

PHYC90045 Introduction to Quantum Computing

Week 10



Lecture 19
Optimization problems, Encoding problems as energies,
Quadratic Binary Optimization (QUBO), Problem embedding

Lecture 20
Quantum Approximate Optimization Algorithm (QAOA),
Variational Quantum Eigensolver (VQE), classical feedback

Lab 9
Optimization problems

1

PHYC90045 Introduction to Quantum Computing



Hybrid Quantum/Classical Optimization Algorithms

Physics 90045
Lecture 20

2

PHYC90045 Introduction to Quantum Computing

Overview



This lecture we will talk about two algorithms to find the minimum energy of a quantum system:

- Quantum Approximate Optimization Algorithm (QAOA) algorithm
- Variational Quantum Eigen-solver (VQE) algorithm

Both algorithms are closely related, combining classical optimization with quantum mechanical states.

Kaye 8.5
Rieffel 13.4.2

3

PHYC90045 Introduction to Quantum Computing

Review of last lecture

Cost function

Optimal value

Ising coupling

local "field"

Encode

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

We can encode problems in the energy of the system, but we had no way of minimizing the energy. Today we will see a hybrid technique which allows us to minimize the energy of a quantum system.

4

PHYC90045 Introduction to Quantum Computing

Recall Total Energy of the System

Consider a system that has an energy function:

$$E = J_{12}z_1z_2 + J_{23}z_2z_3 + J_{13}z_1z_3 + B_1z_1 + B_2z_2 + B_3z_3$$

where the z_i are $+/-1$, and the J 's and B 's are specific parameters defining the particular problem at hand.

To get ready to map to a QC, we write the total energy as the operator " H " (which physicists would call the "Hamiltonian") on a system of qubits as a sum of these terms with $z_i \rightarrow Z_i$ (where Z_i is the Z operator on the i th qubit):

$$H = J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3 + B_1Z_1 + B_2Z_2 + B_3Z_3$$

Pairwise interactions between qubits Bias on individual qubit

5

PHYC90045 Introduction to Quantum Computing

Mapping the Spin Glass form to QC

Optimisation problems can often be cast into an equivalent "spin glass" form:

$$E = \sum_{i \neq j} J_{ij} z_i z_j + \sum_i B_i z_i$$

-> convert to a convenient form to map onto a quantum computer:

Ising coupling

local "field"

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

The Z_i are now operators defined as per our definitions with eigenvalues $+/-1$ (which can be mapped to binary variables 0/1)

6

PHYC90045 Introduction to Quantum Computing

QUBO Problems

QUBO stands for “Quadratic Unconstrained Binary Optimization”

The cost function (which we want to minimize) is:

$$E(x_1, \dots, x_n) = \sum_i c_i x_i + \sum_{i,j} Q_{ij} x_i x_j$$

Where x_i are Boolean (binary) variables, either 0 or 1.
NB. we will use x for binary, z for $+/1$

Quadratic term

7

PHYC90045 Introduction to Quantum Computing

Binary to energy

Typically when we write such energy functions we write in terms of the Z variables:

$$z_i \quad (\text{lower case } z)$$

But the binary variables in terms of 0 or 1:

$$x_i = 0 \quad \text{or} \quad x_i = 1$$

Can convert between x_i and z_i using:

$$x_i \rightarrow \frac{z_i + 1}{2}$$

8

PHYC90045 Introduction to Quantum Computing

Example: Number partitioning

Given a set, S , of numbers:

1, 3, 8, 10, 6, 5, 5

Is there a partition of this set of numbers into two disjoint subsets R and $S - R$, such that the sum of the elements in both sets is the same?

Yes (in this case): {1, 8, 10} and {3, 6, 5, 5}

9

PHYC90045 Introduction to Quantum Computing

Graph Partitioning to QUBO

1, 3, 8, 10, 6, 5, 5

We assign a qubit to each number in the problem set.
The qubit being zero indicates it is one subset.
The qubit being one indicates it is in the other.

Qubits are $|0\rangle$ if they're in subset 0, $|1\rangle$ if they're in subset 1

10

PHYC90045 Introduction to Quantum Computing

Number partitioning as a QUBO problem

1, 3, 8, 10, 6, 5, 5

As an optimization problem: We want

$$\sum_i w_i z_i = 0$$

The i^{th} number ± 1

Unfortunately if we just minimize this, all the qubits will end up with $z_i = -1$!

11

PHYC90045 Introduction to Quantum Computing

Number partitioning as a QUBO problem

But if we square, we should get a positive solution (or zero). We want to find the assignment of spins which has the minimum energy (ie. closest to zero):

$$H = \left(\sum_i w_i Z_i \right)^2 = \sum_{i \neq j} 2w_i w_j Z_i Z_j + \sum_i w_i^2 I$$

Coupling is the product of numbers

Eg. For the set {1, 2, 3}:

$H = 4Z_1Z_2 + 6Z_1Z_3 + 12Z_2Z_3 + 14I$

Finding minimum energy state will solve the problem!

12

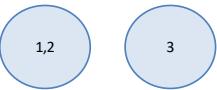
PHYC90045 Introduction to Quantum Computing

Solution for our Number Partitioning



$H = 4Z_1Z_2 + 6Z_1Z_3 + 12Z_2Z_3 + 14I$

Two degenerate solutions: $|110\rangle$ $|001\rangle$



$E = 4 - 6 - 12 + 14 = 0$

And of course, they correctly partition the numbers: $1+2=3$
Other combinations go worse, eg, $|111\rangle$

$E = 4 + 6 + 12 + 14 = 36$

13

PHYC90045 Introduction to Quantum Computing

QAOA Overview



QAOA = “Quantum Approximate Optimization Algorithm”

MIT-CTP/4610

A Quantum Approximate Optimization Algorithm

Edward Farhi and Jeffrey Goldstone
Center for Theoretical Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

Sam Gutmann

Abstract

We introduce a quantum algorithm that produces approximate solutions for combinatorial optimization problems. The algorithm depends on an integer $p \geq 1$ and the quality of the approximation improves as p is increased. The quantum circuit that implements the algorithm consists of unitary gates whose locality is at most the locality of the objective function whose optimum is sought. The depth of the circuit grows linearly with p times (at worst) the number of constraints.

Farhi, Goldstone and Gutmann, 2014

14

PHYC90045 Introduction to Quantum Computing

Structure of Algorithm



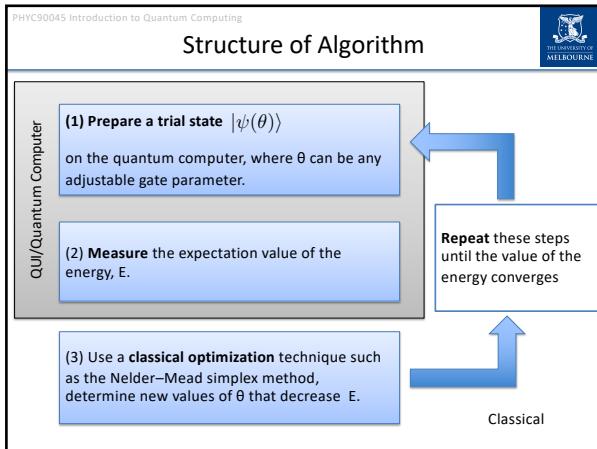
Qu/Quantum Computer

(1) Prepare a trial state $|\psi(\theta)\rangle$
on the quantum computer, where θ represents angles in phase and X rotations.

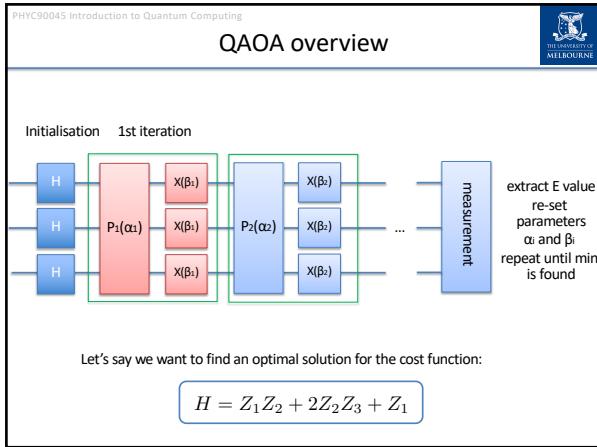
(2) Measure the solution in z basis to obtain the energy, E.

(3) For small depth circuits can analytically calculate optimal values for θ . Original paper found these for a MAX-CUT problem.

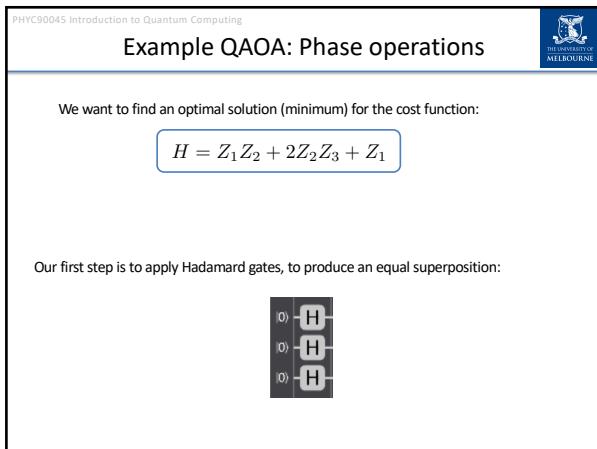
15



16



17



18

PHYC90045 Introduction to Quantum Computing



 THE UNIVERSITY OF
 MELBOURNE

Phase gates in QAOA circuit: $P(\alpha)$

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

For every Z term in the Hamiltonian:



$$H = \dots + B_i Z_i + \dots$$

$$\theta_i = -\frac{B_i \alpha}{2}$$

For every ZZ term in the Hamiltonian:



$$H = \dots + J_{ij} Z_i Z_j + \dots$$

$$\theta_{ij} = -\frac{J_{ij} \alpha}{2}$$

Angles all proportional to their term in the Hamiltonian.

19

PHYC90045 Introduction to Quantum Computing

Phase operation example

Each term's sequence can be placed consecutively. Order of terms does not matter.

$H = Z_1Z_2 + 2Z_2Z_3 + Z_1$

Each term in the cost function gets a gate sequence.

Each rotation angle is proportional to the energy term.

$\theta_{12} = -\frac{\alpha}{2}$

$\theta_{23} = \frac{2\alpha}{2} = -\alpha$

$\theta_1 = -\frac{\alpha}{2}$

20

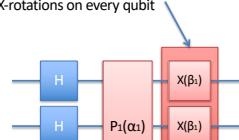
PHYC90045 Introduction to Quantum Computing



 THE UNIVERSITY OF
 MELBOURNE

X-rotations

X-rotations on every qubit



Trial state
 $|\psi(\alpha_1, \beta_1)\rangle$

Preparation of a trial state, for k=1 iterations

21

PHYC90045 Introduction to Quantum Computing


THE UNIVERSITY OF
MELBOURNE

X rotation

After the phase operation, we add x-rotations (again with an angle, β , which we optimize):

A quantum circuit diagram consisting of a single vertical line representing a qubit. Three circular operators, each labeled with an 'X', are positioned along this line. Each operator has a small green arrow pointing to its right, indicating the direction of the rotation.

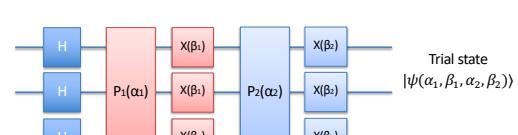
22

PHYC90045 Introduction to Quantum Computing



 THE UNIVERSITY OF
 MELBOURNE

Two iterations



A quantum circuit diagram illustrating the preparation of a trial state for $k=2$ iterations. The circuit consists of four horizontal wires representing qubits. From left to right, the operations are as follows:

- On the first wire (qubit 1), there are three Hadamard gates (H).
- On the second wire (qubit 2), there are two controlled operations: $P_1(\alpha_1)$ followed by a sequence of three $X(\beta_i)$ gates.
- On the third wire (qubit 3), there are two controlled operations: $P_2(\alpha_2)$ followed by a sequence of three $X(\beta_i)$ gates.
- On the fourth wire (qubit 4), there are two controlled operations: $X(\beta_2)$ followed by a sequence of three $X(\beta_i)$ gates.

The final output state is labeled as the Trial state $|\psi(\alpha_1, \beta_1, \alpha_2, \beta_2)\rangle$.

Preparation of a trial state, for $k=2$ iterations

23

PHYC90045 Introduction to Quantum Computing

THE UNIVERSITY OF
MELBOURNE

Measuring the energy

The Hamiltonian of a QUBO problem can be expressed as a sum of several terms:

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

For example:

$$H = B_1 Z_1 + B_2 Z_2 + J_{12} Z_1 Z_2$$

A better approximation to the ground state (depending on the number of steps, k, and the choice of angles) will have a higher probability of measuring the minimum energy, and the lowest energy state.

24

PHYC90045 Introduction to Quantum Computing

One round QAOA

The whole circuit (using just one round, $p=1$) is therefore:

Using values of $\alpha = 0.2\pi$ and $\beta = -0.1\pi$, we get:

Here 101 is the solution. We have not optimized the angles at all, but already you can see (even on our first try) that its amplitude has increased. Optimising the angles would increase it further.

25

PHYC90045 Introduction to Quantum Computing

One round QAOA

The whole circuit (using just one round, $p=1$) is therefore:

Using values of $\alpha = 0.2\pi$ and $\beta = -0.1\pi$, we get:

Work out the average energy, adjust the angles and rerun the experiment, until we come to a minimum energy.

26

PHYC90045 Introduction to Quantum Computing

Calculating the average energy

$$E = \langle Z_1 Z_2 \rangle + 2 \langle Z_2 Z_3 \rangle + \langle Z_1 \rangle$$

$$E = p_{000}E_{000} + p_{001}E_{001} + \dots + p_{111}E_{111}$$

For the $|000\rangle$ state $\begin{cases} Z_1 = 1 \\ Z_2 = 1 \\ Z_3 = 1 \end{cases} \longrightarrow E_{000} = 1 + 2 + 1$

Adjust the circuit parameters (according to classical optimization algorithm) and repeat to minimize the expectation of energy!

27

PHYC90045 Introduction to Quantum Computing

Calculating the energy

$H = Z_1 Z_2 + 2Z_2 Z_3 + Z_1$

State, i	Z_1	Z_2	Z_3	$Z_1 Z_2$	$Z_2 Z_3$	Z_1	E_i
$ 000\rangle$	1	1	1	1	1	1	4
$ 001\rangle$	1	1	-1	1	-1	1	0
$ 010\rangle$	1	-1	1	-1	-1	1	-2
$ 011\rangle$	1	-1	-1	-1	1	1	2
$ 100\rangle$	-1	1	1	-1	1	-1	0
$ 101\rangle$	-1	1	-1	-1	-1	-1	-4
$ 110\rangle$	-1	-1	1	1	-1	-1	-2
$ 111\rangle$	-1	-1	-1	1	1	-1	2

28

PHYC90045 Introduction to Quantum Computing

Calculating the average energy

Obtained from running quantum computer

State, i	E_i	Probability, p_i	$p_i E_i$
$ 000\rangle$	4	0%	0
$ 001\rangle$	0	20%	0
$ 010\rangle$	-2	20%	-0.4
$ 011\rangle$	2	0%	0
$ 100\rangle$	0	10%	0
$ 101\rangle$	-4	40%	-1.6
$ 110\rangle$	-2	0%	0
$ 111\rangle$	2	10%	0.2

*Made up probabilities for demonstration!

Calculate the average energy: $E = \sum_i p_i E_i = -1.8$

29

PHYC90045 Introduction to Quantum Computing

Measure to find energy

Measure Z:



In the QUI you can look directly at probabilities rather than measure and building statistics!

Unlike for QEC codes, you don't need to add an extra qubit to measure correlations. Eg. For ZZ you can just multiply yourself for a given state!

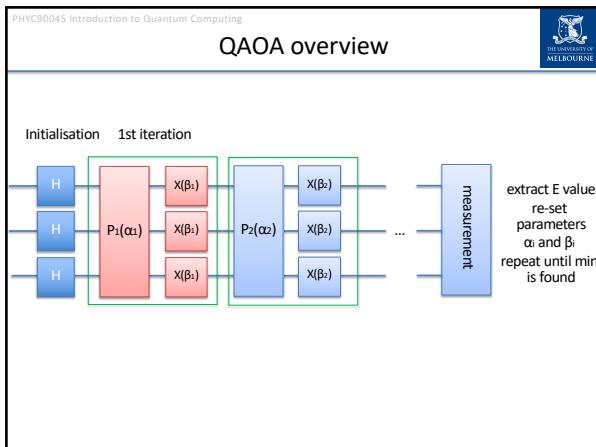
30

PHYC90045 Introduction to Quantum Computing

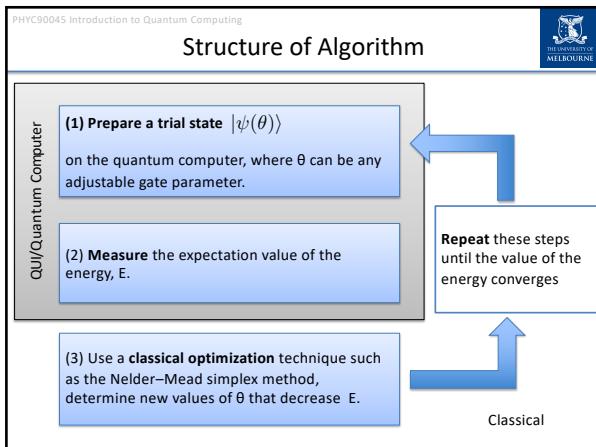

THE UNIVERSITY OF
MELBOURNE

Multiple measurements

31



32



33

PHYC90045 Introduction to Quantum Computing

THE UNIVERSITY OF
MELBOURNE

VQE overview

VQE = Variational Quantum Eigensolver

We need not confine ourselves to Ising/Z terms. Many interesting quantum systems have a Hamiltonian, H , which includes terms in X and Y (and might not even come from a qubit system at all!).

Or perhaps we have a Hermitian matrix, and we just want to find the smallest eigenvalue. How do we do that?

- 1) Pick a convenient basis to express H
- 2) Write out the total energy, H , as a matrix
- 3) Convert your matrix a linear combination of Pauli matrices
- 4) Parameterize an "Ansatz" wavefunction candidate solution to problem
- 5) Use hybrid classical/quantum optimization to find the lowest energy and lowest energy state.

34

PHYC90045 Introduction to Quantum Computing

Structure of Algorithm

```
graph TD; A["(1) Prepare a trial state |ψ(θ)⟩"] --> B["(2) Measure the expectation value of the energy, E."]; B --> C["(3) Use a classical optimization technique such as the Nelder–Mead simplex method, determine new values of θ that decrease E."]; C --> B; D["Repeat these steps until the value of the energy converges"]
```

The diagram illustrates the structure of an algorithm for quantum computing. It consists of three main steps enclosed in a large grey box:

- (1) Prepare a trial state $|\psi(\theta)\rangle$**

on the quantum computer, where θ can be any adjustable gate parameter.
- (2) Measure the expectation value of the energy, E.**
- (3) Use a classical optimization technique such as the Nelder–Mead simplex method, determine new values of θ that decrease E.**

Blue arrows indicate a feedback loop from step 3 back to step 2. To the left of the box, the text "Q# / Quantum Computer" is written vertically. To the right, a blue arrow points upwards with the label "Classical" below it, pointing towards step 3. Above the box, the text "Repeat these steps until the value of the energy converges" is written, with a blue arrow pointing to it from the top right.

35

PHYC90045 Introduction to Quantum Co Hamiltonian as
linear combination of Pauli operators



36

PHYC90045 Introduction to Quantum Computing

Find the expectation value of H

We can express the expectation value of the energy as a sum of expectation values of the Paulis:

$$\langle H \rangle = \sum_i E_i \langle \sigma_i \rangle$$

For our example:

$$\langle H \rangle = B_1 \langle X_1 \rangle + B_2 \langle X_2 \rangle + J_{12} \langle Z_1 Z_2 \rangle$$

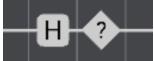
For a given trial state, these can be found directly from experiment (or through the QUI)

37

PHYC90045 Introduction to Quantum Computing

Reminder: How to measure Paulis

Measure X:



Measure Y:



In the QUI you record probabilities rather than measure and building statistics!

Measure Z:



Unlike for QEC codes, you don't need to add an extra qubit to measure correlations. Eg. For ZZ you can just multiply yourself given the state which is measured!

38

PHYC90045 Introduction to Quantum Computing

VQE: Jordan Wigner Transformation

A classic of physics from 1928, by Jordan and Wigner. You've got a system of qubits. You want to use it to simulate fermions (eg. someone's given you a chemistry problem involving electrons). Electrons do not behave the same as qubits.

How do we do this?

Tempting solution:

$$\sigma_j^+ \rightarrow \frac{X_j + iY_j}{2} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}_j = f_j^+ \quad \text{Create a fermion at the } j^{\text{th}} \text{ site?}$$

$$\sigma_j^- \rightarrow \frac{X_j - iY_j}{2} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}_j = f_j^- \quad \text{Destroy a fermion at the } j^{\text{th}} \text{ site?}$$

This is close but **WRONG!** The commutation relations between different sites are wrong (fermions anti-commute). $[f_j, f_k] = 0$

39

PHYC90045 Introduction to Quantum Computing



THE UNIVERSITY OF
MELBOURNE

Jordan Wigner Transformation

Correct solution:

$$\sigma_j^+ \rightarrow Z_1 Z_2 \dots Z_{j-1} \frac{X_j + iY_j}{2}$$

$$\sigma_j^- \rightarrow Z_1 Z_2 \dots Z_{j-1} \frac{X_j - iY_j}{2}$$

Jordan and Wigner: Images from Wikipedia

40

PHYC90045 Introduction to Quantum Computing

Picking a VQE Ansatz



QAOA State

Use a combination of X rotations and phase rotations.

Adiabatic Methods

Slowly vary the Hamiltonian, in a parameterized way, to obtain an approximation to the ground state.

Coupled Cluster Methods

First start in a (often unentangled) reference state, which can be calculated classically, eg. with mean field methods.

Consider successively more complicated perturbations away from this reference state: First we consider just (parameterized) single qubit rotations away from the reference state. Then we consider unitaries with both single qubit rotations and two body interactions, then one, two and three body interactions. As with QAOA we can consider several rounds of interaction.

41

PHYC90045 Introduction to Quantum Computing



 THE UNIVERSITY OF
 MELBOURNE

Nelder-Mead Classical Optimization

A classical method of optimization.

- Classical optimization technique
- Requires only the calculation of few points at each step

Based on simplex:

A *simplex* S in n dimension is defined as the convex hull of $n+1$ vertices: x_0, \dots, x_n

Eg. Triangle in 2D



42

PHYC90045 Introduction to Quantum Computing

Nelder-Mead operations

Start with an initial simplex
Repeat until the convergence is reached:
Test if we've reached convergence
If not then transform the working simplex

Four types of transformation to test:

1) Reflection

Worst point Centroid of all other points

43

PHYC90045 Introduction to Quantum Computing

Nelder-Mead operations

2) Expand

Worst point Centroid of all other points

3) Contract

Worst point Centroid of all other points

4) Shrink

44

PHYC90045 Introduction to Quantum Computing

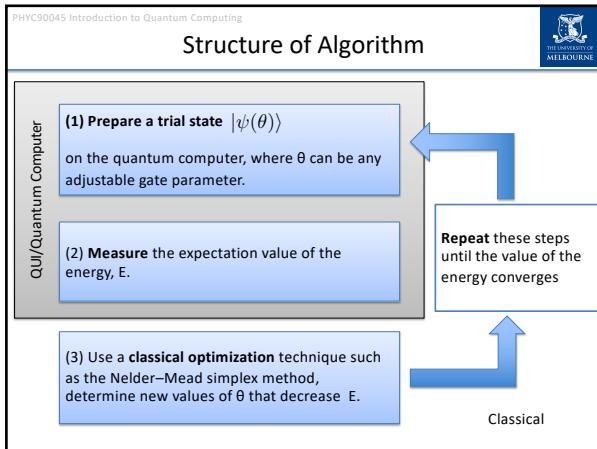
Visualization

x_1

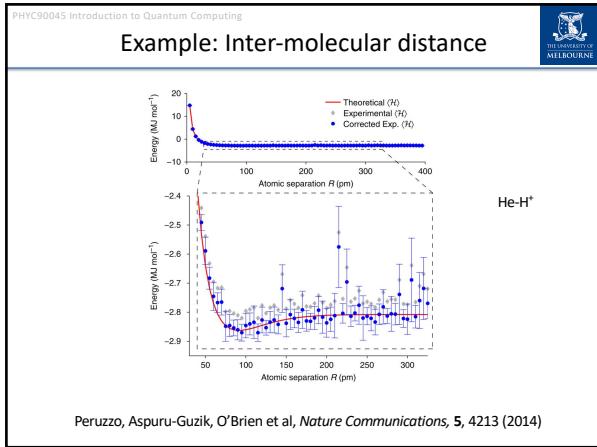
x_2

Image: Nicoguaro, Wikipedia

45



46



47

PHYC90045 Introduction to Quantum Computing

Week 10

Lecture 19
Optimization problems, Encoding problems as energies, Quadratic Binary Optimization (QUBO), Problem embedding

Lecture 20
Quantum Approximate Optimization Algorithm (QAOA), Variational Quantum Eigensolver (VQE), classical feedback

Lab 9
Optimization problems

48