WACQT Wallenberg Centre for Quantum Technology

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Protein folding with QAOA

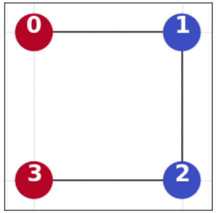
Hanna Linn, PhD student | Applied Quantum Physics Laboratory and WACQT

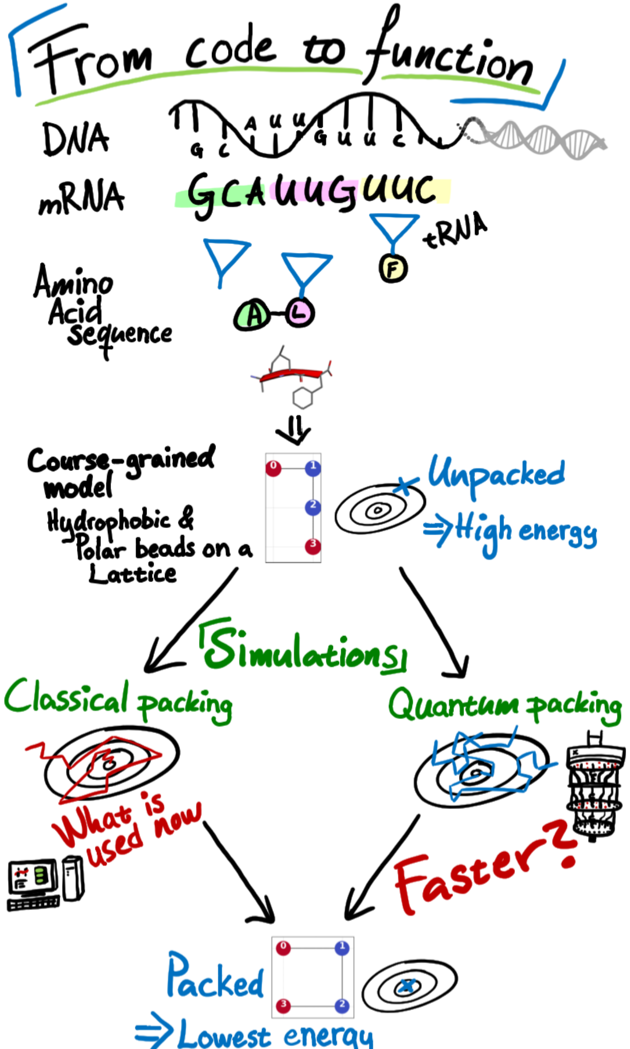
Overview

- Protein folding
- Gate based quantum computer: Quantum Approximate Optimisation Algorithm (QAOA)
- Initial parameters in QAOA inspired by quantum annealing
- What kind of quantum computers would be needed to challenge classical computers in folding proteins?

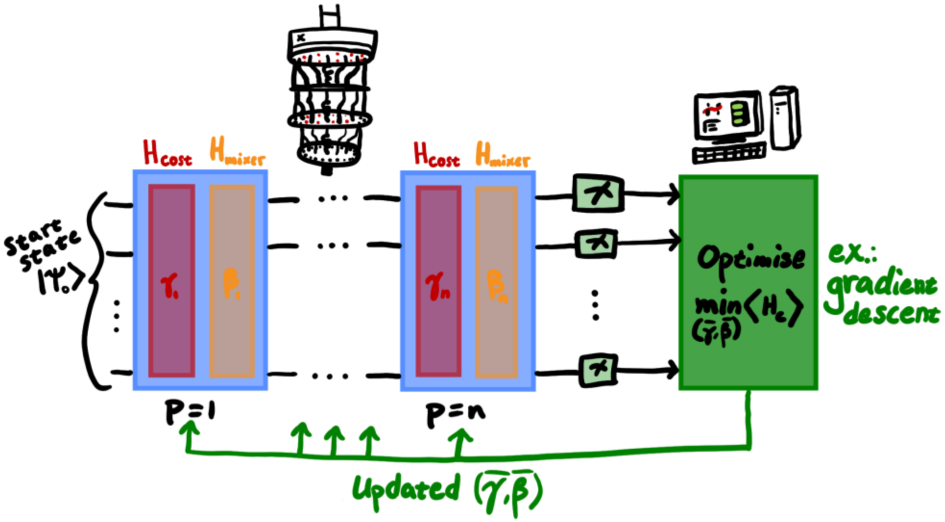
Protein folding simulations

- From DNA to amino acid sequence.
- Amino acid sequence folds to functioning protein.
- Course-graining models for simplifications.
- Hydrophobic-Polar model on a lattice.

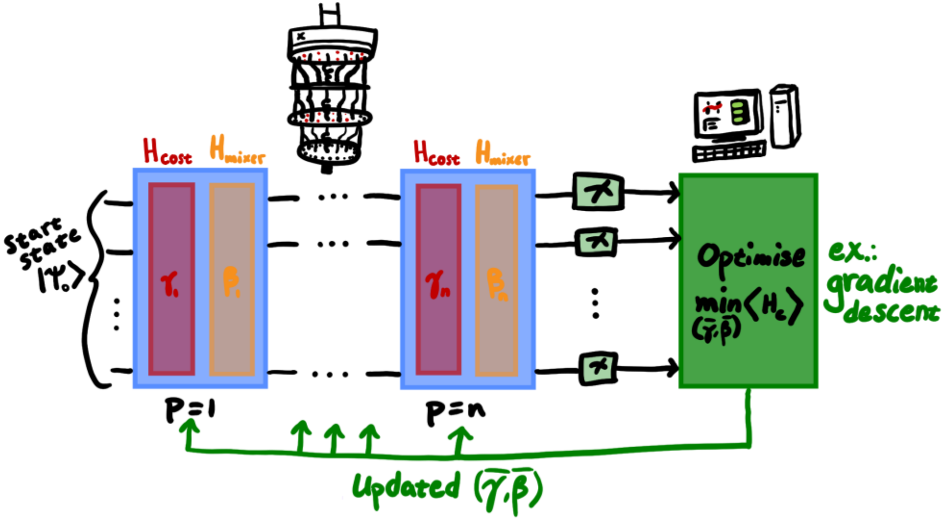


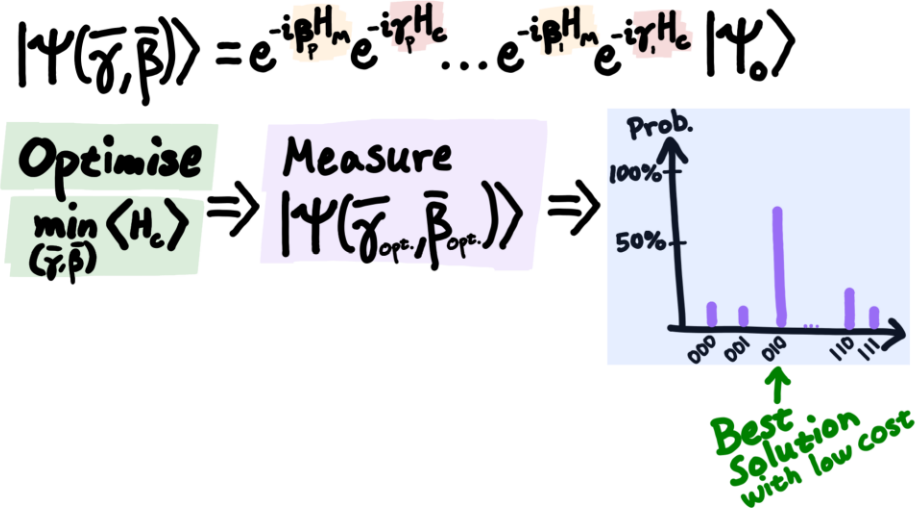


QAOA


start state $|\psi_0\rangle$
H_{cost}
H_{mixer}
γ_1
β_1
γ_n
β_n
P=1
P=n
Optimise
$\min_{(\vec{\gamma},\vec{\beta})}\langle H_c\rangle$
ex.: gradient descent
Updated $(\vec{\gamma},\vec{\beta})$

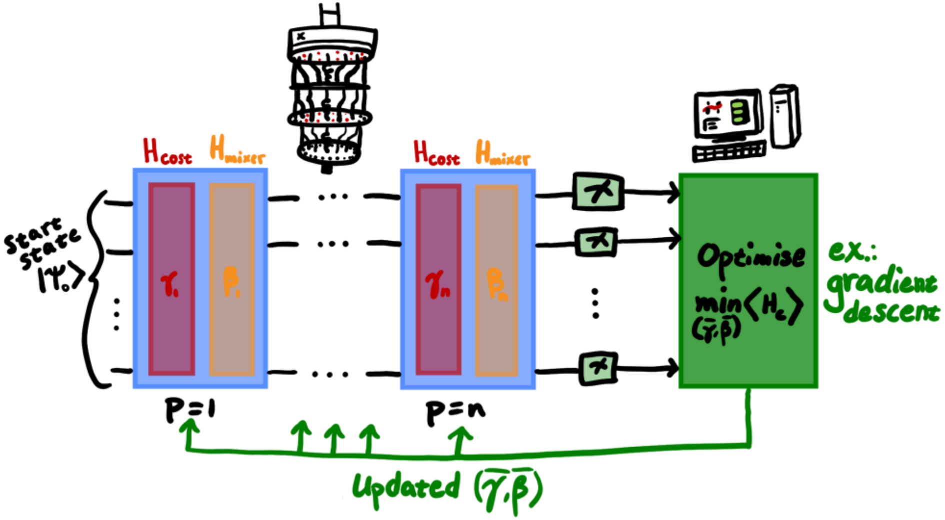
QAOA

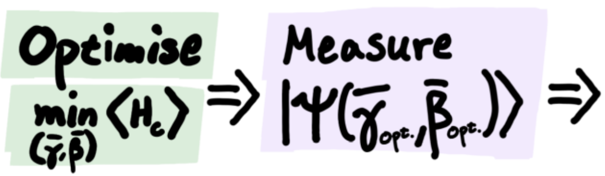

Start state |ψ₀⟩
H cost
H mixer
γ₁
β₁
γₙ
βₙ
P=1
P=n
Optimise min⟨H_c⟩ (γ̄,β̄)
ex.: gradient descent
Updated (γ̄,β̄)

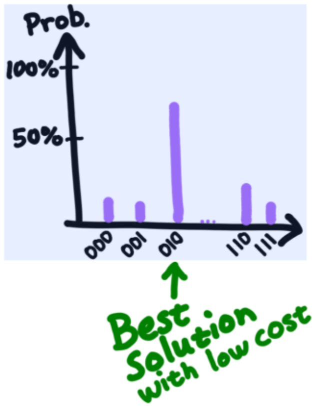

|ψ(γ̄,β̄)⟩ = e^{-iβ_p H_m} e^{-iγ_p H_c} ... e^{-iβ_1 H_m} e^{-iγ_1 H_c} |ψ₀⟩
Optimise
min ⟨H_c⟩ (γ̄,β̄)
Measure
|ψ(γ̄_opt., β̄_opt.)⟩
Prob.
100%
50%
000
001
010
110
111
Best Solution with low cost

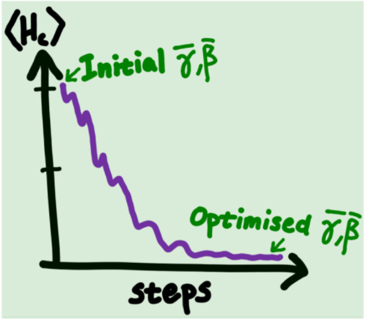
QAOA

$$|\Psi(\bar{\gamma},\bar{\beta})\rangle = e^{-i\beta_p H_m} e^{-i\gamma_p H_c} \ldots e^{-i\beta_1 H_m} e^{-i\gamma_1 H_c} |\Psi_0\rangle$$

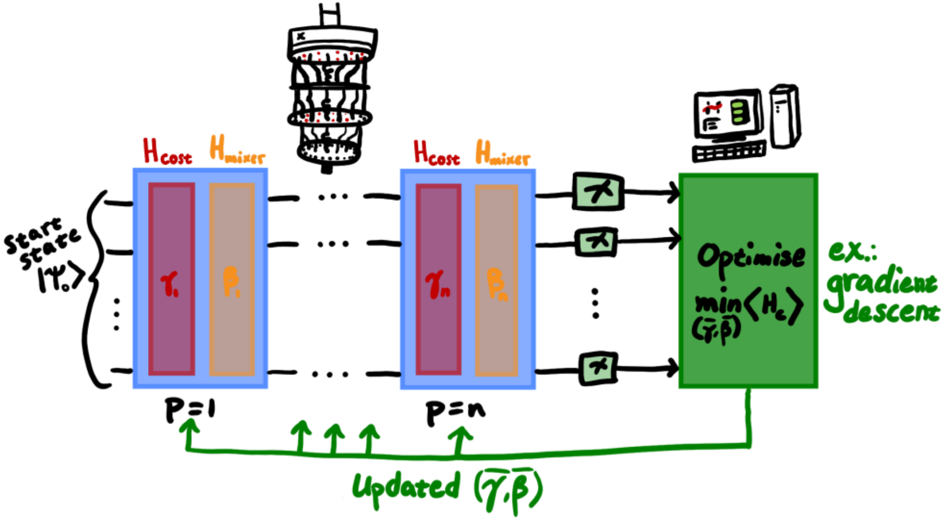




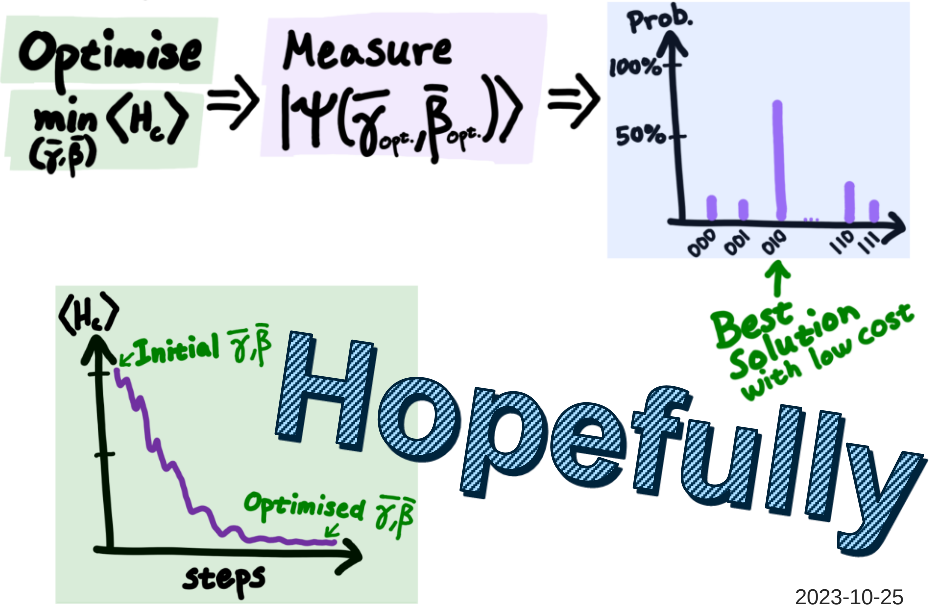




QAOA



$$|\psi(\bar{\gamma},\bar{\beta})\rangle = e^{-i\beta_p H_m} e^{-i\gamma_p H_c} \dots e^{-i\beta_1 H_m} e^{-i\gamma_1 H_c} |\psi_0\rangle$$



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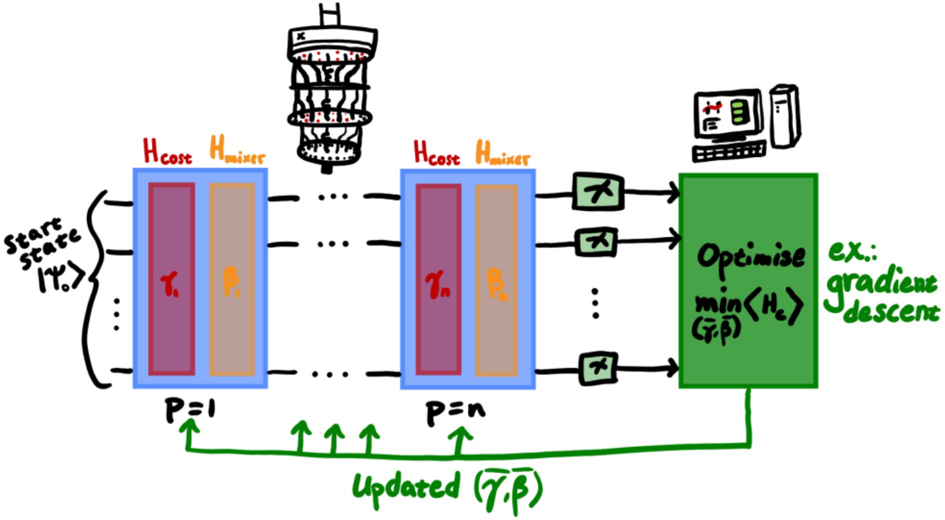

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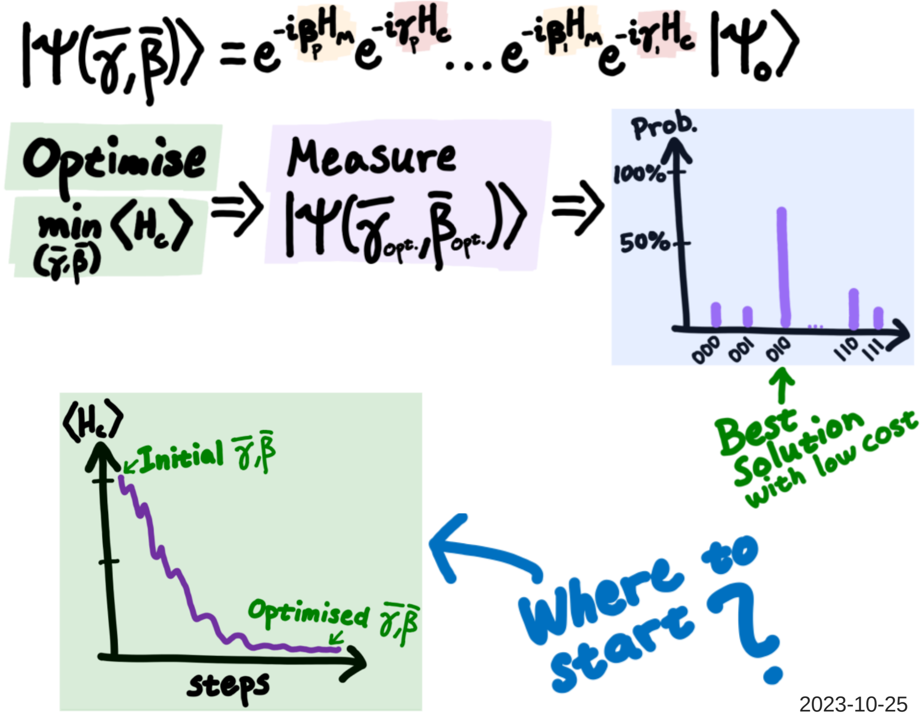

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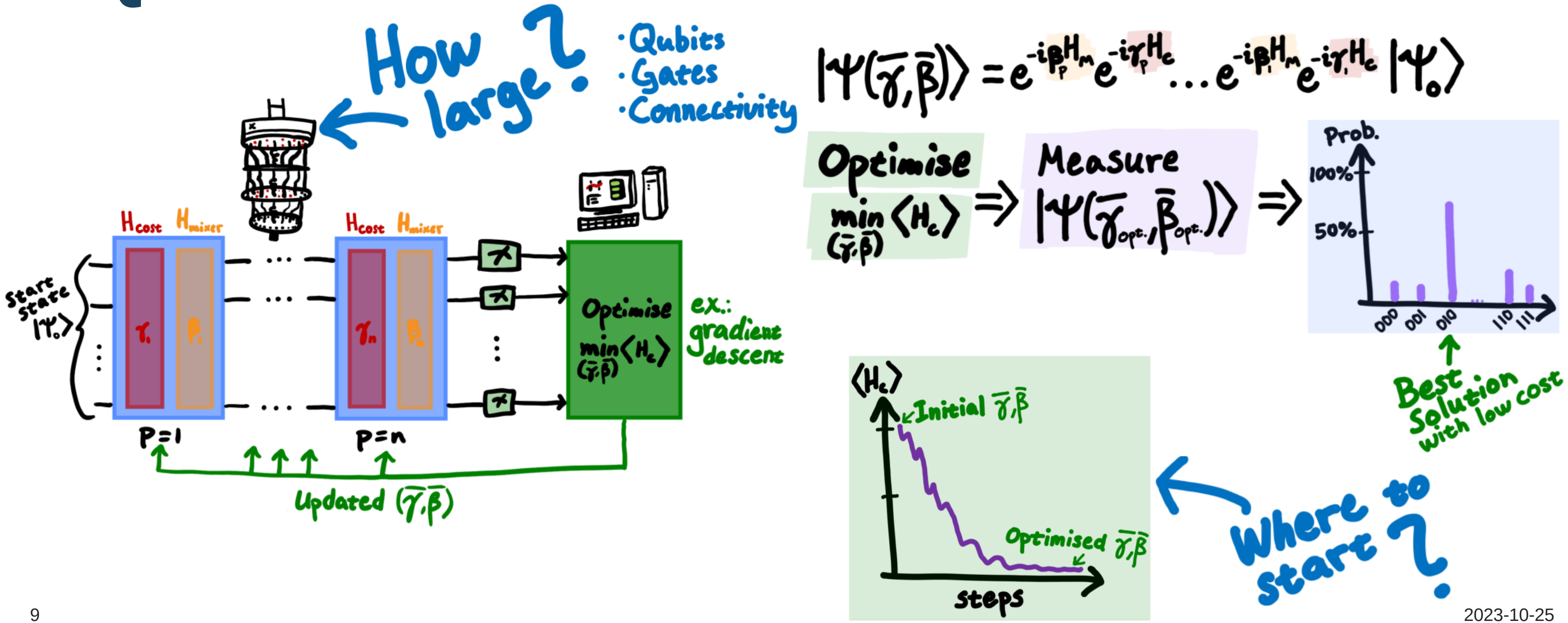
$\min_{(\bar\gamma,\bar\beta)} \langle H_c \rangle$
Measure
$|\psi(\bar\gamma_{opt.},\bar\beta_{opt.})\rangle$
Prob.
100%
50%
000
001
010
110
111
Best Solution with low cost
$\langle H_c \rangle$
Initial $\bar\gamma,\bar\beta$
Optimised $\bar\gamma,\bar\beta$
steps
Where to start?

QAOA


How large?
· Qubits
· Gates
· Connectivity
$|\Psi(\bar{\gamma},\bar{\beta})\rangle = e^{-i\beta_p H_m} e^{-i\gamma_p H_c} \dots e^{-i\beta_1 H_m} e^{-i\gamma_1 H_c} |\Psi_0\rangle$
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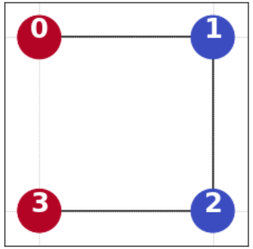
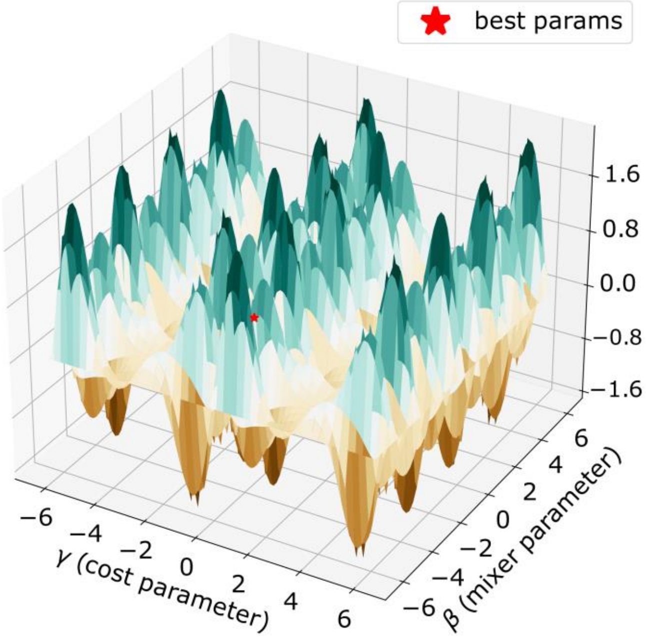
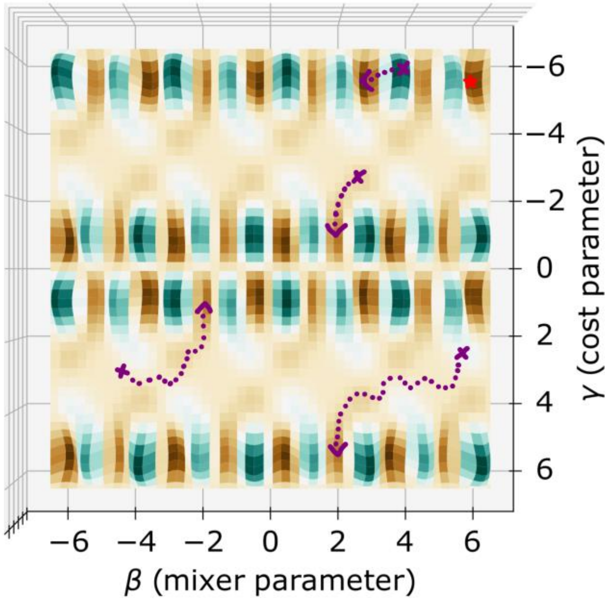
ex.: gradient descent
Updated $(\bar{\gamma},\bar{\beta})$
$\langle H_c \rangle$
Initial $\bar{\gamma},\bar{\beta}$
Optimised $\bar{\gamma},\bar{\beta}$
steps
Where to start?

Energy landscape p=1

Success of measuring best solution $\approx 38\%$



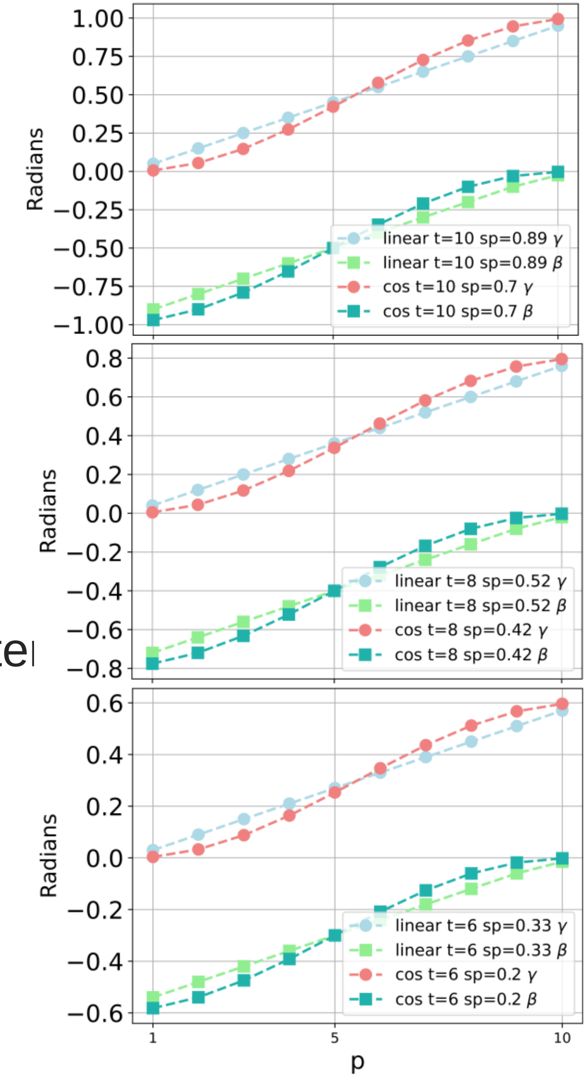




Initial parameters p>1

Where to start?

- Annealing parameters [Sack et al. arXiv:2101.05742 **[quant-ph]**]
  - Linear
  - Cosine (from seeing what it trained to)
- Annealing time t becomes a hyperparameter



Lattice size:

(2,2)

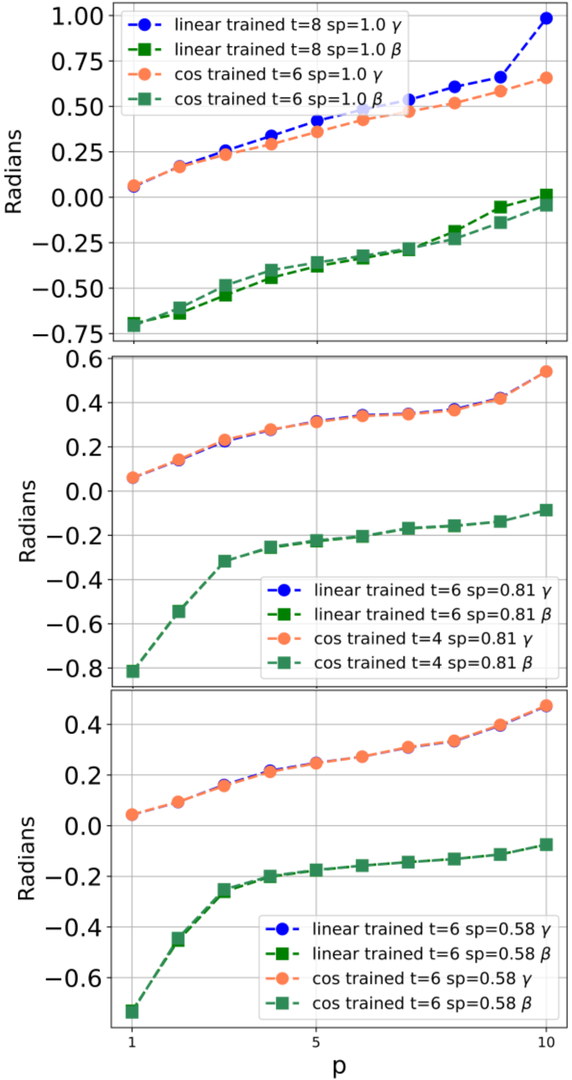
(3,2)

(3,3)

Initial parameters p>1

Where to start?

- Train for 100 steps with Adam optimiser (gradient descent).
- Finds same minima.
- Gives a suggestion of what the best annealing schedule could be.



Lattice size:

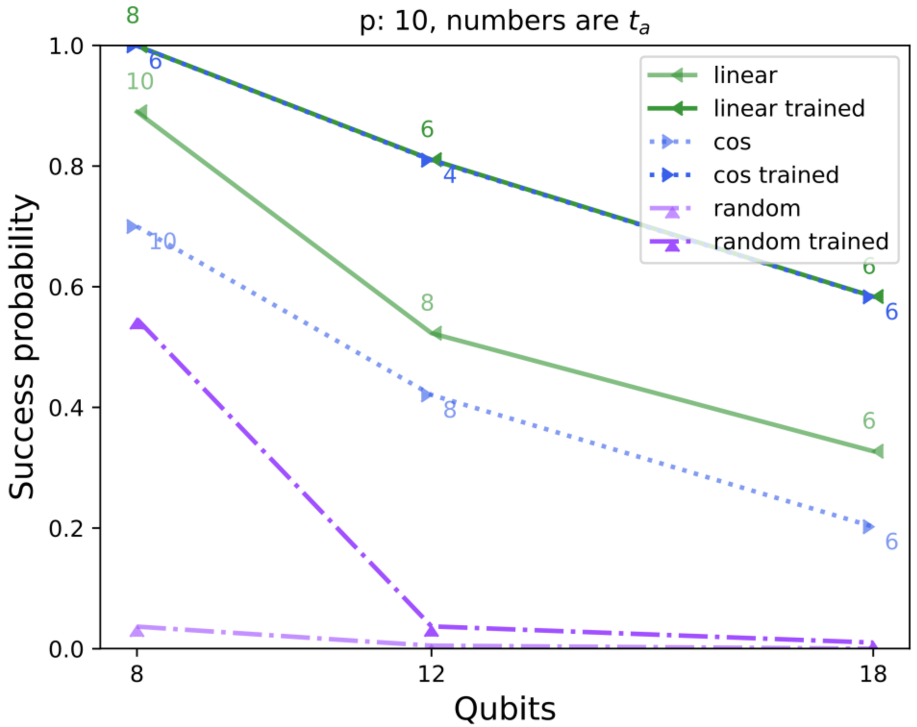
(2,2)

(3,2)

(3,3)

Initial parameters p>1

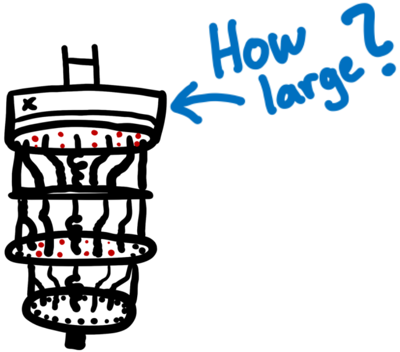
Larger lattices needs more qubits and thereby harder to optimise.



From current proofs of principle to future practical implementations

Resources in a quantum computer

- Resources:
  - Number of qubits
  - Connectivity of the qubits
  - Number of gates
- Protein models:
  - Side-chain conformation-based model
  - HP-Lattice model
    - Turn-based
    - Coordinate-based
- Bit strings encodings:
  - One-Hot
  - Binary
  - BUBinary



Decimal	One-hot	Binary	$\text{BUBinary}_{g=3}$
0	10000	000	00 01
1	01000	001	00 10
2	00100	010	00 11
3	00010	011	01 00
4	00001	111	10 00

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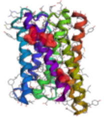
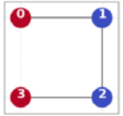
Resources in a quantum computer





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  - Number of qubits
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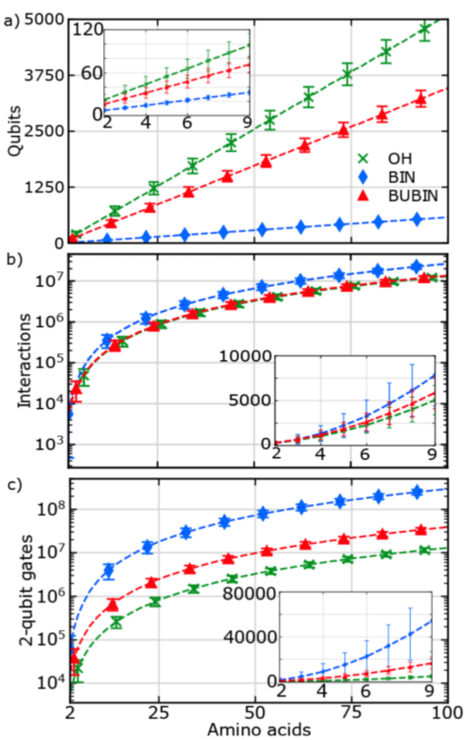
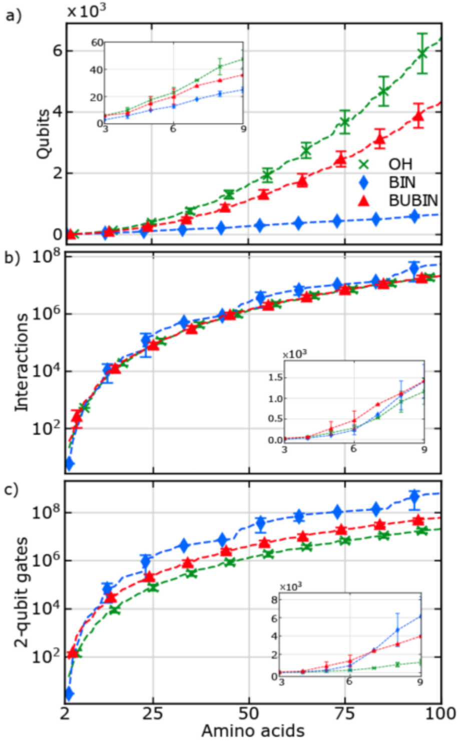
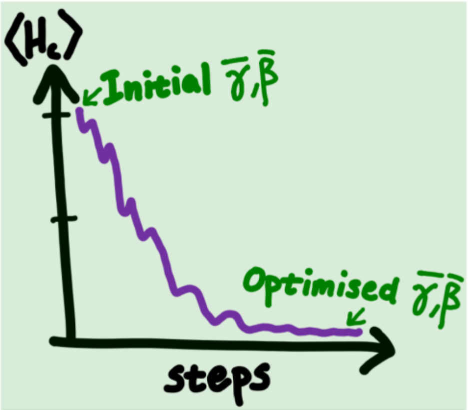
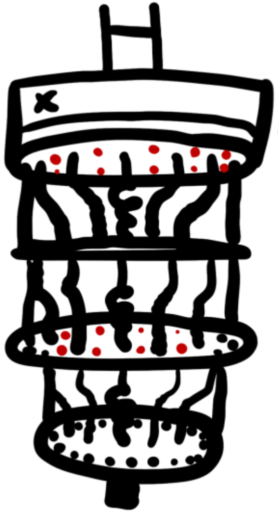




Summary

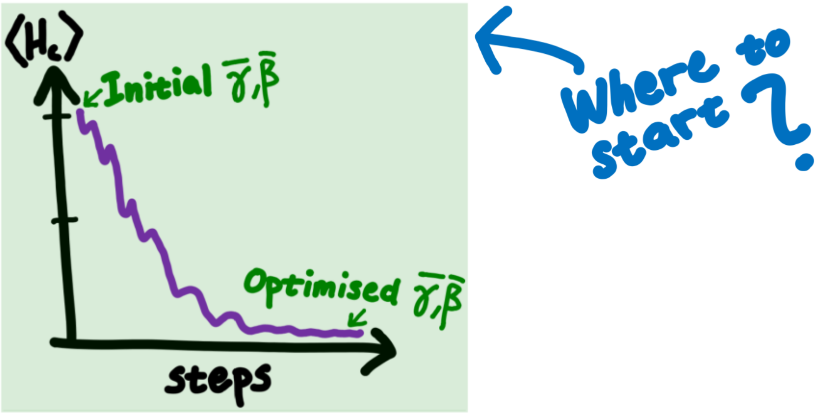


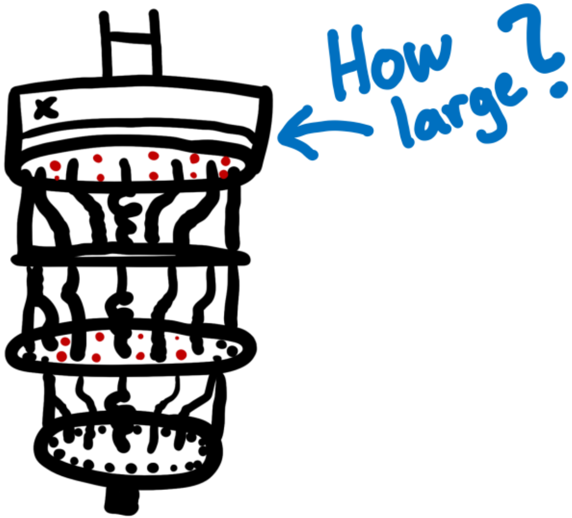
Where to start?



How large?

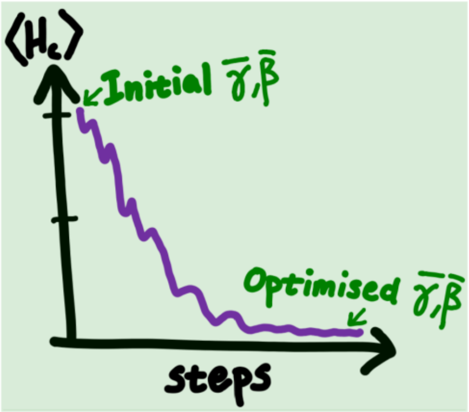
Summary





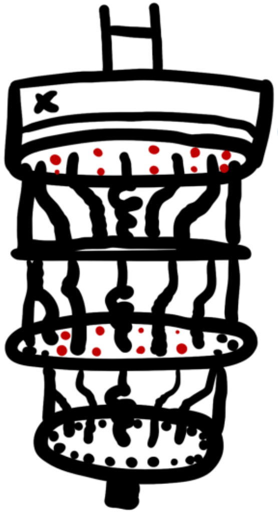
Annealing parameters

Summary



Where to start?

Annealing parameters



How large?

Very large

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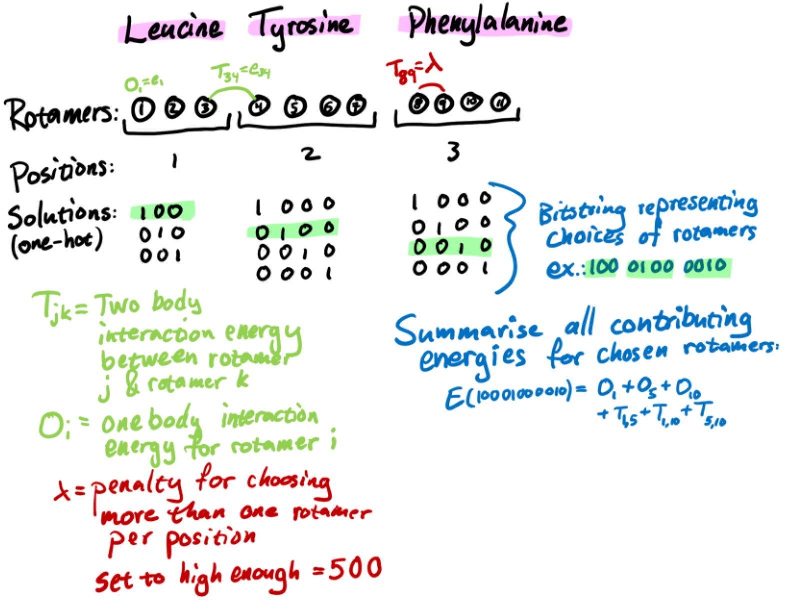
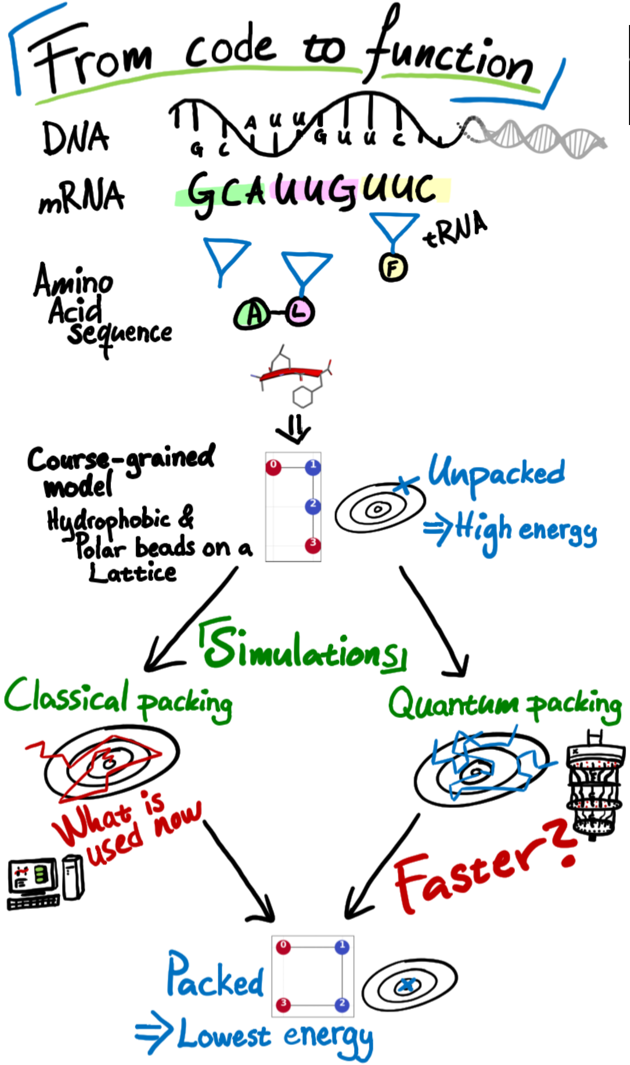
Protein folding simulations

- Rotamer model





Comparison with quantum annealing: Soft suppression