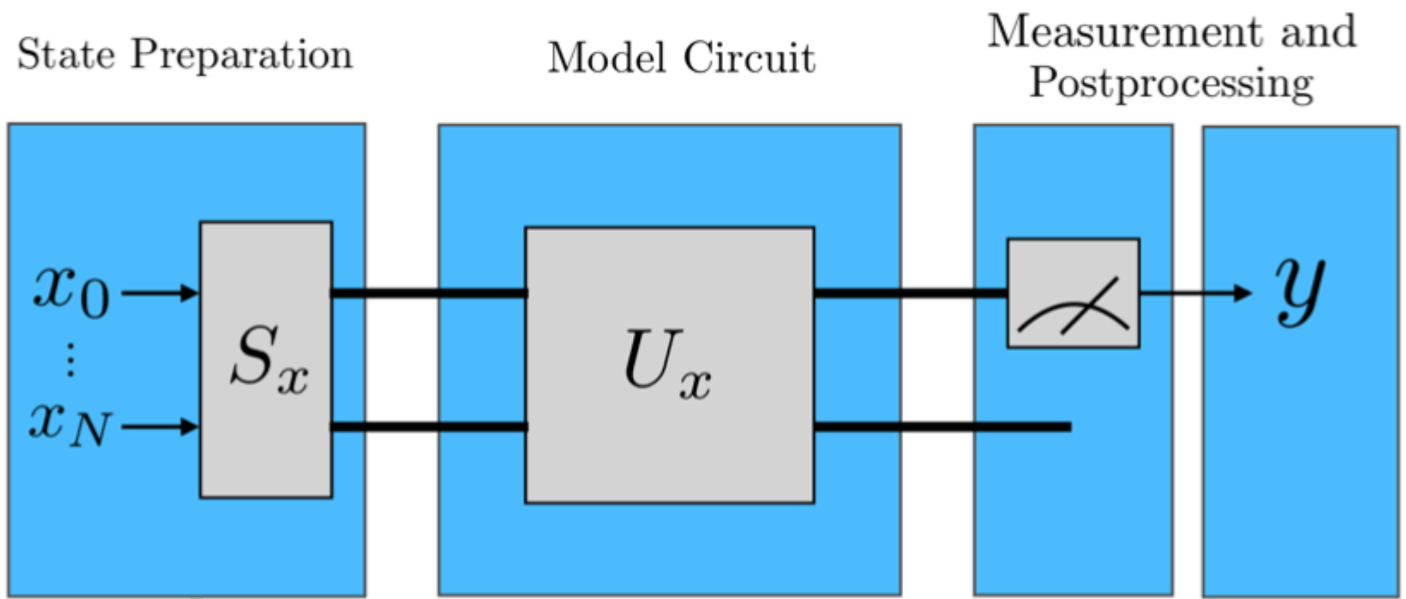
[Farhi, Neven '18]

[Schuld et al '20]

[Blance, MS '20]



Quantum Machine Learning with a Variational Quantum Circuit



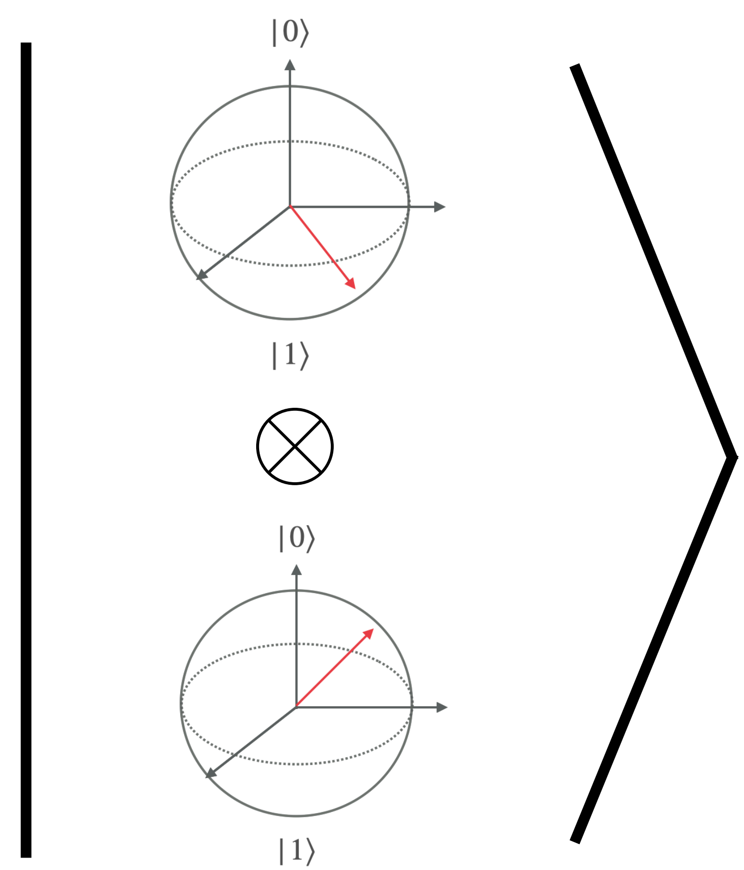
state preparation

n corresponds to # features

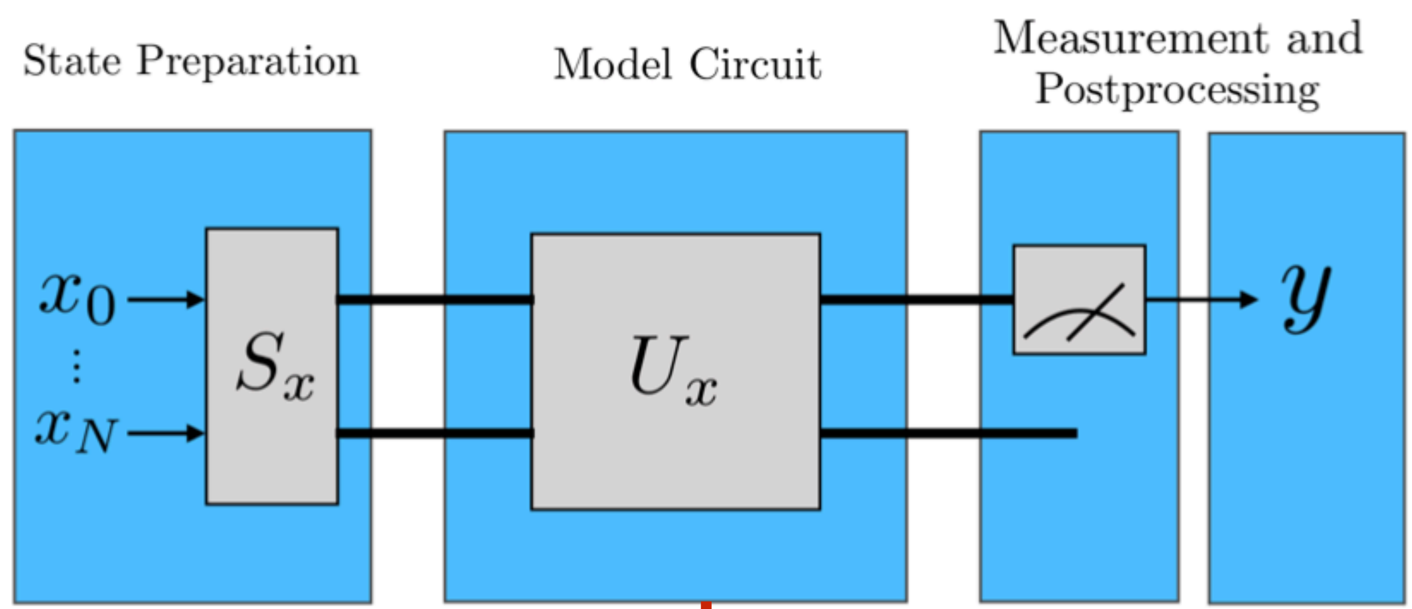
$$x \mapsto S_x|\phi\rangle = S_x|0\rangle^{\otimes n} = |x\rangle$$

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



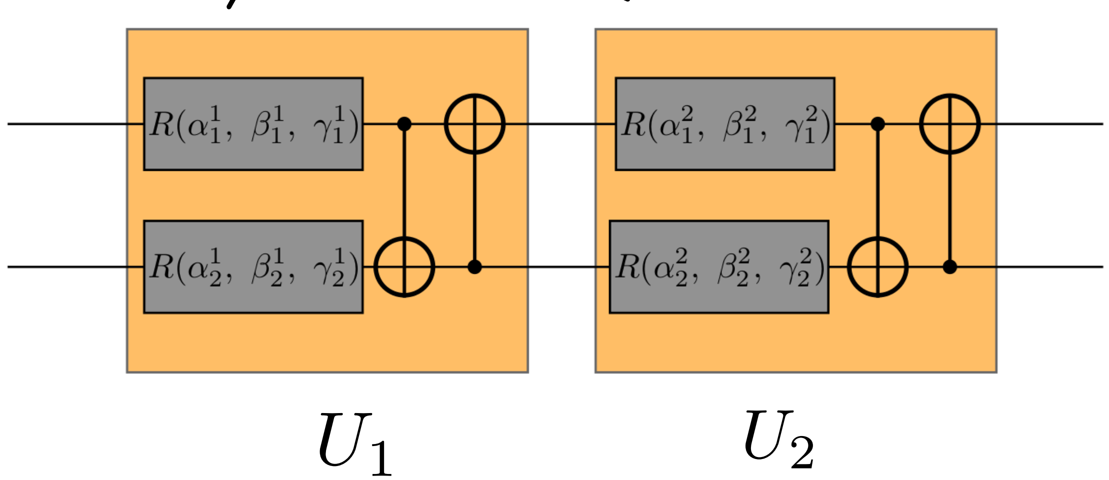
$$|\psi\rangle = U(w)|x\rangle$$ with $$U(w) = U_{l_{\max}}(w_{l_{\max}})...U_l(w_l)...U_1(w_1)$$

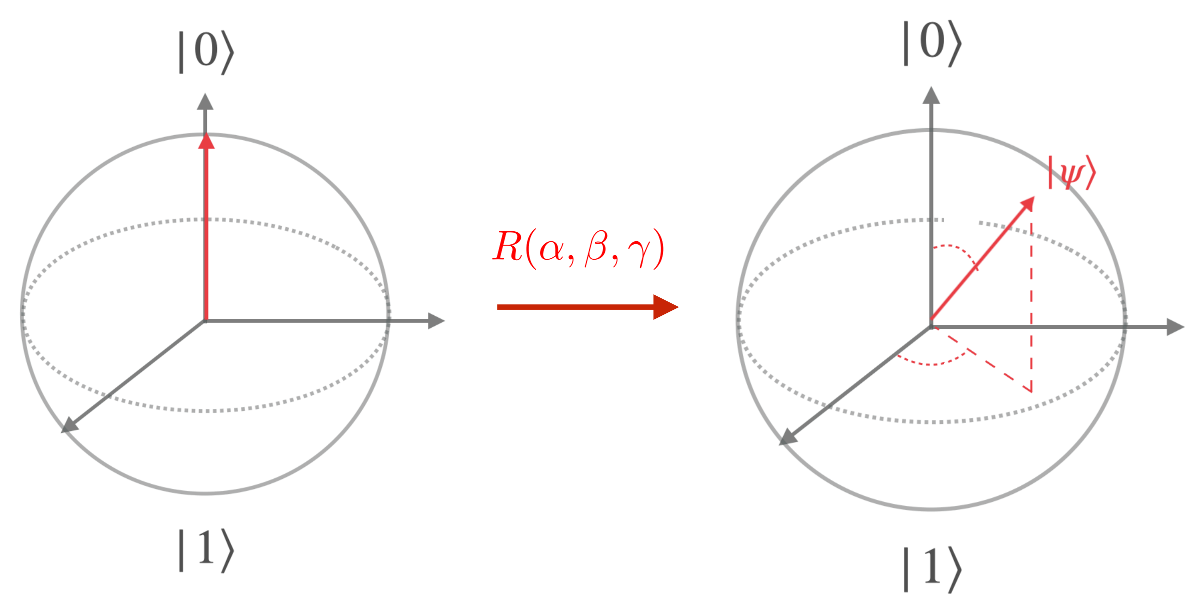
model circuit

trainable parameters

prepared state

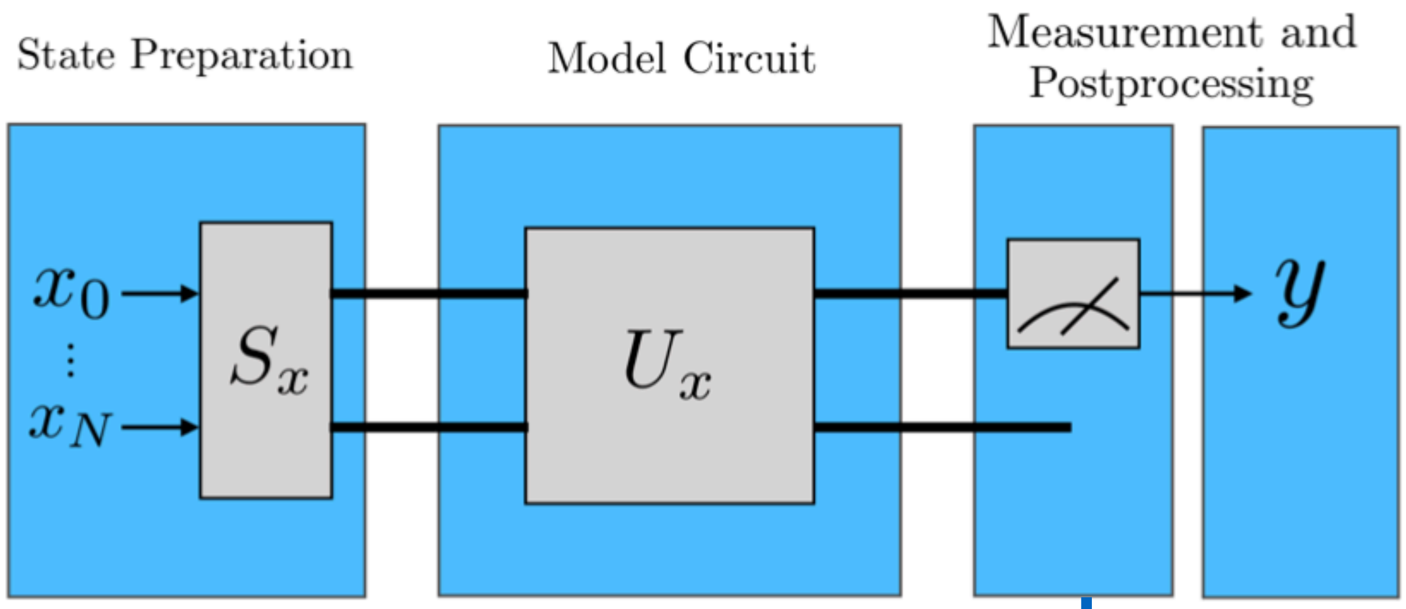
2-layer Variational Quantum Circuit





→ Rotation + CNOT -> Entanglement

Quantum Machine Learning with a Variational Quantum Circuit



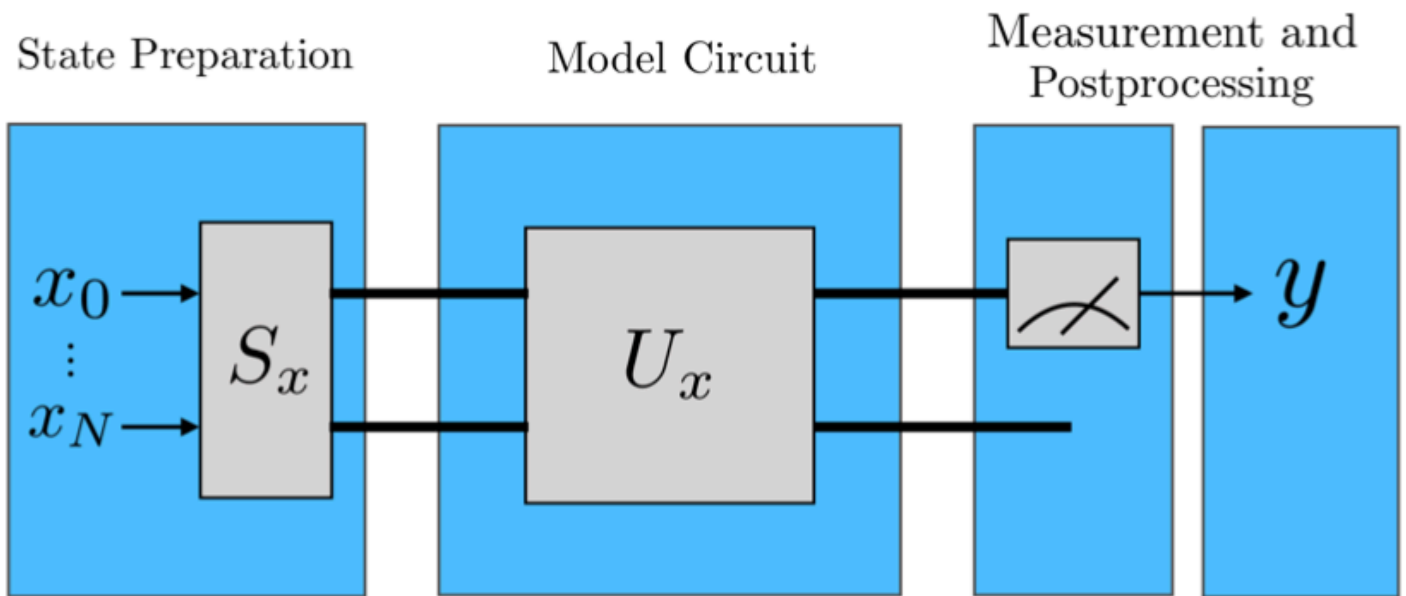
- Entangled state shares information across qubits
- Evaluate expectation value of qubits to construct loss

  for supervised S vs B classification one qubit sufficient

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

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

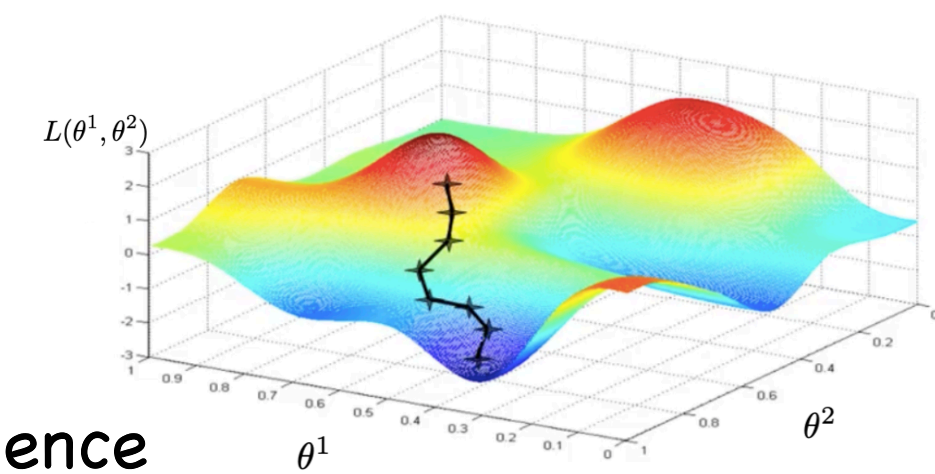
Quantum Machine Learning with a Variational Quantum Circuit



- 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

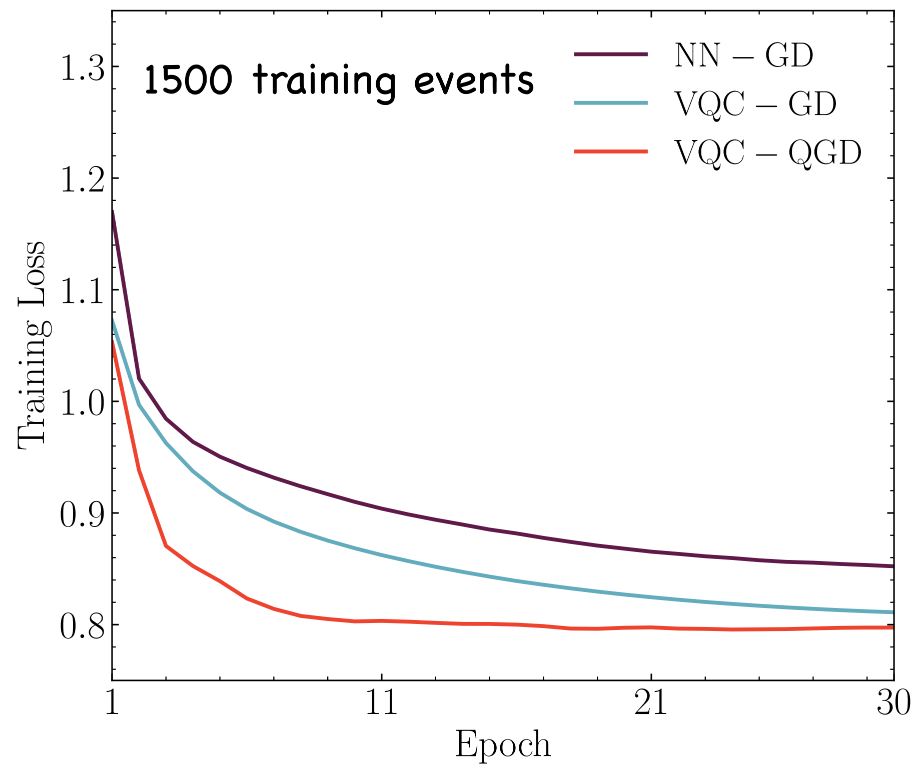
  Fubiny-Study metric underlies geometric structure of VQC parameter space: $\theta_{t+1} = \theta_t - \eta g^{+}\nabla L(\theta)$

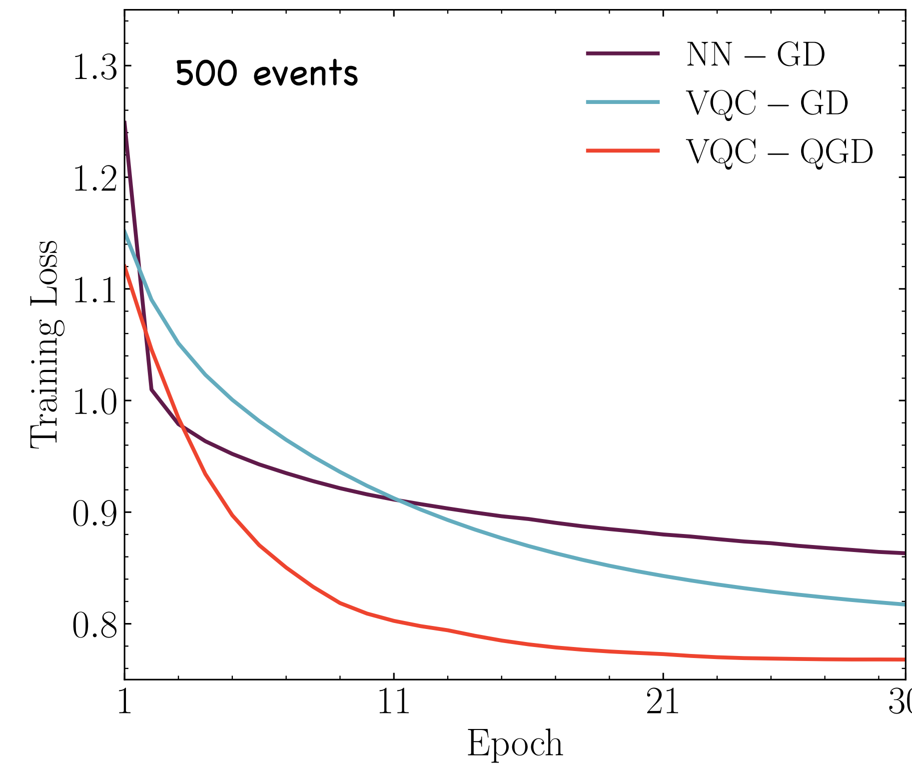
[Cheng '10]

[Blance, MS '20]

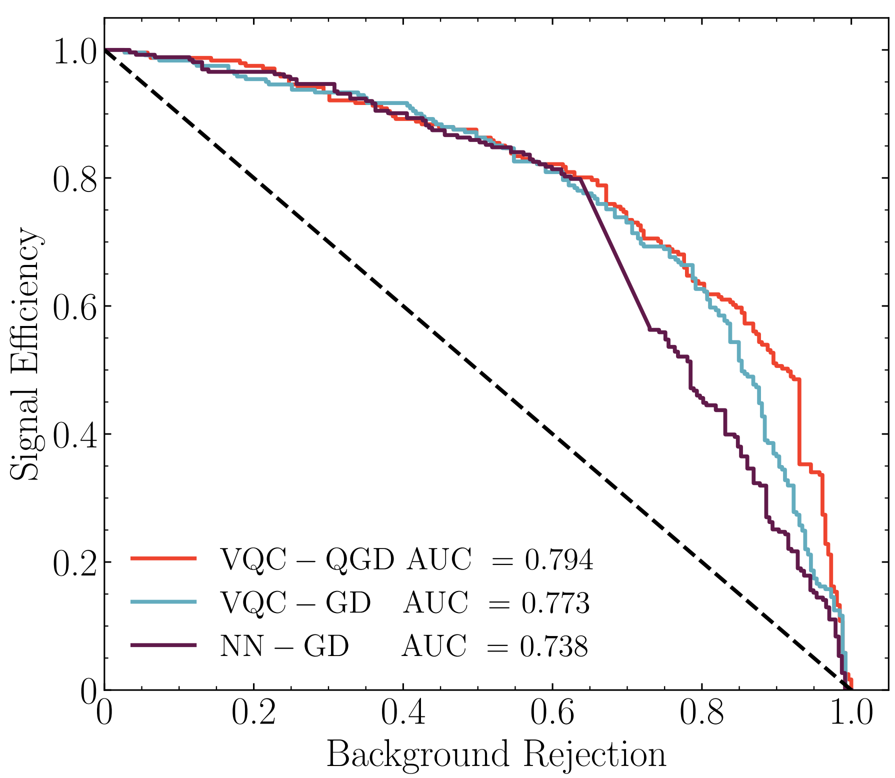
[Abbas et al '20]

Gate quantum machine learning in action





[Blance, MS '20]



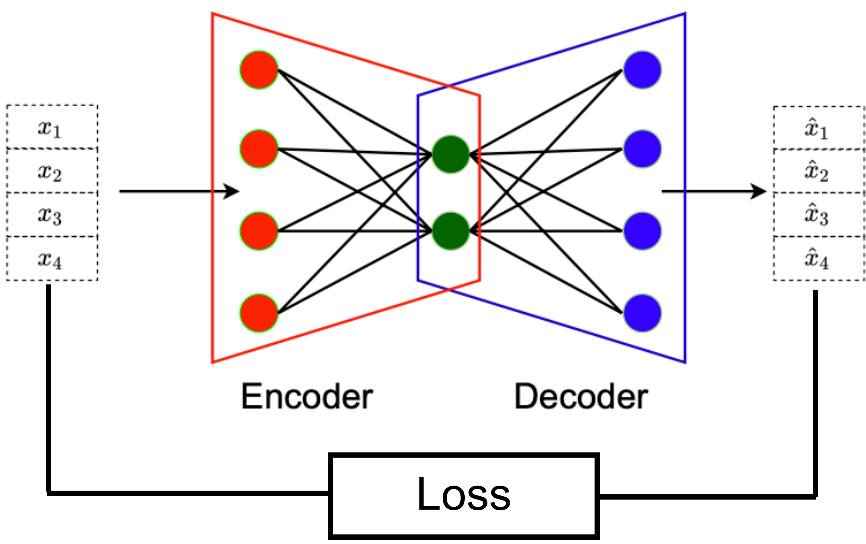
QC device vs simulator

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

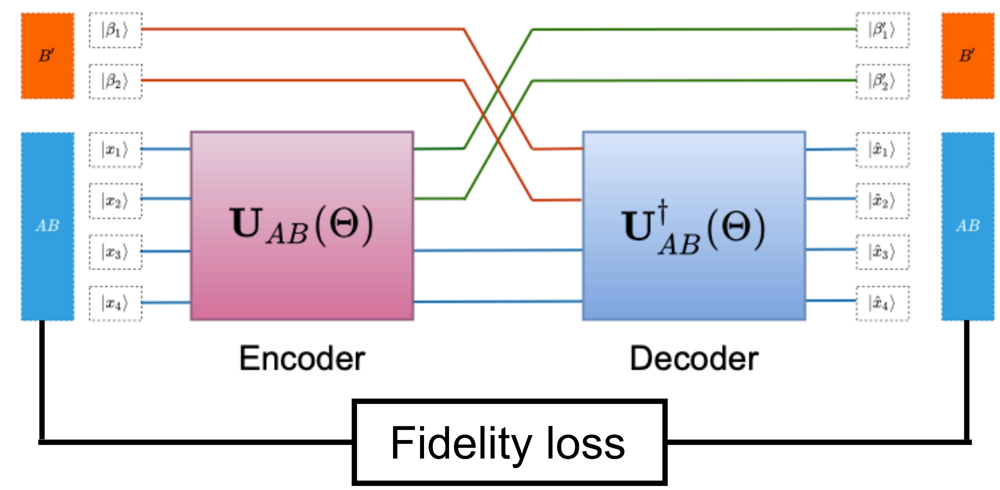
- Applied to $pp \to t\bar{t}$ vs $pp \to Z' \to t\bar{t}$ lept. top dec for 2d feature space only p_{T,b_1} and $\not{E}_T$

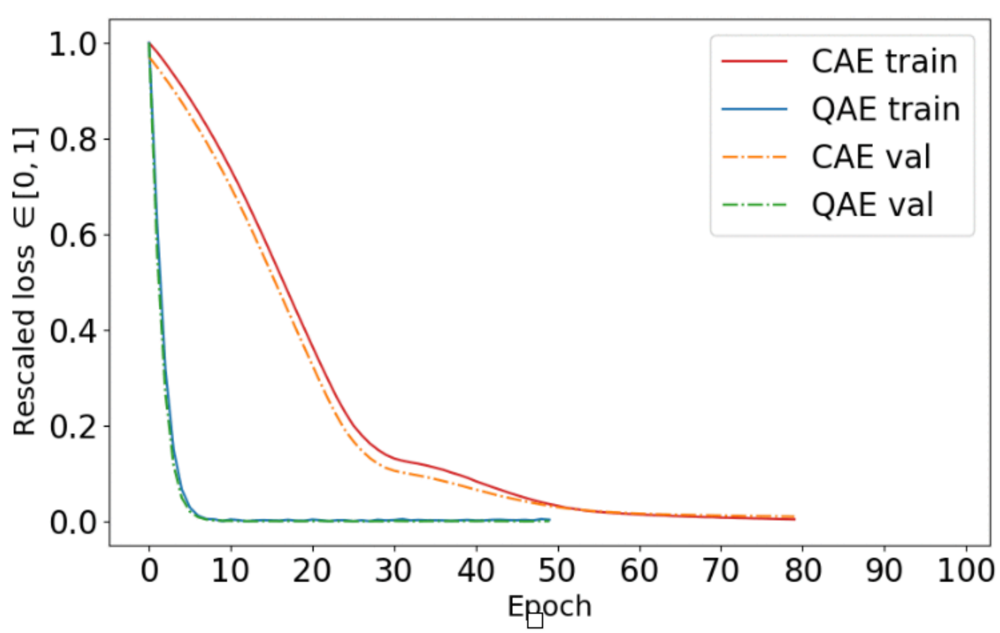
Anomaly detection with a Quantum Autoencoder

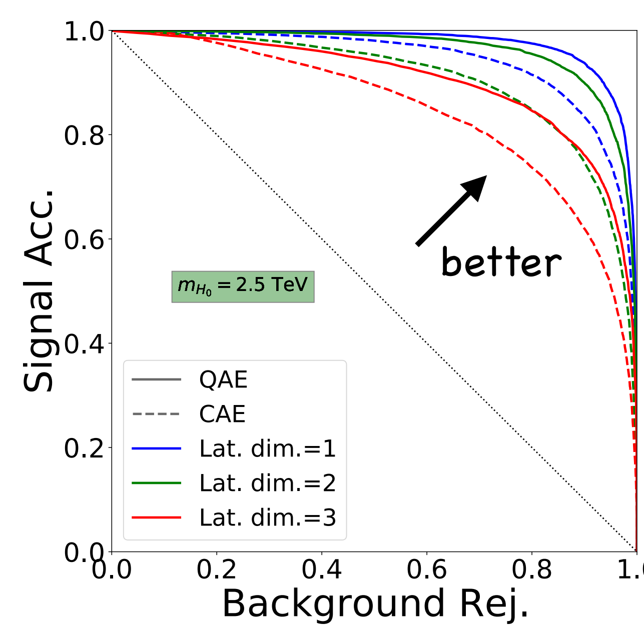
Classical autoencoder



Quantum autoencoder





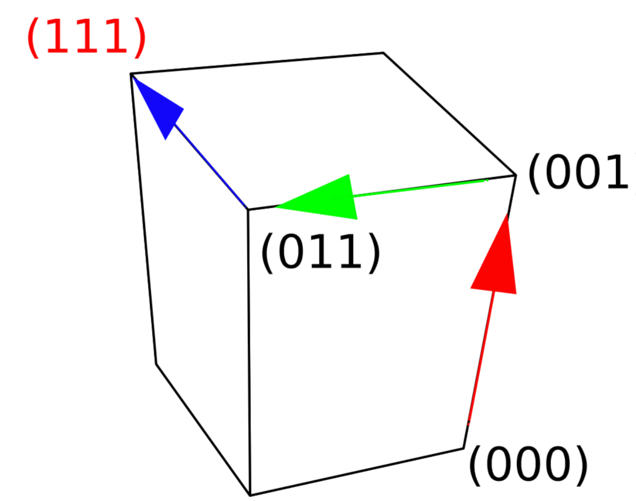


[Ngairangbam, MS, Takeuchi '21]

→ Much faster training and better performance for Quantum AE

→ Result persists despite full hyper-parameter scan for much larger CAE

Quantum annealing:
Non-universal but universally powerful?



- Problem needs to be encoded as Ising model

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

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

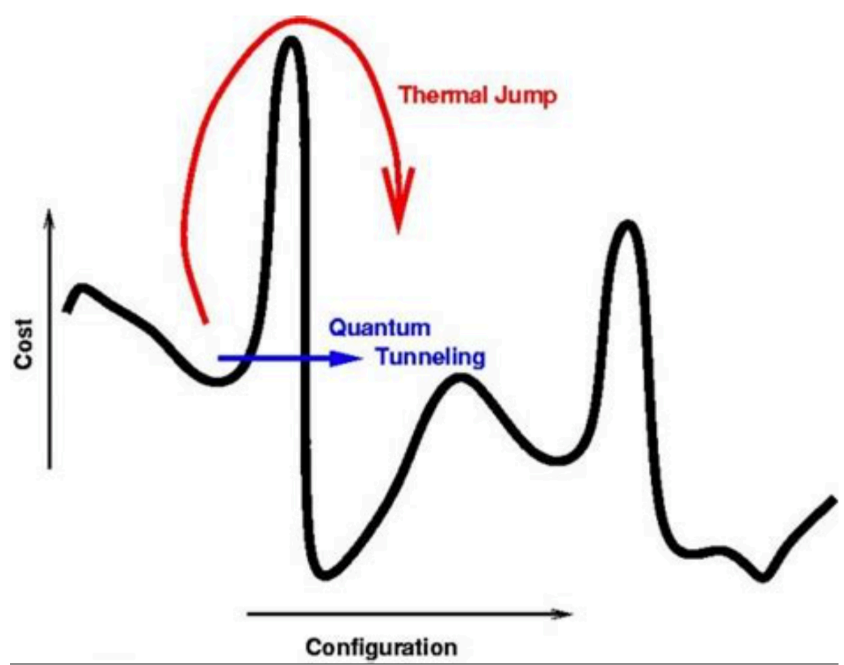
- Anneal idea: transition from initial Hamiltonian into ground state of problem Hamiltonian

- Thermal tunnelling is fast over broad shallow potentials $\sim e^{-\mathrm{height}/T}$

- Quantum tunnelling is fast through tall thin potentials $\sim e^{-\sqrt{\mathrm{height}}\times \mathrm{width}/\hbar}$

- Papers showing quantum dynamics on annealer

[Boixo et al, ’14 Nature] [King et al, ’21 Nature]



A quantum laboratory for QFT and QML

- 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] [Abel, Chancellor, 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.

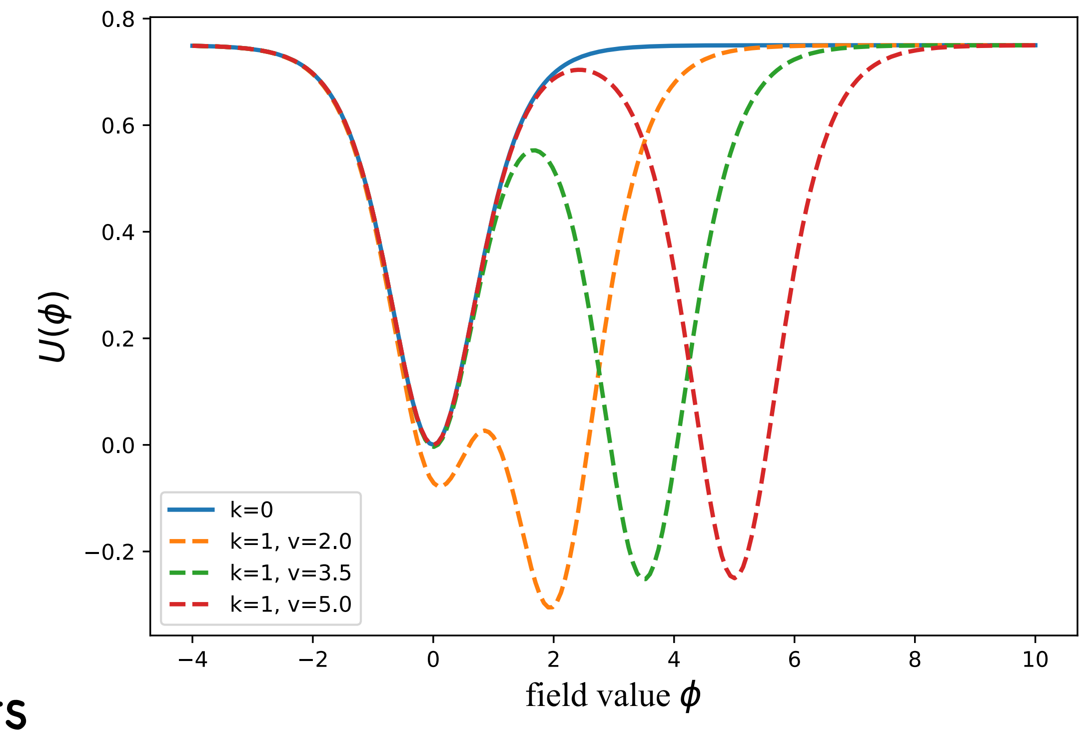
- Choose a potential of interest:

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

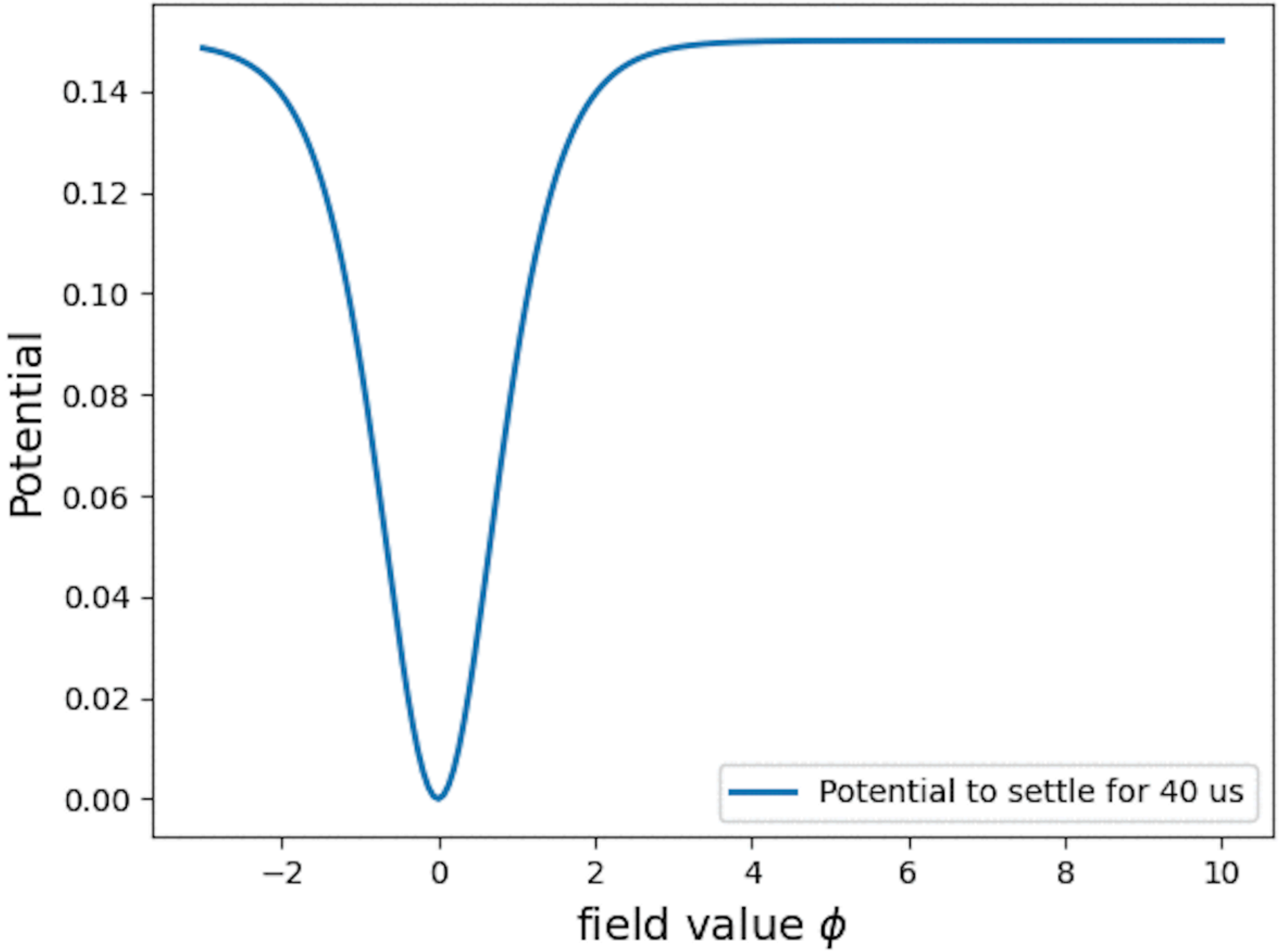
time dependent

where $\phi = \eta/\eta_0$

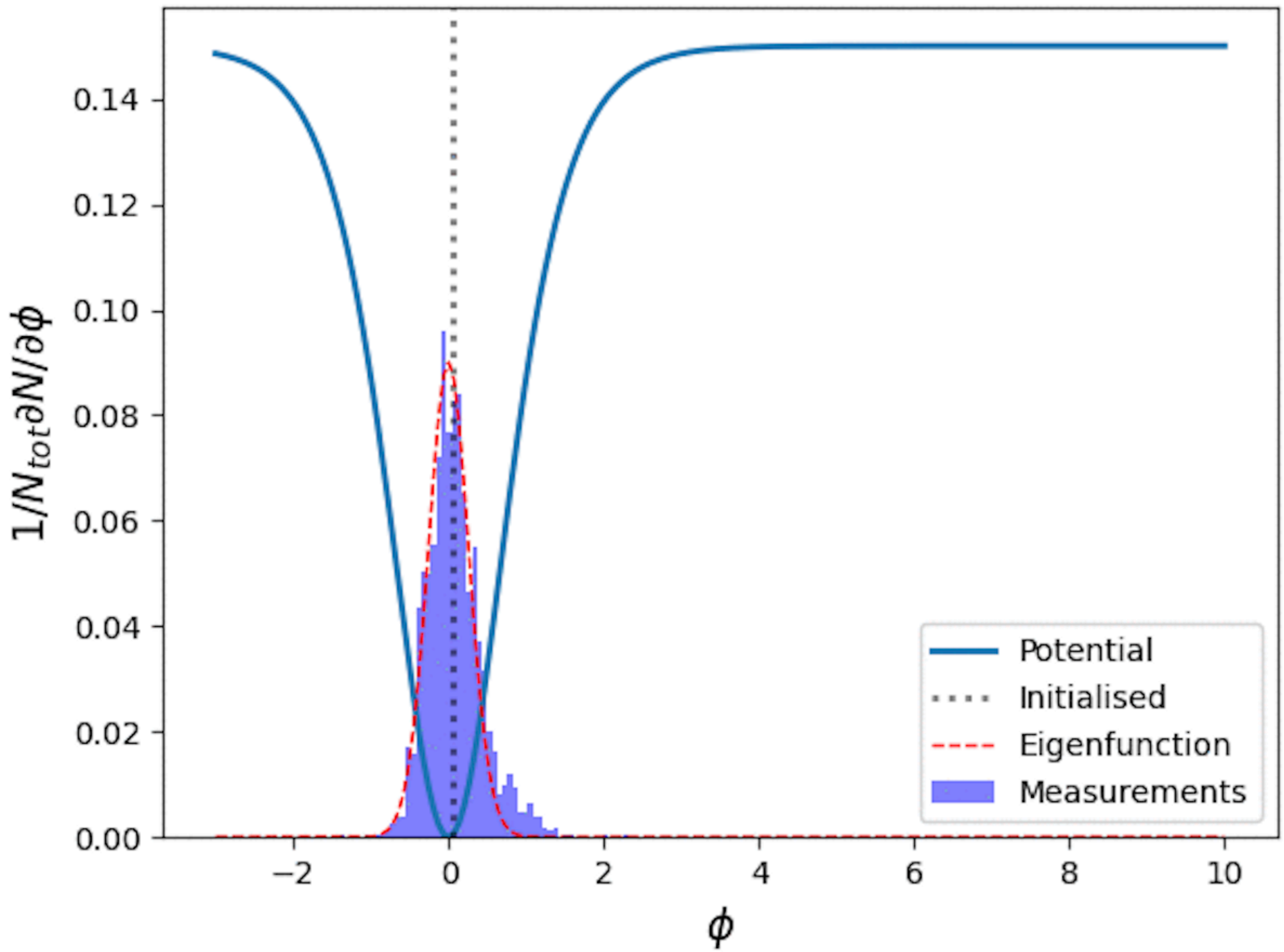
$\phi(t)$ is the field and c, v are dimless constants



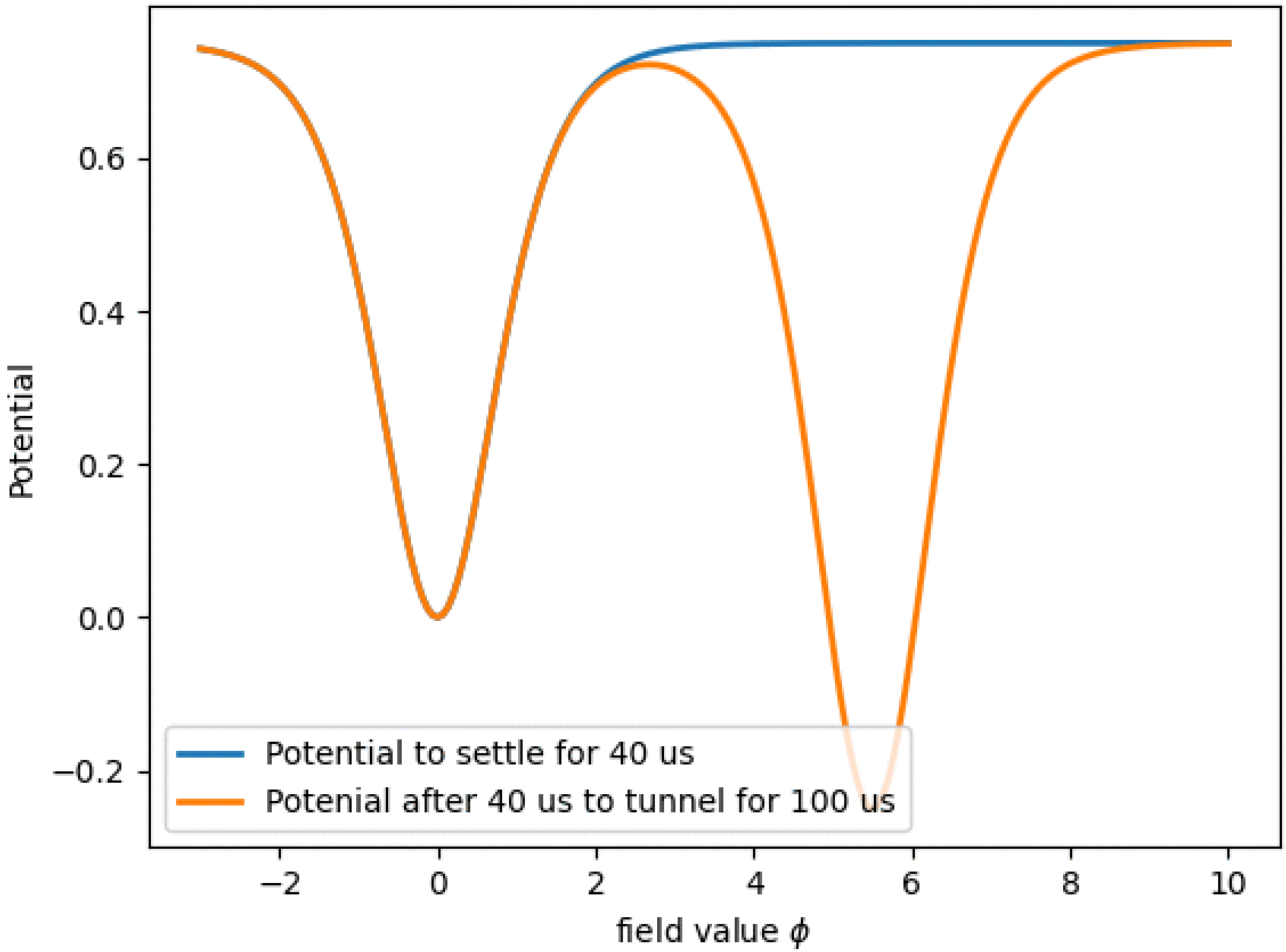
Implemented and executed on D-Wave Q2000 machine



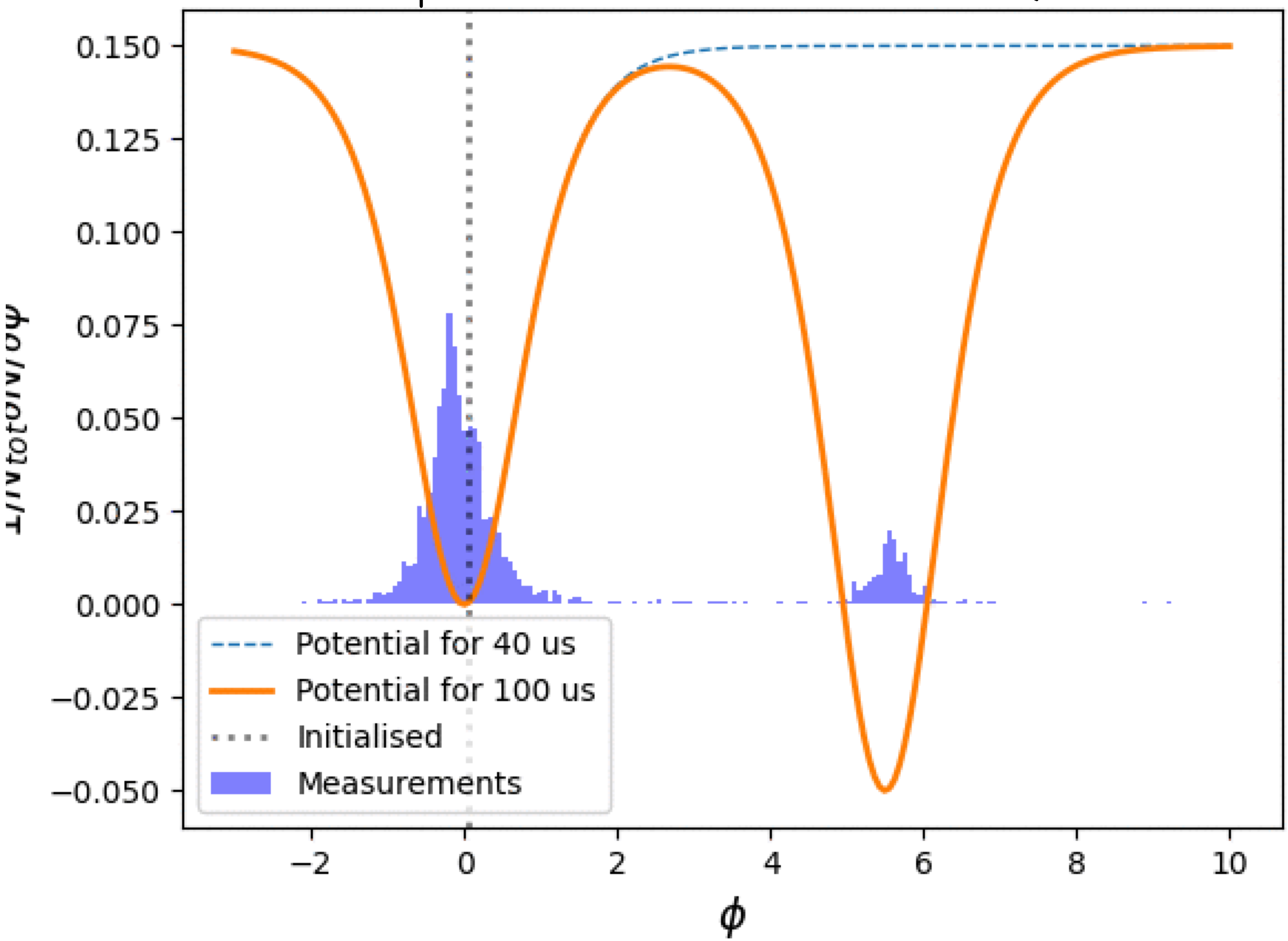
Implemented and executed on D-Wave Q2000 machine



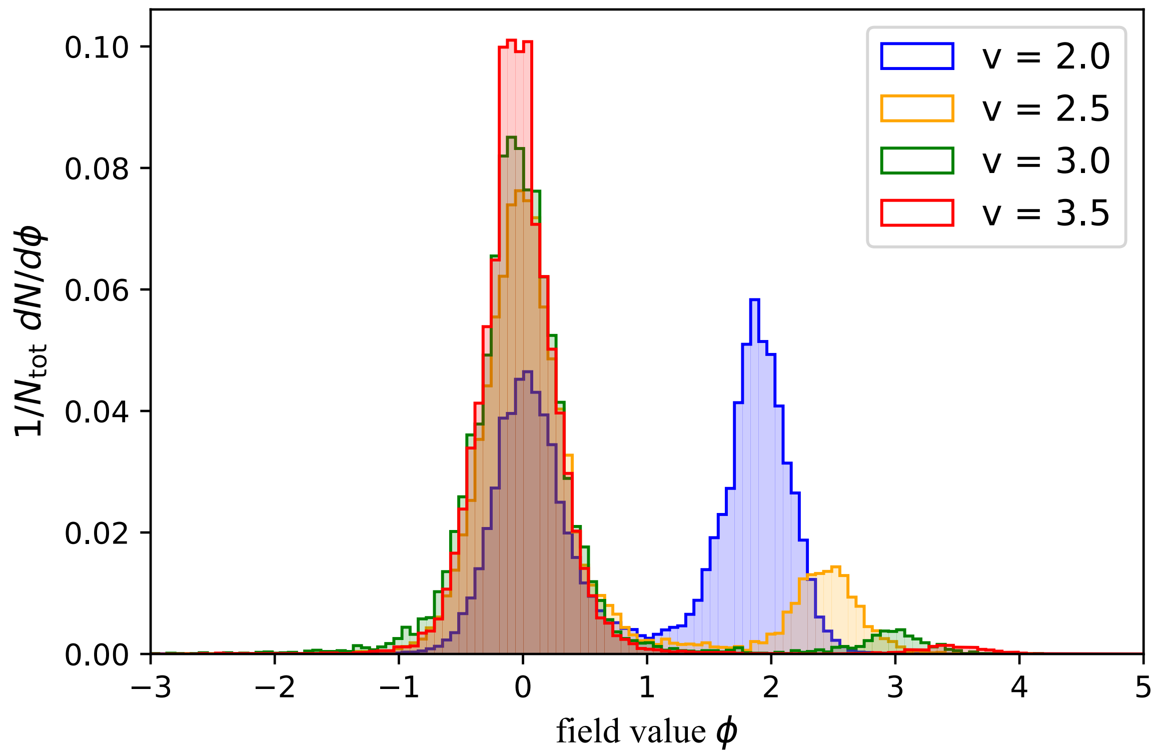
Implemented and executed on D-Wave Q2000 machine



Implemented and executed on D-Wave Q2000 machine



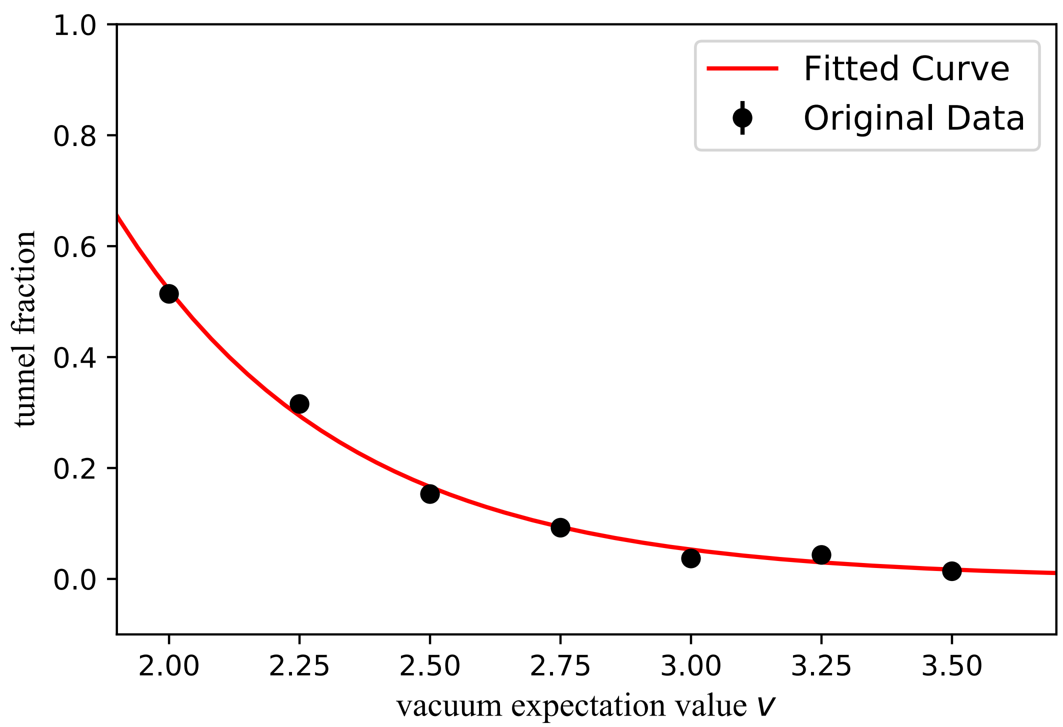
Results: it decays with v as expected



Perform tunnelling for

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

[Abel, MS '20]



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

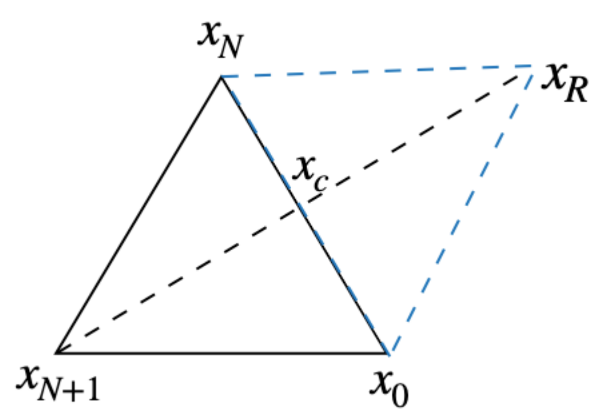
Exp: $\log\Gamma = 2.29 \times (1.71 - v)$

Optimisation algorithm comparison quantum vs classical

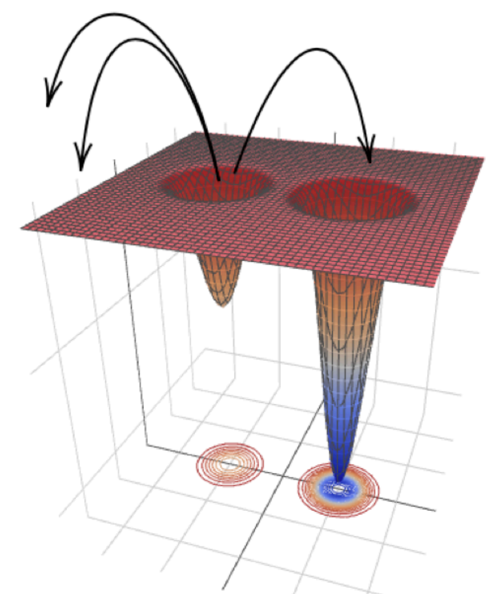
gradient descent

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

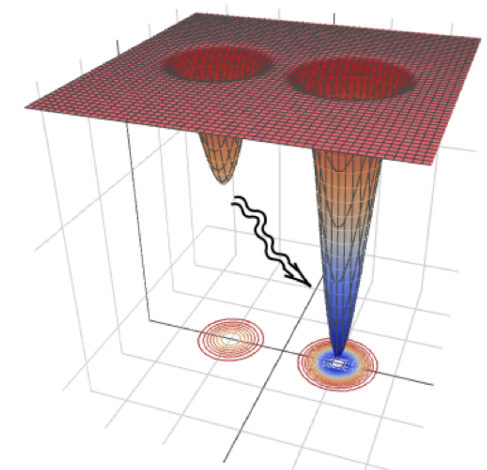
Nelder-Mead



Thermal Annealing

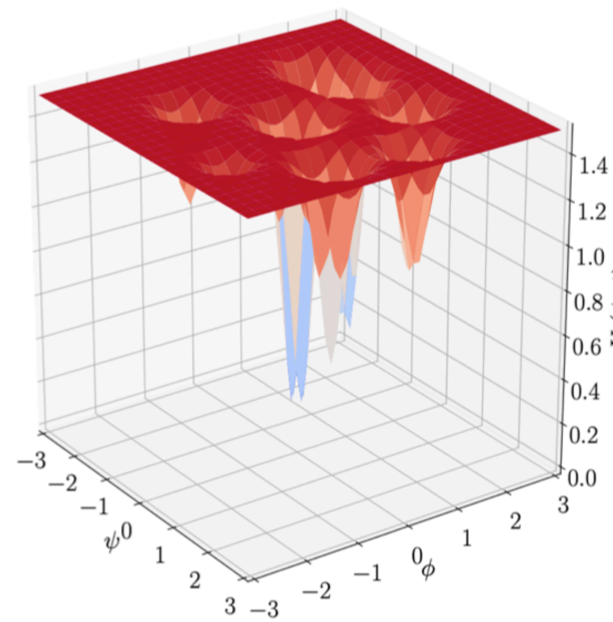


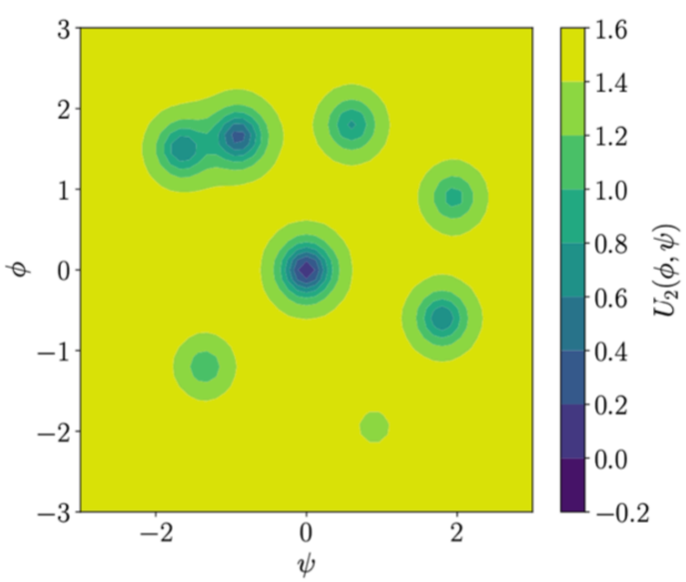
Quantum Annealing



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

Multi-well potential



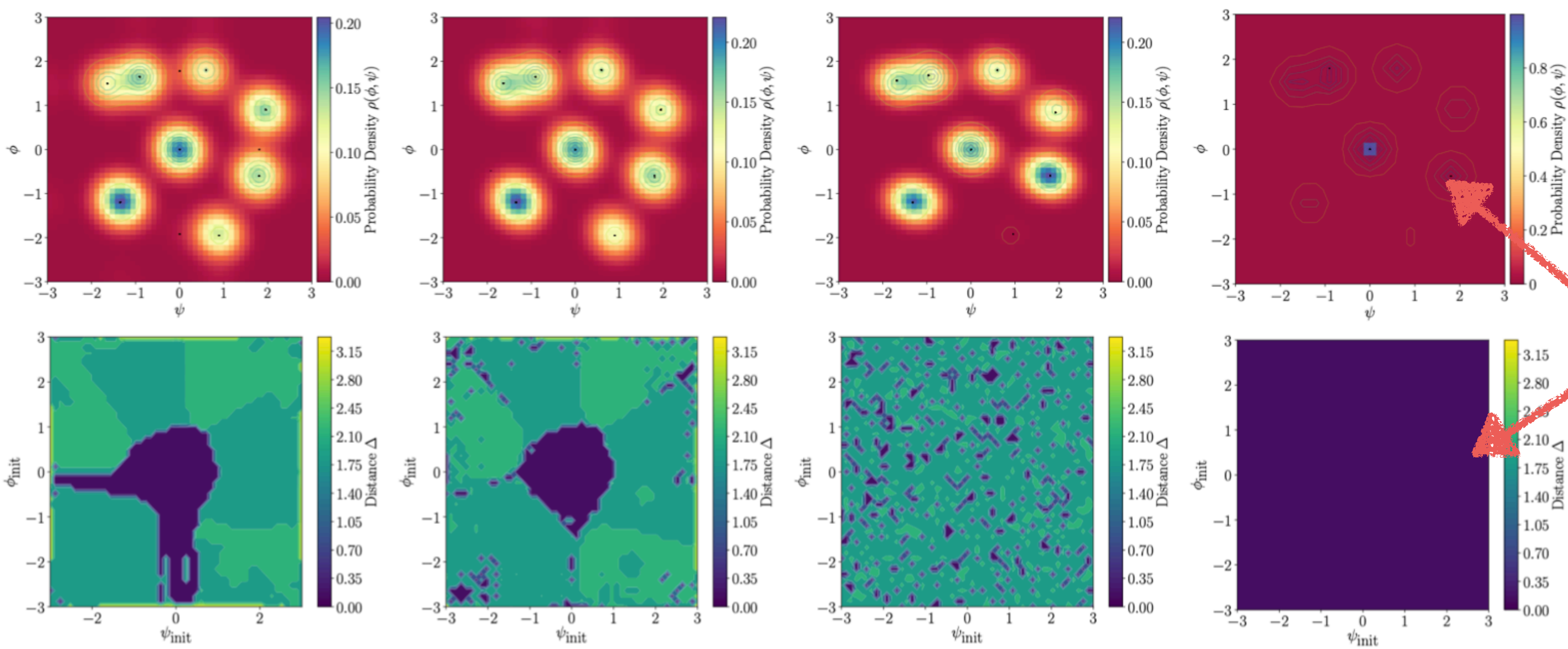


Results for Multi-well potential

- 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

→ Significant quantum advantage on current device

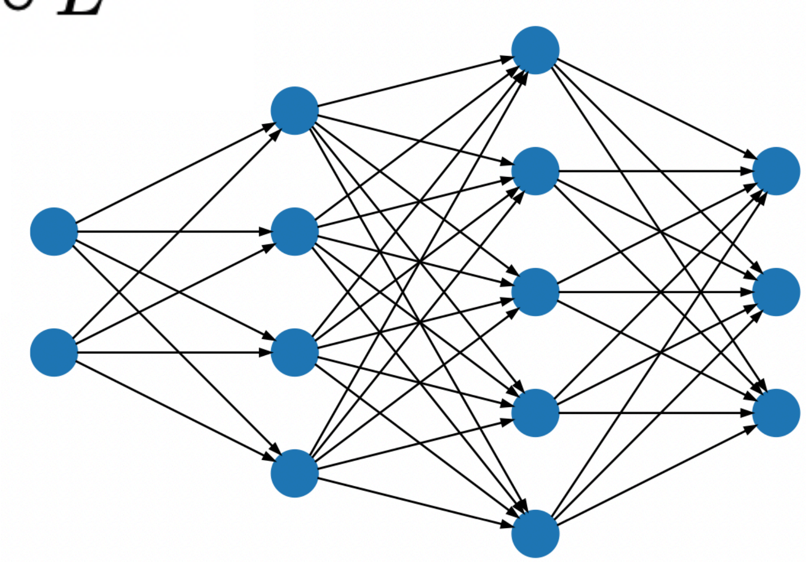
Completely Quantum Neural Networks

- Output of a classical NN is a function of functions depending on trainable weights

→ Encode NN on quantum annealer and train with quantum dynamics [Abel, Criado, MS '22]

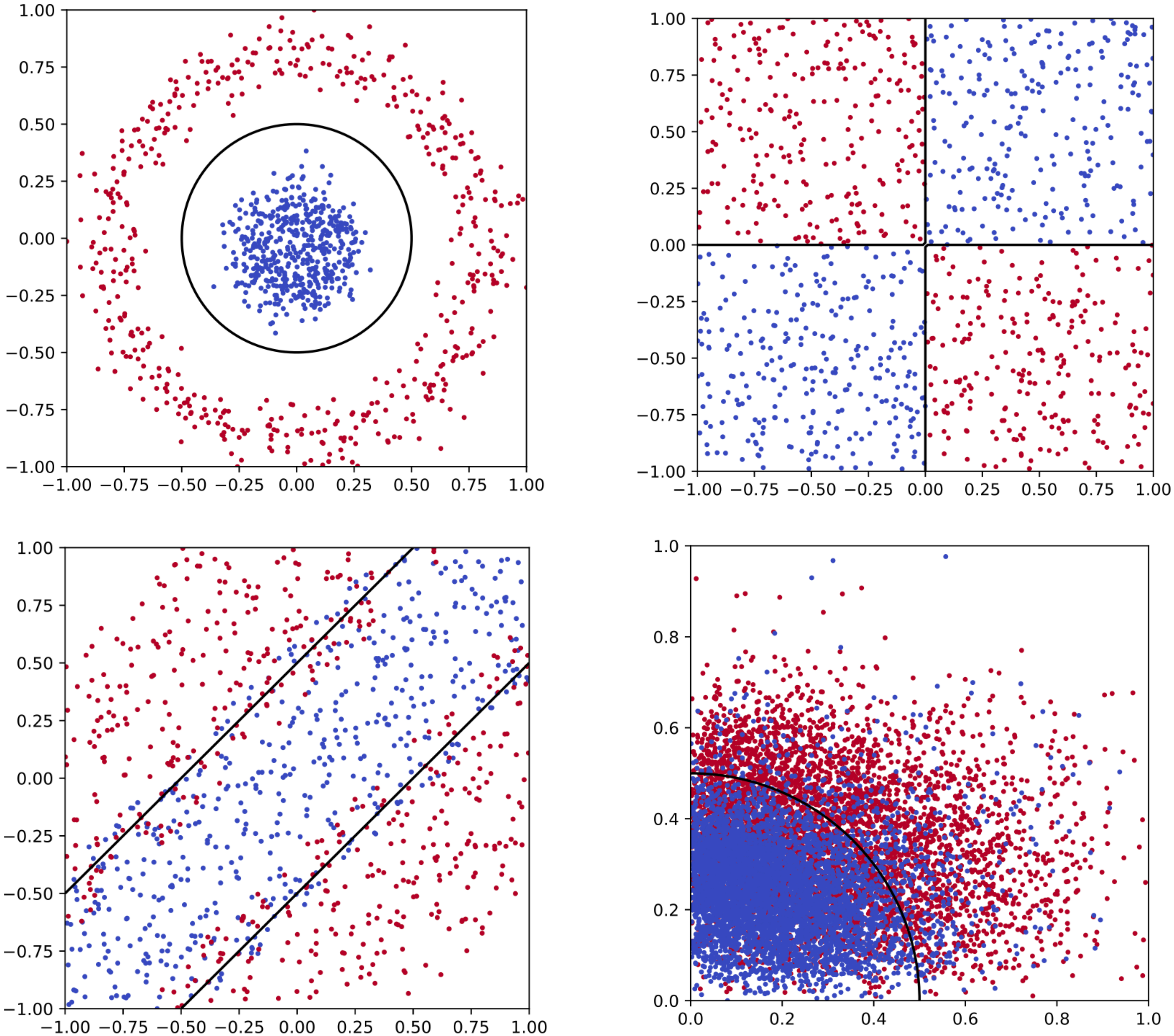
Network output in final layer $Y = L^{(n)} \circ \ldots \circ L^{(0)}$

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

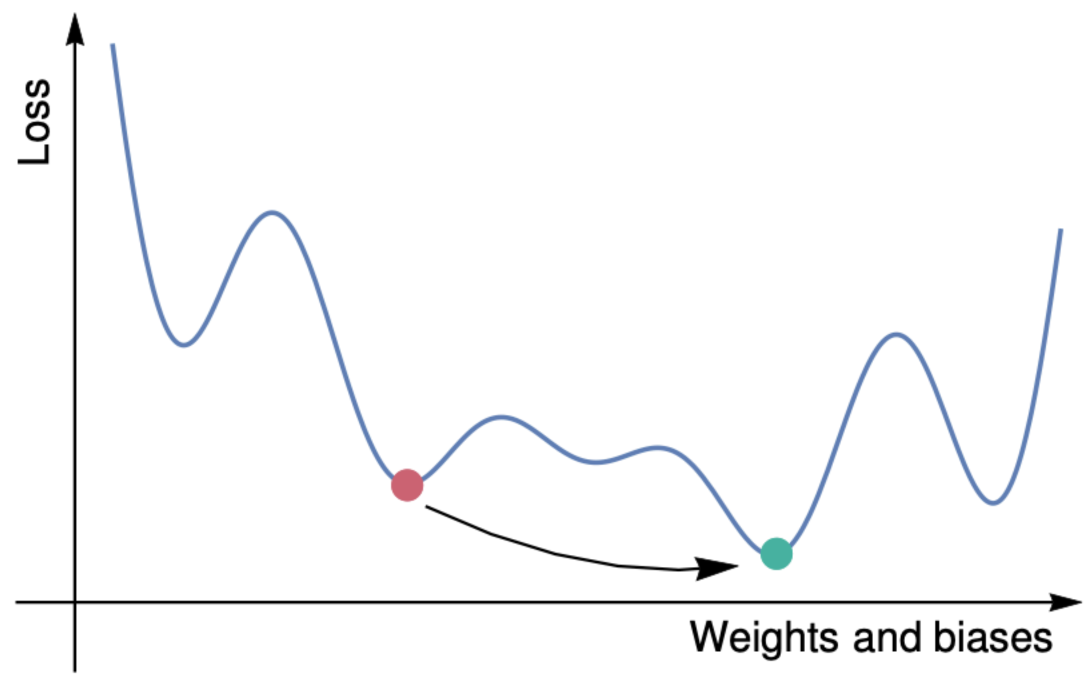


- Currently some simplifications needed due to technical limitations (#qubits, connections etc)

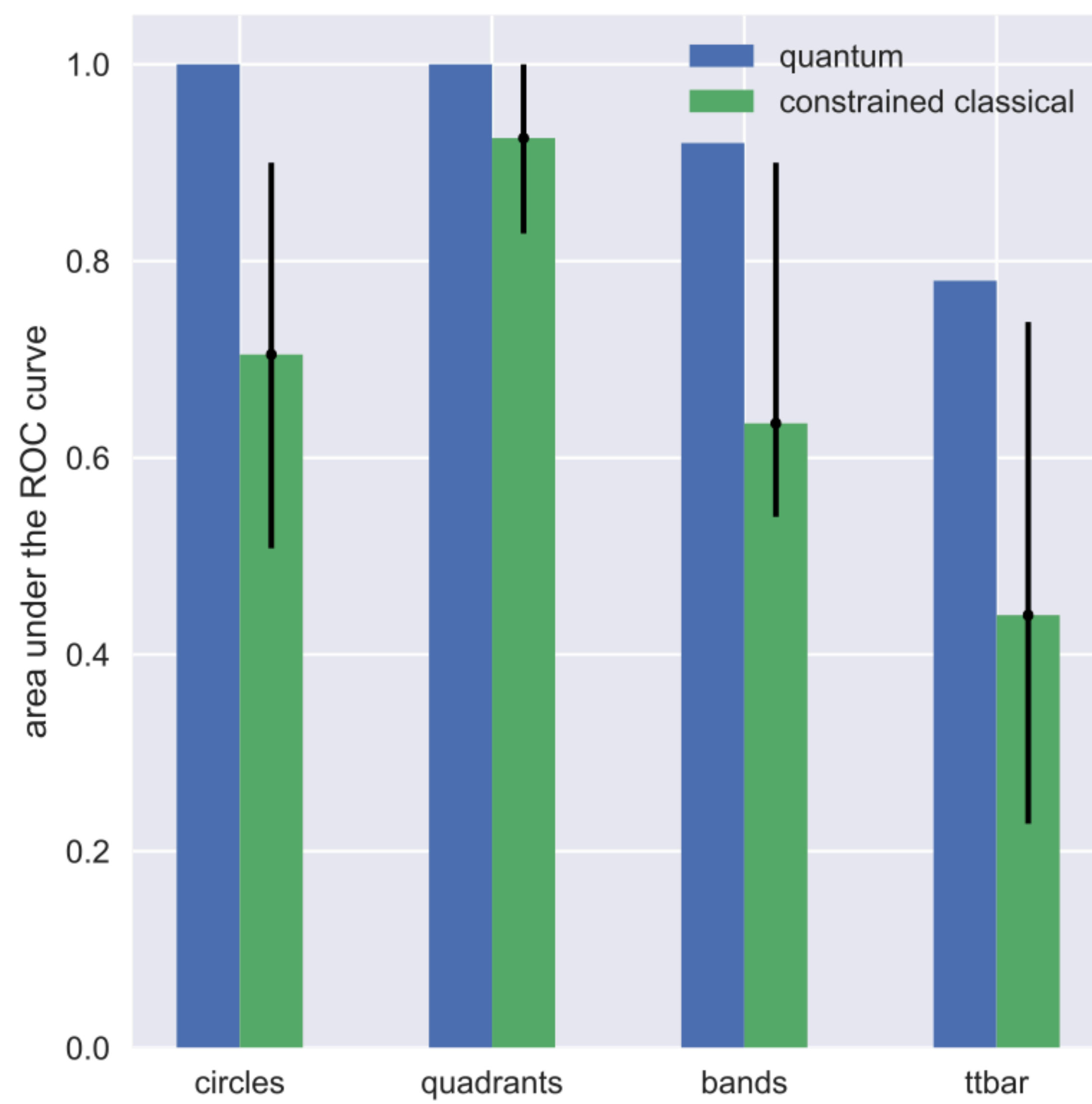
- Train NN weights in no time optimally on quantum computer (annealer) -> export them for deployment using classical NN framework


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

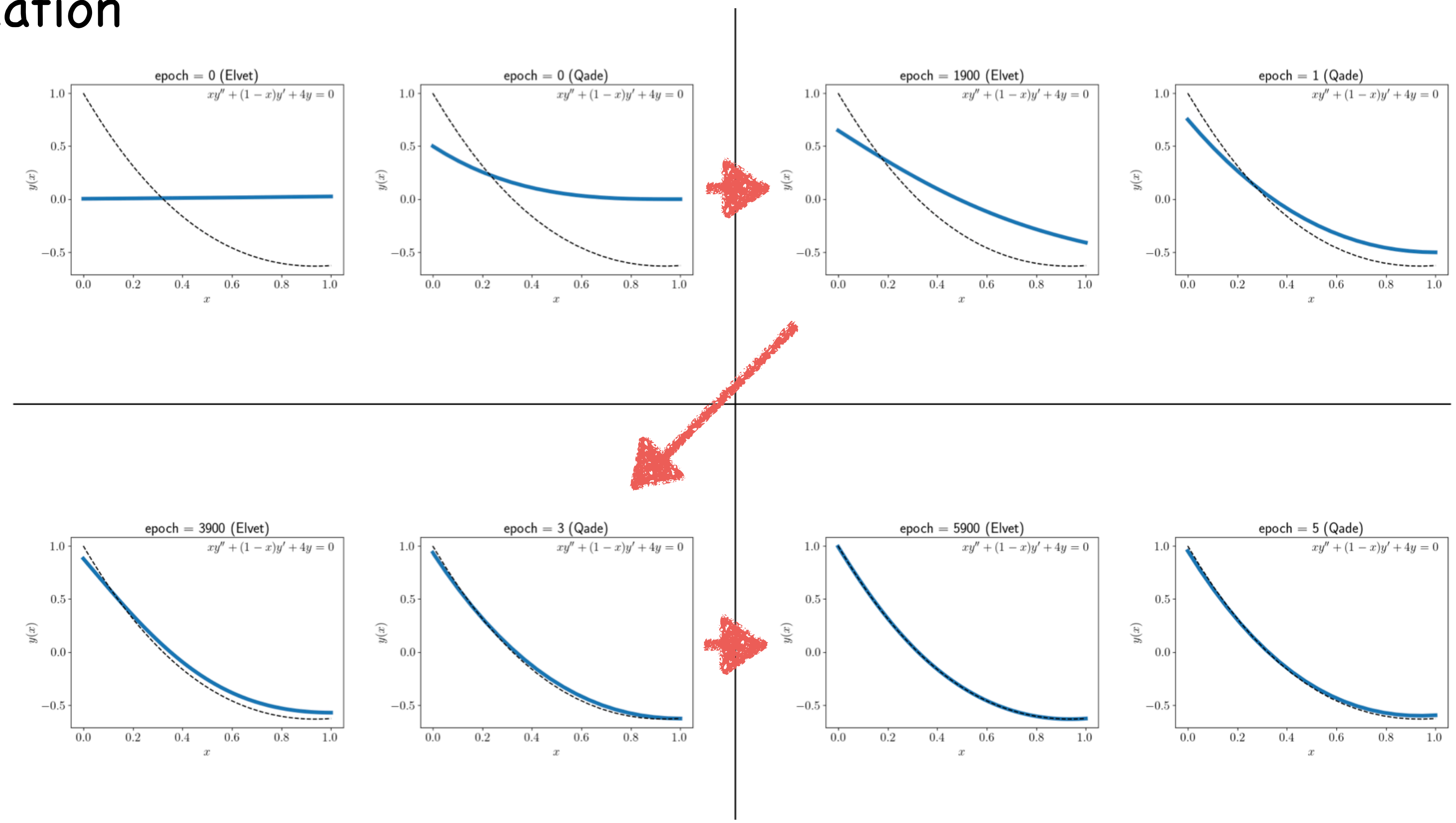


Optimal network training

QADE: Solving differential equations with a quantum annealer

Define Loss as: $\mathscr{L} = \sum_i \mathrm{E}_i(f, \partial f, \ldots)^2 + \sum_j \mathrm{BC}_j(f, \ldots)^2$

Example Laguerre differential equation $xy'' + (1-x)y' + 4y = 0$ with $y(0) = 1$ and $y(1) = L_4(1)$



Classical Neural Network approach (Elvet)

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

https://gitlab.com/elvet/elvet

Quantum algorithm (QADE)

gitlab.com/jccriado/qade [Criado, MS '22]

QFitter

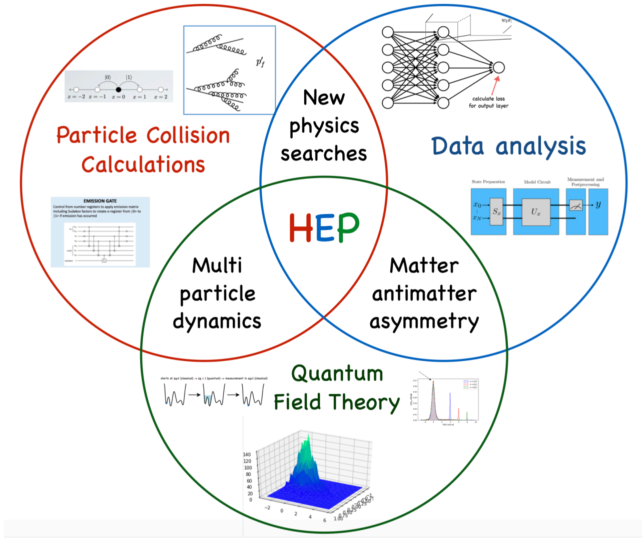
Example Higgs EFT fit: [Criado, Kogler, MS '22]

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

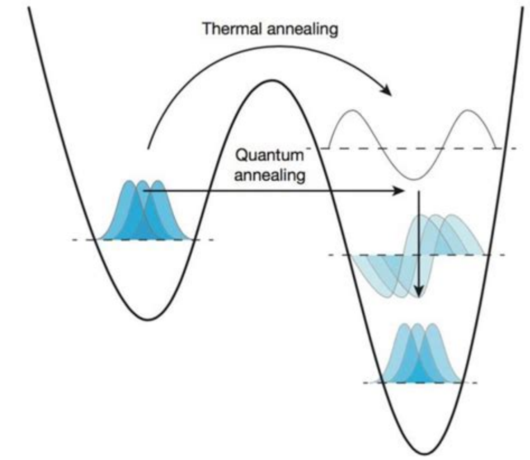
$$\chi^2 = \sum_{ij} V_a C^{-1}_{ab} V_b \qquad V_a = O_a^{(\text{exp})} - O_a^{(\text{th})}(c)$$

- 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

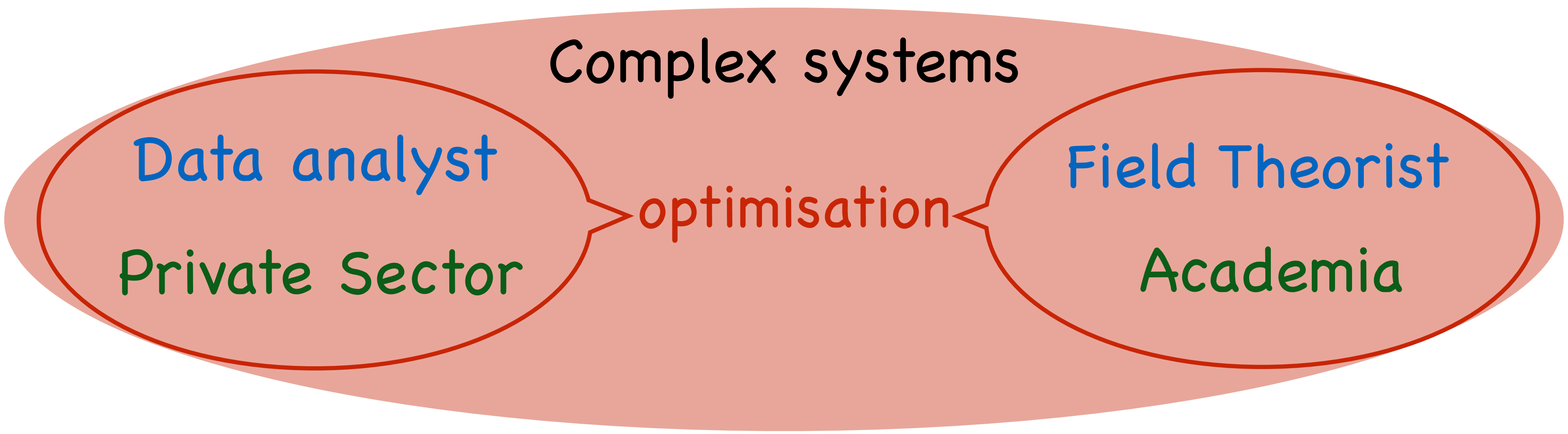
Formulation	Method	Fit time	c_{HW}	c_H	c_g	c_γ	χ^2
Standard	Minuit (initial $c_{HW} = 0$)	2.0 s	-0.009	0.100	1.4×10^{-5}	3.2×10^{-6}	4110
	Minuit (initial $c_{HW} = -0.05$)	2.4 s	-0.050	0.039	-9.7×10^{-6}	-1.0×10^{-4}	135
	Simulated annealing (initial $c_{HW} = 0$)	642 s	-0.009	0.100	1.4×10^{-5}	3.7×10^{-6}	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



Summary



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



- Neural Networks, Tensor Networks and Variational Quantum Algorithms share conceptual and structural similarities.
  Terence: "when two do the same, the result is not identical", see [Araz, MS '22]

- Exciting times to develop novel algorithms for data analysis and QFT