PHYC90045 Introduction to Quantum Computing

Week 10

Lecture 19
Quantum Approximate Optimization Algorithm (QAOA), Variational Quantum Eigensolver (VQE), classical feedback

Lecture 20
Exponentials, and Quantum Optimization

Lab 10
Optimization problems

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Matrix Exponentiation

Physics 90045
Lecture 19

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Overview

This lecture we will introduce useful tools for mapping problems to a quantum computing framework:

- Power series
- Gates as exponentials
- Rotations as exponentials
- BCH Formula
- "Trotter" to add exponents
- Cartan Decomposition

Kaye 8.5
Reiffel 13.4.2

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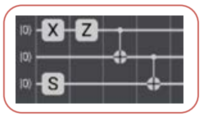
Hamiltonians and gates...

We've been using matrices to represent both gates and Hamiltonians.

Gates on the QC



Operators are represented by a **unitary** matrix

$$V^\dagger V = I$$

Operators form a *group*.

Problem Hamiltonians

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

Observables (like total energy) are represented by a **Hermitian** matrix

$$H^\dagger = H$$

Observables form an algebra.

Beware, "H" is used for Hadamard and Hamiltonian, but they are different!

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Exponentiation of Operators

There is a deep relationship in QM between the Hamiltonian and gates in a circuit.

A circuit represents "evolution" of a quantum state through the action of gate operators.

In general a system evolves via an operator U through the exponentiation of an underlying Hamiltonian:

$$U = \exp(iHt)$$

Evolution operator

e.g. a gate in the circuit

Hamiltonian – two types

1. Of the QC itself to implement a gate, e.g. Z

2. Of the problem being mapped to the QC

We will first look at what exponentiation of operators (matrices) means mathematically...

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Power series

Power series (Taylor/Maclaurin series):

$$\exp(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

Power series for trigonometric functions:

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \ldots$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} \ldots$$

Complex Numbers: Exponential form

We can use this to prove useful things. For example consider:

$$\exp(i\theta) = 1 + i\theta - \frac{\theta^2}{2} - i\frac{\theta^3}{3!} + \frac{\theta^4}{4!} + i\frac{\theta^5}{5!} - \dots$$

Comparing to power series for trigonometric functions:

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} \dots$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \dots$$

We can prove that

$$\exp(i\theta) = \cos\theta + i\sin\theta$$

Matrix Exponentiation

By analogy we can define the exponential of a matrix to be:

$$\exp(A) = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \dots$$

Matrix equation

Compare to the equation for real/complex numbers

$$\exp(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

Rotations as a matrix exponential

Consider:

$$\exp(i\theta Z) = I + i\theta Z - \frac{\theta^2 Z^2}{2} - i\frac{\theta^3 Z^3}{3!} + \frac{\theta^4 Z^4}{4!} + i\frac{\theta^5 Z^5}{5!} - \dots$$

Using the fact that $Z^2 = I$

$$\begin{aligned}\exp(i\theta Z) &= I + i\theta Z - \frac{\theta^2}{2}I - i\frac{\theta^3}{3!}Z + \frac{\theta^4}{4!}I + i\frac{\theta^5}{5!}Z - \dots \\ &= (1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!} + \dots)I + i(\theta - \frac{\theta^3}{3!} + \dots)Z \\ &= \cos(\theta)I + i\sin(\theta)Z\end{aligned}$$

i.e. the rotation matrix around Z-axis!

Z-rotations

$$\exp(i\theta Z) = I + i\theta Z - \frac{\theta^2}{2}I - i\frac{\theta^3}{3!}Z + \frac{\theta^4}{4!}I + i\frac{\theta^5}{5!}Z - \ldots$$
$$= (1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!} + \ldots)I + i(\theta - \frac{\theta^3}{3!} + \ldots)Z$$
$$= \cos(\theta)I + i\sin(\theta)Z$$

$$R_z(\theta) = \exp\left(-\frac{i\theta}{2}Z\right)$$

put in
-ve sign

Compare with our R-gate
(with zero global phase)

$$R_z(\theta_R) = e^{i\theta_g}\left(I\cos\left(\frac{\theta_R}{2}\right) - iZ\sin\left(\frac{\theta_R}{2}\right)\right)$$

Rotations around other axes

The only fact we used the fact that Z squares to the identity. Other axes work in a similar way.

$$R_x(\theta) = \exp\left(-\frac{i\theta}{2}X\right)$$

$$R_y(\theta) = \exp\left(-\frac{i\theta}{2}Y\right)$$

$$R_z(\theta) = \exp\left(-\frac{i\theta}{2}Z\right)$$

Arbitrary axis rotation as matrix exponential

Consider any unit vector, n:

$$(n_xX + n_yY + n_zZ)^2 = (n_x^2 + n_y^2 + n_z^2)I +$$
$$n_xn_z(XZ + ZX) + n_yn_z(YZ + ZY) + n_xn_z(XZ + ZX)$$
$$= (n_x^2 + n_y^2 + n_z^2)I$$
$$= I$$

Like Z, this squares to the identity.

An arbitrary rotation of one qubit can be expressed:

$$R_n(\theta) = \exp\left(-\frac{i\theta}{2}\hat{n}\cdot\sigma\right) = \cos\frac{\theta}{2} - i\sin\frac{\theta}{2}(\hat{n}\cdot\sigma)$$

Exponentiation of two qubit operators

Not only do single qubit operators square to the identity, we can consider:

If $$(Z \otimes Z)(Z \otimes Z) = I$$

So just like for a single qubit rotations, we could use a power series to show:

Then $$\exp\left(i\theta Z \otimes Z\right) = \cos(\theta) I + i \sin(\theta) Z \otimes Z$$

Eigenvalues and exponentiation

Consider an eigenvalue decomposition of a matrix, A

$$A = VDV^\dagger$$

Here V is unitary, D is diagonal and real. We can find powers:

$$\begin{aligned} A &= VDV^\dagger \\ A^2 &= VDV^\dagger VDV^\dagger = VD^2V^\dagger \\ A^3 &= \ldots = VD^3V^\dagger \\ A^n &= VD^nV^\dagger \end{aligned}$$

And taking powers of a diagonal matrix is the same as taking the power of each of the diagonal entries.

Applied to exponentiation

U is unitary, D is diagonal with the entries on the diagonal equal to the eigenvalues.

$$\exp(A) = I + A + \frac{A}{2} + \frac{A^3}{3!} + \frac{A^4}{4!} + \ldots$$

So, using the powers of A from the previous slide:

$$\begin{aligned} \exp(A) &= I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \frac{A^4}{4!} + \ldots \\ &= V\left(I + D + \frac{D^2}{2} + \frac{D^3}{3!} + \frac{D^4}{4!} + \ldots\right)V^\dagger \\ &= V\exp(D)V^\dagger \end{aligned}$$

Simply exponentiate the eigenvalues/diagonal of D matrix.

Conjugating with V and V inverse

$$\exp(A) = \exp(VDV^\dagger) = V\exp(D)V^\dagger$$

Conjugating in the exponent

Conjugating with a gate and its inverse eg. In QUI.

Example: CZ gate

$$CZ = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} e^{i0} & 0 & 0 & 0 \\ 0 & e^{i0} & 0 & 0 \\ 0 & 0 & e^{i0} & 0 \\ 0 & 0 & 0 & e^{i\pi} \end{bmatrix}$$

$$CZ = \exp\left(i\pi \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\right)$$

Matrix as linear combination of Pauli operators

Always possible decompose a matrix as a sum of Pauli products. If you have a matrix only:

$$E_i = \frac{\mathrm{Tr}\left[\sigma_i H\right]}{d} \qquad \sigma_i = XI, IX, ...XZ, ...ZZ$$

Where d is the dimension of the system (d=4 for 2 qubits), H is the Hamiltonian and σ_i is the Pauli. If the matrix is Hermitian, the co-efficients you find, E_i, should be real.

Express the Hamiltonian as linear combination of Pauli matrix products:

$$H = \sum_i E_i \sigma_i$$

For example: $H = B_1X_1 + B_2X_2 + J_{12}Z_1Z_2$

CZ Gate continued

$$CZ = \exp\left(i\pi\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{bmatrix}\right)$$

$$\frac{II - IZ - ZI + ZZ}{4}$$

$$CZ = \exp\left(i\frac{\pi}{4}II - i\frac{\pi}{4}ZI - i\frac{\pi}{4}IZ + i\frac{\pi}{4}ZZ\right)$$

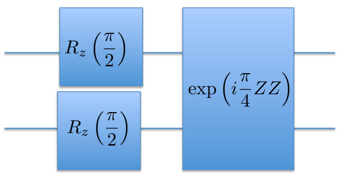
All the terms commute, so

$$CZ = \exp\left(i\frac{\pi}{4}II\right)\exp\left(-i\frac{\pi}{4}ZI\right)\exp\left(-i\frac{\pi}{4}IZ\right)\exp\left(+i\frac{\pi}{4}ZZ\right)$$

Global phase Single qubit rotations Interaction

CZ Circuit

$$CZ = \exp\left(i\frac{\pi}{4}II\right)\exp\left(-i\frac{\pi}{4}ZI\right)\exp\left(-i\frac{\pi}{4}IZ\right)\exp\left(+i\frac{\pi}{4}ZZ\right)$$



Using $R_z(\theta) = \exp\left(-\frac{i\theta}{2}Z\right)$

Example: CNOT gate in exponent form

$$CZ = \exp\left(i\frac{\pi}{4}II\right)\exp\left(-i\frac{\pi}{4}ZI\right)\exp\left(-i\frac{\pi}{4}IZ\right)\exp\left(+i\frac{\pi}{4}ZZ\right)$$

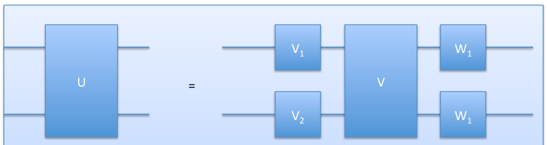
Global phase Single qubit rotations Interaction

We can work out how CNOT can be expressed as an exponent:

$$\begin{aligned} CNOT &= I\otimes H \quad CZ \quad I\otimes H \\ &= I\otimes H \quad \exp\left(i\pi\frac{II - ZI - IZ + ZZ}{4}\right) \quad I\otimes H \\ &= \exp\left(i\pi\frac{II - ZI - IX + ZX}{4}\right)\end{aligned}$$

Cartan Decomposition

Known as the Cartan or KAK decomposition:



The interacting part, V, depends on just three parameters:

$$V = \exp(i\theta_x XX + i\theta_y YY + i\theta_z ZZ)$$

All of these terms commute, so the order doesn't matter. Can be implemented separately.

Warning about non-commuting operators

Warning:

$$\exp(A)\exp(B) \neq \exp(A+B)$$

Unless A and B commute! (see CZ example)

Baker-Campbell-Hausdorff formula

First few terms of the BCH formula:

$$\exp(A)\exp(B) = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}([A,[A,B]] + [B,[B,A]] + \ldots\right)$$

Higher order terms involve commutators

Where the commutator is given by

$$[A,B] = AB - BA$$

Question for you

$$[X,Y] = ?$$
$$[Y,Z] = ?$$
$$[Z,X] = ?$$

Given:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\boxed{[A,B] = AB - BA}$$

Commutators of Paulis

$$[X,Y] = 2iZ$$
$$[Y,Z] = 2iX$$
$$[Z,X] = 2iY$$

Baker-Campbell-Hausdorff formula

First few terms of the BCH formula:

$$\exp(A)\exp(B) = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}([A,[A,B]] + [B,[B,A]] + \ldots\right)$$

Higher order terms involve commutators

Where the commutator is given by

$$\boxed{[A,B] = AB - BA}$$

Trotter Approximation

But what if you do want to create the gate:

$$\exp(A+B)$$

We might try:

$$\exp(A+B) \approx \exp(A)\exp(B)$$

$$\exp(A+B) \approx \exp\left(\frac{A}{2}\right)\exp\left(\frac{B}{2}\right)\exp\left(\frac{A}{2}\right)\exp\left(\frac{B}{2}\right)$$

$$\boxed{\exp(A+B) \approx \left(\exp\left(\frac{A}{n}\right)\exp\left(\frac{B}{n}\right)\right)^n}$$

This is called the Trotter (sometimes Trotter-Suzuki) approximation – useful!

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Lie Algebras and Lie Groups

$$U = \exp(iHt)$$

$SU(n)$

"Special" unitary Lie group

Det(U) = 1
U is unitary

These operations you can implement using QUI

$\mathfrak{su}(n)$

Lie algebra

iHt is anti-Hermitian
Traceless

Like using phase in complex numbers, this can help!

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Problem Hamiltonians

Now consider the "Hamiltonian" associated with a particular problem, e.g.

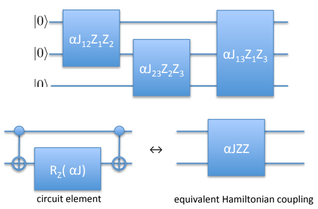
$$H = J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3$$

(set t = - α/2, to absorb factor of 2)

Evolution operator is:

$$U = \exp[-iH\alpha/2] = \exp[-(i\alpha/2)(J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3)]$$
$$= \exp[-(i\alpha/2)(J_{12}Z_1Z_2)]\exp[-(i\alpha/2)(J_{23}Z_2Z_3)]\exp[-(i\alpha/2)(J_{13}Z_1Z_3)]$$

Equivalent circuit is:



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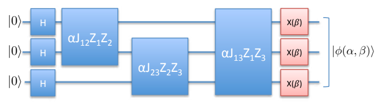
$$H = J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3$$

(set t = - α/2, to absorb factor of 2)

Evolution operator is:

$$\begin{aligned} U &= \exp\left[-iH\alpha/2\right] = \exp\left[-(i\alpha/2)\left(J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3\right)\right] \\ &= \exp\left[-(i\alpha/2)\left(J_{12}Z_1Z_2\right)\right]\exp\left[-(i\alpha/2)\left(J_{23}Z_2Z_3\right)\right]\exp\left[-(i\alpha/2)\left(J_{13}Z_1Z_3\right)\right] \end{aligned}$$

This is the basis for encoding the QAOA trial state for the problem Hamiltonian:



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