Tricks

$H_f|x\rangle = f(x)|x\rangle$ - eigenvalue equation

$|\psi\rangle = \sum_x \alpha_x |x\rangle$ - eigen vectors are complete
linear combination of basis vectors

$\langle x|\psi\rangle = \langle x|\sum_y \alpha_y|y\rangle = \sum_y \langle x|y\rangle = \alpha_x\langle x|x\rangle = \alpha_x$

Expectation Value

eigenvalue

$$\langle\psi|H_f|\psi\rangle = \sum_{x,y} \alpha_y^* \alpha_x \langle y|H_f|x\rangle = \sum_{x,y} \alpha_y^* \alpha_x f(x)\langle y|x\rangle$$

$$= \sum_x \alpha_x^* \alpha_x f(x) = \sum_x |\alpha_x|^2 f(x)$$

Probability: $|\alpha_x|^2 = |\langle x|\psi\rangle|^2$

Operators

$A|\lambda_j^k\rangle = \lambda_j|\lambda_j^k\rangle$ multiple eigenvectors per eigenvalue

- Hermitian Operators: $A^\dagger = A$
- Guarenteed real eigenvalues
- Possible measurement are $\lambda_1 \dots \lambda_j$
- generic superposition: $\sum_j \alpha_j^k|\lambda_j^k\rangle$ collapse: $\dfrac{\sum_k \alpha_j^k|\lambda_j^k\rangle}{\sqrt{\sum_k|\alpha_j^k|^2}}$

measure first qubit as zero

2 qubit: $\dfrac{a_{00}|00\rangle + a_{01}|01\rangle}{\sqrt{|a_{00}|^2 + |a_{01}|^2}}$

Computational Basis Operators

$N = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ $\quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ← 1 qubit

$\lambda = 0, 1$ $\quad \lambda = -1, 1$

Expectation Value

$$\langle A\rangle_\psi = \sum_{j,k} \overset{\text{probability}}{\left|\langle \lambda_j^k|\psi\rangle\right|^2} \overset{\text{value}}{\lambda_j}$$ - typical expected value

$$= \sum_{j,k} \langle \lambda_j^k|\psi\rangle^* \langle \lambda_j^k|\psi\rangle \lambda_j$$

$$= \sum_{j,k} \langle \psi|\lambda_j^k\rangle \langle \lambda_j^k|\psi\rangle \lambda_j$$

$$= \sum_{j,k} \langle \lambda_j^k|\psi\rangle \langle \psi|\lambda_j^k\rangle \lambda_j$$

$$= \sum_{j,k} \langle \lambda_j^k|\psi\rangle \langle \psi|\overset{\text{eigenvalue}}{\lambda_j}|\lambda_j^k\rangle$$

$$= \sum_{j,k} \langle \lambda_j^k|\psi\rangle \langle \psi|A|\lambda_j^k\rangle$$

$$= \langle \psi|A \sum_{j,k} \langle \lambda_j^k|\psi\rangle |\lambda_j^k\rangle$$

$$= \langle \psi|A \sum_{j,k} \alpha_j^k |\lambda_j^k\rangle$$

$$= \langle \psi|A|\psi\rangle$$

Variational Principle

$$\langle A \rangle_\psi = \sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2 \lambda_j \geq \underbrace{\sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2}_{\text{all prob} = 1} \lambda_0 = \lambda_0$$

→ Any observable can be represented as the tensor product of pauli matrices

Example: $\langle \psi | \frac{1}{2} Z \otimes I \otimes X - 3 I \otimes Y \otimes Y | \psi \rangle$ (linearity)

$= \frac{1}{2} \langle \psi | Z \otimes I \otimes X | \psi \rangle - 3 \langle \psi | I \otimes Y \otimes Y | \psi \rangle$

VQE General Buildup

1) Eigenvalue Equation

$$H|x\rangle = f(x)|x\rangle$$

2) Wavefunction can be decomposed into linear combination of eigenstates

$$|\psi\rangle = \sum_x \alpha_x |x\rangle$$

3) An expectation value can be calculated as follows:

$$\langle\psi|H|\psi\rangle = \sum_{x,y} \alpha_y^* \alpha_x \langle y|H|x\rangle = \sum_{x,y} \alpha_y^* \alpha_x \overbrace{f(x)}^{\text{eigenvalue eq}}\langle y|x\rangle = \sum_x |\alpha_x|^2 f(x)$$

4) Superscript notation: we are considering multiple eigenvectors for the same eigenvalue

$$A|\lambda_j^k\rangle = \lambda_j|\lambda_j^k\rangle$$

5) Probability for a given state x:

$$\langle x|\psi\rangle = \alpha_x$$

6) Expectation Value for any Hermitian Operator:

$$\langle A\rangle_\psi = \sum_{j,k} |\langle\lambda_j^k|\psi\rangle|^2 \lambda_j = \langle\psi|A|\psi\rangle$$

7) Linearity Trick (A has multiple terms) $A = \frac{1}{2} Z\otimes I\otimes X - 3 I\otimes Y\otimes Y$

$$\langle\psi|A|\psi\rangle = \langle\psi|(\tfrac{1}{2}Z\otimes I\otimes X - 3I\otimes Y\otimes Y)|\psi\rangle = \tfrac{1}{2}\langle\psi|Z\otimes I\otimes X|\psi\rangle - 3\langle\psi|I\otimes Y\otimes Y|\psi\rangle$$

8)Eigenvectors of each component tensored are the states of the tensored operator (we can find eigenvectors and eigenvalues for multiplication)

Example: $Z\otimes I\otimes X$

Eigenvectors	Eigenvalues	Eigenvectors	Values
$\|0\rangle\otimes\|0\rangle\otimes\|+\rangle$	$1\cdot1\cdot1=1$	$\|1\rangle\otimes\|0\rangle\otimes\|+\rangle$	$-1\cdot1\cdot1=-1$
$\|0\rangle\otimes\|0\rangle\otimes\|-\rangle$	$1\cdot1\cdot-1=-1$	$\|1\rangle\otimes\|0\rangle\otimes\|-\rangle$	$-1\cdot1\cdot-1=1$
$\|0\rangle\otimes\|1\rangle\otimes\|+\rangle$	$1\cdot-1\cdot1=-1$	$\|1\rangle\otimes\|1\rangle\otimes\|+\rangle$	$-1\cdot-1\cdot1=1$
$\|0\rangle\otimes\|1\rangle\otimes\|-\rangle$	$1\cdot-1\cdot-1=1$	$\|1\rangle\otimes\|1\rangle\otimes\|-\rangle$	$-1\cdot-1\cdot-1=-1$

9) There is a set of pauli matrices, called the change of basis operator, for which any given probability representation for an eigenstate can be transformed to 000

Example: $Z\otimes X\otimes Z$ eigenstate: $|0\rangle|+\rangle|0\rangle$ Probability: $|(\langle 0|\langle +|\langle 0|)|\psi|^2$

Since $|0\rangle|+\rangle|0\rangle = (I\otimes H\otimes I)|0\rangle|0\rangle|0\rangle$, :

$$|(\langle 0|\langle +|\langle 0|)|\psi\rangle|^2 = |\langle 0|\langle 0|\langle 0|(I\otimes H\otimes I)^\dagger|\psi\rangle|^2$$

→ $(I\otimes H\otimes I)|\psi\rangle = \overset{\text{(hermitian)}}{(I\otimes H\otimes I)^\dagger}|\psi\rangle$ For any eigenvector: $|\lambda_A\rangle = (I\otimes H\otimes I)|\lambda_C\rangle$ computational basis

→ For any tensor product of pauli matrices, we can create a change of basis operator which maps every eigenstate to an eigenstate of the computational basis

→ Example: prepare $(I\otimes H\otimes I)^\dagger|\psi\rangle$. $|000\rangle$ represents $|0\rangle|+\rangle|0\rangle$

10) Goal: $|\langle\lambda_A|\psi\rangle|^2$

$$\langle\lambda_C|(I\otimes H\otimes I)^\dagger|\psi\rangle = \langle\lambda_A|(I\otimes H\otimes I)(I\otimes H\otimes I)^\dagger|\psi\rangle = \langle\lambda_A|\psi\rangle$$

11) Each eigenvalue doesn't need to be run individually. We prepare the state and calculate relative ferquencies for a great enough number of shots

12) Each individual matrix has a change of basis matrix. These matrices can be tensored together to form a deterministic way of switching to the computational basis

$Z\to Y$: SH $\quad Y\to Z$ $(SH)^\dagger$

$Z\to X$: H $\quad X\to Z$: $(H)^\dagger$

$Z\to Z$: I $\quad I\to Z$: I

Example: $\langle\psi|Z\otimes I\otimes X|\psi\rangle$

↳ Prepare: $(I\otimes I\otimes H)|\psi\rangle$

13) Prepararation and Measurement are done on a quantum computer. Energy Estimation and Parameter Minimization done on a classical computer

14) Fermionic Hamiltonians --> qubit hamiltonians to be run on quantum computers

Eigenvalue Equation

$H|x\rangle = f(x)|x\rangle$ $\quad$ $|x\rangle$ = computational basis state

Eigenvectors

Since we are building this matrix from the tensor product of Z's and I's, $|x\rangle$ ($|0\rangle, |1\rangle$ for 1 qubit) are guarenteed to be eigenstates

Wavefunction

→ Can be decomposed into linear combination of basis states

$|\psi\rangle = \sum_x \alpha_x |x\rangle$ $\quad$ ~ α_x is complex coefficient associated w/ each state

Alternate Probability relation

→ typically, the probability of $|x\rangle$ is $|\alpha_x|^2$

$$\langle x|\psi\rangle = \langle x| \sum_y \alpha_y |y\rangle = \sum_y \alpha_y \langle x|y\rangle = \begin{matrix} 0 \text{ for } y \neq x \\ 1 \text{ for } y = x \end{matrix} = \alpha_x$$

→ Thus, $|\alpha_x|^2 = |\langle x|\psi\rangle|^2$

Expectation Value Derivation

$\langle\psi|H|\psi\rangle =$

$\sum_y \alpha_y^* \langle y| H \sum_x \alpha_x |x\rangle =$

$\sum_{x,y} \alpha_x \alpha_y^* \langle y|H|x\rangle =$

$\sum_{x,y} \alpha_x \alpha_y^* f(x) \langle y|x\rangle =$ $\quad$ Eigenvalue: $\langle y|H = f(x)\langle y|$

$\sum_x \alpha_x \alpha_x^* f(x) =$ $\quad$ same trick as above

$\sum_x |\alpha_x|^2 f(x) = \sum_x |\langle x|\psi\rangle|^2 f(x)$

↳ agrees with statistical intepretation (sum of prob · value)

→ For any observable, we are guarenteed to find a set of eigenvectors with attached real eigenvalues. The same arguments from the last page would still apply for any eigen-basis. I chose $|x\rangle$, similar to the book, since optimization problems use $I \otimes Z \otimes I \otimes Z \ldots$

Similar, for any observable: $\langle A \rangle_\psi = \sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2 \lambda_j$

$$= \langle \psi | A | \psi \rangle$$

Variational Principle

$$\langle A \rangle_\psi = \sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2 \lambda_j \geq \sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2 \lambda_0$$

$$= \lambda_0$$

Sum of all probabilities

$$\sum_{j,k} |\langle \lambda_j^k | \psi \rangle|^2 = 1$$

Linearity

Assume a matrix $A = \frac{1}{2} Z \otimes I \otimes X - 3 I \otimes Y \otimes Y$

Additive

$$\langle \psi | A | \psi \rangle = \langle \psi | \left(\tfrac{1}{2} Z \otimes I \otimes X - 3 I \otimes Y \otimes Y \right) | \psi \rangle$$

$$= \frac{1}{2} \langle \psi | (Z \otimes I \otimes X) | \psi \rangle - 3 \langle \psi | I \otimes Y \otimes Y | \psi \rangle$$

Tensor Product

$$(Z \otimes I \otimes X) |\lambda\rangle = \lambda |\lambda\rangle$$

$|\lambda\rangle = |\lambda_Z\rangle \otimes |\lambda_I\rangle \otimes |\lambda_X\rangle$ for all states of Z, I, X

$\lambda = \lambda_Z \cdot \lambda_I \cdot \lambda_X$ for all values of Z, I, X

Transformations

→ Change of basis operator, for any tensor product of pauli matrices transforms the eigenstates of our Hamiltonian into computational basis states

Observable: $Z \otimes X \otimes Z$ eigenstate: $|0\rangle \otimes |+\rangle \otimes |0\rangle$

$$|0\rangle \otimes |+\rangle \otimes |0\rangle = (I \otimes H \otimes I)(|0\rangle \otimes |0\rangle \otimes |0\rangle)$$

→ this is true for any state

inversely, $\langle 0| \otimes \underbrace{\langle +|}_{\langle x|} \otimes \langle 0| = \langle 0| \otimes \langle 0| \otimes \langle 0| (I \otimes H \otimes I)^{\dagger}$

$|\lambda_A\rangle$ - our basis $|\lambda_C\rangle$ - computational basis

$|\lambda_A\rangle = (I \otimes H \otimes I)|\lambda_C\rangle$ $I \otimes H \otimes I$ is change of basis operator for $Z \otimes X \otimes Z$

$$|\langle \lambda|\psi\rangle|^2 = |(\langle 0|\langle +|\langle 0|)|\psi\rangle|^2 = |\langle 0|\langle 0|\langle 0|(I \otimes H \otimes I)^{\dagger}|\psi\rangle|^2$$

(for example)

→ Prepare (change of basis)$|\psi\rangle$ and measure in computational basis
↳ given the result vary $|\psi\rangle$

Probability equivalence

$\langle \lambda_C|(I \otimes H \otimes I)^{\dagger}|\psi\rangle =$

$\langle \lambda_A|(I \otimes H \otimes I)(I \otimes H \otimes I)^{\dagger}|\psi\rangle =$

$\langle \lambda_A|\psi\rangle$

probability of any eigenstate of our system

Qiskit

→ Transforming Max 3SAT Problem

* Convert to ising: 3 terms: linear, quadratic, constant

$$H = -\sum_{j,k} J_{jk} Z_j Z_k - \sum_j h_j Z_j - \text{constant}$$

Linear: Z on j^{th} qubit I on else
Z_j

Quadratic: 2 Z's on i^{th}, j^{th} qubit I on else
$Z_i Z_j$

Constant: I on every qubit

Ansatz: ($|\psi\rangle$) Efficient SU2

Multiple runs

Stored the final parameters for the ansatz
Plugged into the SU2 gate and measurement

→ Did that for 500 runs of VQE