Class 2: PWF 2021 - QML 11/30/2021

Based on the postulates, some properties of QM:

- Schrödinger's equation is <u>deterministic</u>

$$\underset{t}{|\psi\rangle} \longrightarrow \underset{t'}{|\psi'\rangle = U(t)\,|\psi\rangle}$$

measurement outcomes are <u>probabilistic</u>.

- Superposition principle: $|\psi\rangle$ can be expressed as a linear combination of eigenvectors of a given observable (Hermitian operator)

  The coefficients in this expansion determine the probabilities of measurement outcomes

$$\{|0\rangle, |1\rangle\}^{\otimes n} = \{|0\cdots0\rangle, |10\cdots0\rangle, \ldots, |1\cdots1\rangle\}$$

$$|\psi\rangle = \sum_i \tilde{c}_i |z\rangle \qquad z \in \{0,1\}^{\otimes n}$$

computational basis

$$\boxed{\begin{aligned} Z|0\rangle &= |0\rangle \\ Z|1\rangle &= -|1\rangle \end{aligned}}$$

$$A|a_i\rangle = a_i|a_i\rangle \qquad |\psi\rangle = \sum_i c_i |a_i\rangle$$

 $\rightarrow$ measurement in the z-basis.

- Interference: wave functions can interfere coherently or destructively.

- Entanglement: for many body quantum systems, the wave function of its constituents only provides partial information about the state whole system

$$|\psi\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$$

$$|\psi\rangle = \sum_i c_i \bigotimes_{j=1}^{n} |\psi_{ij}\rangle$$

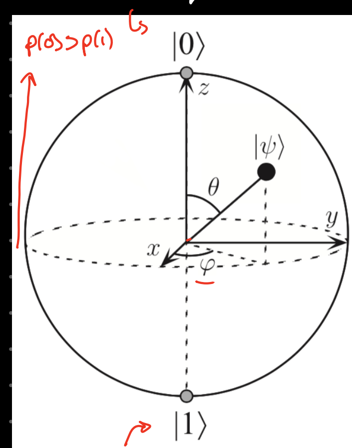
Single Qubit [and then generalize to n-qubit system].

Quantum system that only has 2 degrees of freedom

$|\psi\rangle = a_0|0\rangle + a_1|1\rangle \qquad a_0, a_1 \in \mathbb{C}$

$|a_0|^2 + |a_1|^2 = 1$

$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \quad \rightarrow \quad |\psi\rangle = \begin{pmatrix}a_0\\a_1\end{pmatrix}$



wikipedia

1) Pure states belong to the surface of the Bloch sphere

$\rho = |\psi\rangle\langle\psi| \quad \rightarrow \quad Tr[\rho^2] = 1$

$\rho^2 = \rho = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{1}\langle\psi| = |\psi\rangle\langle\psi|$

Mixed states live inside the Bloch Sphere

$\rightarrow a_0 = \cos\left(\frac{\theta}{2}\right)$

$a_1 = e^{i\varphi}\sin\left(\frac{\theta}{2}\right)$

$M_0 = |0\rangle\langle 0| = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$

$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$

$\langle 0| = (1\ 0)$

$p(0) = Tr[M_0\rho]$

$= Tr[M_0|\psi\rangle\langle\psi|] = Tr[|0\rangle\langle 0|\psi\rangle\langle\psi|]$

$= \langle 0|\psi\rangle\langle\psi|0\rangle$

$= |\langle 0|\psi\rangle|^2$

$= |\langle 0|(a_0|0\rangle + a_1|1\rangle)|^2$

$= |a_0|^2$

$= \cos^2\left(\frac{\theta}{2}\right)$

$p(1) = \sin^2\left(\frac{\theta}{2}\right)$

$\boxed{\begin{array}{l}\underline{\text{Trick \# 1}}\\ Tr[|\varphi\rangle\langle\varphi|O]\\ = \langle\varphi|O|\varphi\rangle\end{array}}$

$Tr[A] = \sum_i \langle i|A|i\rangle$

$\langle i|j\rangle = \delta_{ij}$

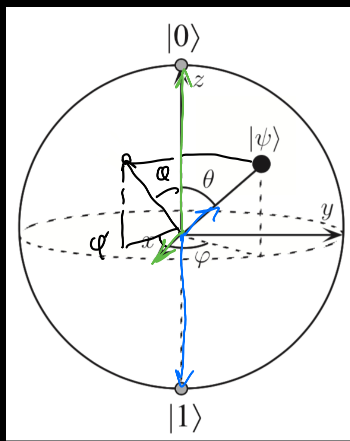
$\{|\varphi\rangle, |\varphi_j^\perp\rangle\}$

$Tr[|\varphi\rangle\langle\varphi|O]$

$= \sum_i \langle i|\varphi\rangle\langle\varphi|O|i\rangle$

$= \underbrace{\langle\varphi|\varphi\rangle}_{1}\langle\varphi|O|\varphi\rangle$

$+ \sum_j \underbrace{\langle\varphi_j^\perp|\varphi\rangle}_{=0}\langle\varphi|O|\varphi_j^\perp\rangle$



$= \langle \varphi | a | \varphi \rangle$

Extremely important for QML implementation for the hands-on exercises.

$$|\psi\rangle \xrightarrow{\text{measurements}} \begin{array}{ll} |0\rangle & p(0) \\ |1\rangle & p(1) \end{array}$$

$$\langle Z \rangle_{|\psi\rangle} = \langle \psi | Z | \psi \rangle = (a_0^* \; a_1^*) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

$\langle X \rangle$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad Z = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i| = 1\,|0\rangle\langle 0| - 1\,|1\rangle\langle 1| = |0\rangle\langle 0| - |1\rangle\langle 1|$$

$$\begin{aligned}\langle Z \rangle = \langle \psi | Z | \psi \rangle &= \langle \psi | (|0\rangle\langle 0| - |1\rangle\langle 1|) | \psi \rangle \\ &= \langle \psi | 0 \rangle\langle 0 | \psi \rangle - \langle \psi | 1 \rangle\langle 1 | \psi \rangle \\ &= |\langle 0 | \psi \rangle|^2 - |\langle 1 | \psi \rangle|^2 \\ &= p(0) - p(1)\end{aligned}$$

N times → we get outcome 0 N_0 times

" " " 1 N_1 times

$N_0 + N_1 = N$

$$\langle Z \rangle \simeq \frac{N_0}{N} - \frac{N_1}{N}$$

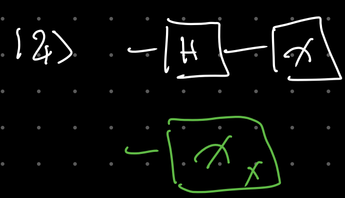
$|\psi\rangle$ —

$$X = |+\rangle\langle+| - |-\rangle\langle-| \qquad |\pm\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \pm |1\rangle\right)$$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad H^\dagger = H \qquad H|0\rangle = |+\rangle \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Hadamard operator $\qquad H|1\rangle = |-\rangle$

$$R_y\left(\frac{\pi}{2}\right)$$



$$M_0 = |0\rangle\langle 0| \xrightarrow{H} H M_0 H^\dagger = H M_0 H = |+\rangle\langle+|$$

$$M_1 = |1\rangle\langle 1| \qquad H M_1 H = |-\rangle\langle-|$$

$$\langle X\rangle = |\langle+|\psi\rangle|^2 - |\langle-|\psi\rangle|^2$$

$$= \frac{N_0}{N} - \frac{N_1}{N}$$

> TIP #2:
> Change of basis prior to measurement allows me to compute expectation value of any Pauli operator

~ o ~

Transition from QM to QC

Schrödinger's equation $\qquad i\,\frac{\partial|\psi\rangle}{\partial t} = H|\psi(t)\rangle \qquad \hbar = 1$

from a Quantum (physical) system to quantum interactions to QC

DiVicenzo

1) A scalable physical system with well characterized qubits

Physical interaction $\{H_k\} \rightarrow$ Unitary evolutions $\{e^{-itH_k}\}$

$\rightarrow$ possible states

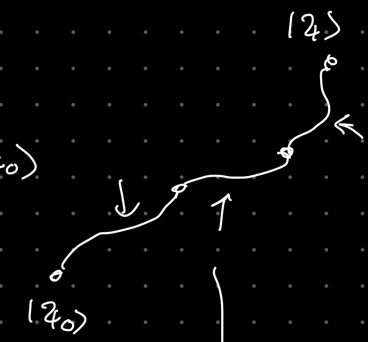
2) The ability to initialize qubits to a simple initial state

$|\psi_0\rangle = |0\rangle^{\otimes n}$

$$|\psi(t)\rangle = e^{-iH_k t}|\psi_0\rangle$$

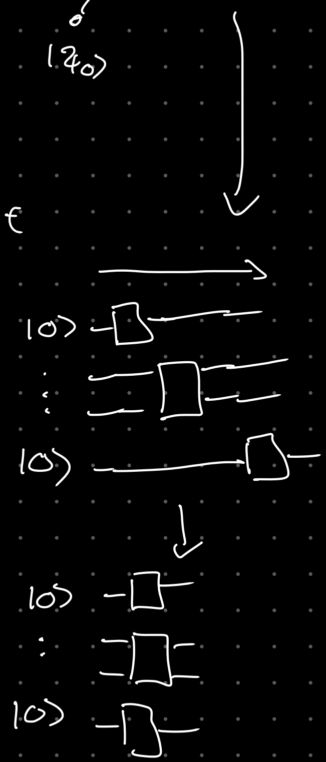
$$|\psi(t')\rangle = e^{-iH_{k'}t'}|\psi(t)\rangle = e^{-iH_{k'}t}e^{-iH_k t}|\psi_0\rangle$$

$$|\psi\rangle = \prod_t e^{-iH_k t}\,\underline{|\psi_0\rangle}$$



3) A universal set of gates

$$\underline{U = \prod U_t^k} \qquad U_t^k = e^{-iH_k t}$$



We want to implement the textbook Quantum Fourier Transform Alg

U_{QFT}

$$|U_{QFT} - \prod U_t^k| \le \varepsilon$$

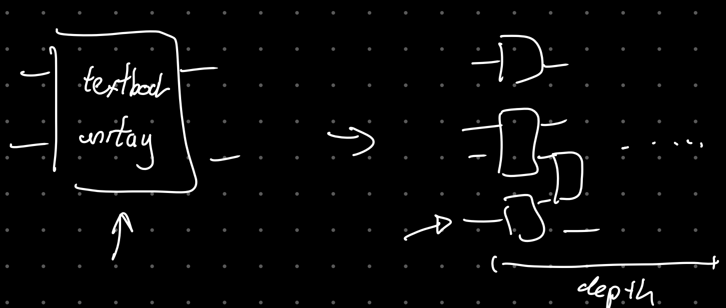
Universal QC → implement any operaⁿ

Universal set of quantum gates $S = \{U_k\}$

Solovay (2000) Kitaev (1997) Russ. Math Surv. 52 1191

A quantum circuit of m constant-qubit gates, can be approximated to ε error by a quantum circuit with

$$O\left(m \log\left(\frac{m}{\varepsilon}\right)\right) \text{ gates from a universal set}$$



Unitary operations preserve purity

$U|\psi_0\rangle\langle\psi_0|U^\dagger$

$\rho^2 = \rho$ (1)

$U|\psi_0\rangle\langle\psi_0|U^\dagger U|\psi_0\rangle\langle\psi_0|U$

$U|\psi_0\rangle\langle\psi_0|\psi_0\rangle\langle\psi_0|U^\dagger$, $\langle\psi_0|\psi_0\rangle = 1$

$U|\psi_0\rangle\langle\psi_0|U^\dagger$

Set of universal quantum gates $\{R_x, R_y, R_z, P(\varphi), CNOT\}$ $\begin{pmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&0&1\\ 0&0&1&0 \end{pmatrix}$

$\downarrow$

$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix}$

$CNOT|00\rangle = |00\rangle$

$CNOT|01\rangle = |01\rangle$

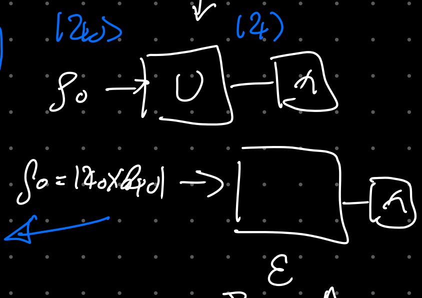
$CNOT|10\rangle = |11\rangle$

$CNOT|11\rangle = |10\rangle$

4) A qubit specific measurement capability

Tip #3.1 The natural sort of initialization evolution & measurement will lead me to compute quantities in the QC

$\rho_0 = |\psi_0\rangle\langle\psi_0|$ $\quad Tr[U \rho_0 U^\dagger O]$



$Tr[\mathcal{E}(\rho) O]$

$\mathcal{E}_U(\rho) = U \rho U^\dagger$

5) Long relevant decoherence times

TIP #3.2:

$O = \sum_i \alpha_i \, \sigma_\mu^{(1)} \otimes \cdots \sigma_\mu^{(n)}$ $\quad \sigma_\mu^{(k)} \in \{X, Y, Z\}$

$Z_1, \quad X_2 X_3, \quad X_1 Y_4 Z_5$ $\quad |\vec{0}\rangle = |0 \cdots 0\rangle$

$O = \sum_i e_i \, |Z_i\rangle\langle Z_i|$ $\quad \rightarrow \quad O = |0 \cdots 0\rangle\langle 0 \cdots 0|$

$Tr[U \rho_0 U^\dagger |\vec{0}\rangle\langle\vec{0}|]$

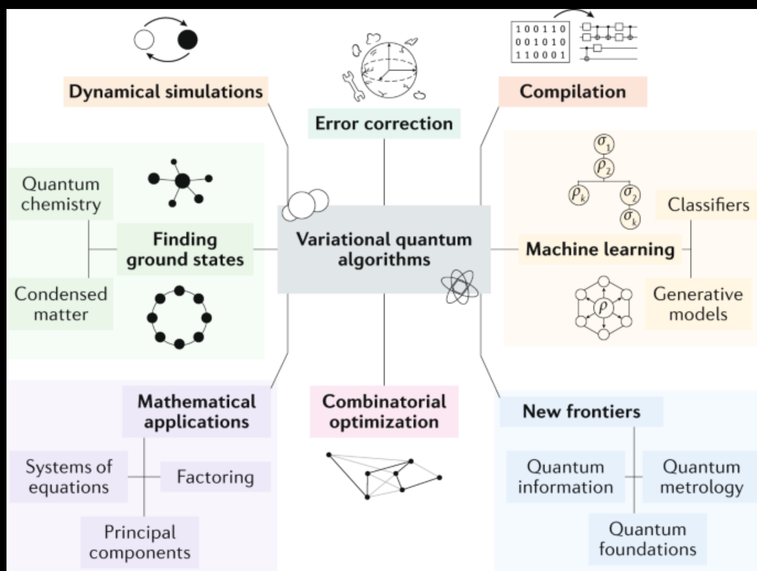
$= \langle\vec{0}| U \rho_0 U^\dagger |\vec{0}\rangle$

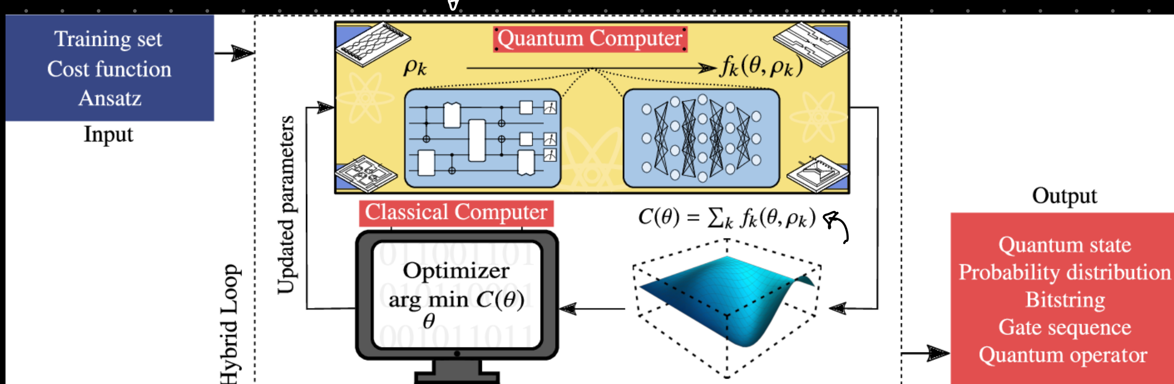
$= p(0) \sim \frac{N_0}{N}$

O is expanded into poly(n) terms.

How to build a Variational Quantum Algorithm (VQA) & Quantum machine learning (QML) model

Make practical use of near-term QC.





1) Given a problem of interest, we want to encode this problem into an optimization task, define a cost function $C(\vec{\theta})$

- Faithful $\quad \underline{C(\theta^*) = 0}$

$$\theta^* = \arg\min_{\theta} C(\theta)$$

- Operationally meaningful: $C(\theta_1) < C(\theta_2)$
  ↳ closer to the solution & better quality

- Cannot be efficiently estimated on a classical computer.
- Has to be " " " " " quantum computer.
- Trainable
- Noise resilient

↳ Computational complexity $O(\text{poly}(n))$ and not in $O(2^n)$ ←

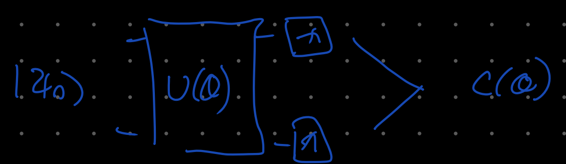
Example: Given a one qubit system $|\psi_0\rangle (= |0\rangle)$.

Goal: Prepare the ground-state of Z

$$\mathrm{Tr}[U|\psi_0\rangle\langle\psi_0|U^\dagger O] \rightarrow \mathrm{Tr}[U|\psi_0\rangle\langle\psi_0|U^\dagger Z] = C(\theta) \cong \frac{N_0}{N} - \frac{N_1}{N}$$

TIP #4: Many VQA's encode the optimization problem onto the task of finding the ground-state Hamiltonian H.

$$C(\theta) = \mathrm{Tr}[U(\theta)|\psi_0\rangle\langle\psi_0|U^\dagger(\theta) H]$$



Faithful: $C(\theta) = \mathrm{Tr}[U(\theta)|\psi_0\rangle\langle\psi_0|U^\dagger(\theta) H]$

$$H = \sum_i E_i |E_i\rangle\langle E_i| \qquad |\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$$

$$C(\theta) = \mathrm{Tr}\Big[|\psi(\theta)\rangle\langle\psi(\theta)| \sum_i E_i |E_i\rangle\langle E_i|\Big]$$

$$= \sum_i E_i \,\mathrm{Tr}[|\psi(\theta)\rangle\langle\psi(\theta)||E_i\rangle\langle E_i|]$$ weighted sum of eigenvalues of H by the probability of the state $|\psi(\theta)\rangle$ collapsing to the associated energy level

$$= \sum_i \underset{\uparrow}{E_i} \; \underset{1 \geq \uparrow \geq 0}{|\langle\psi(\theta)|E_i\rangle|^2}$$

$|\psi(\theta)\rangle \rightarrow E_{d-1}, \ \vdots, \ E_1, \ E_0$

$p(E_0) = |\langle E_0|\psi(\theta)\rangle|^2$

$\rightarrow$ $E_0 \le C(\theta)$ the equality holds $(C(\theta) = E_0)$ when $|\psi(\theta)\rangle = |E_0\rangle$.

Variational Principal

$|\psi(\theta)\rangle = a_0|E_0\rangle + a_1|E_1\rangle$

$|\psi(\theta')\rangle = a_0|E_0\rangle + a_1|E_{d-1}\rangle$

$C(\theta) < C(\theta')$

2) Define an ansatz $U(\theta)$

↳ := assumption about the form

setting what are the gates in $U(\theta)$ and how they are placed.

$\boxed{U(\vec{\theta})}$

Parametrized Quantum Circuit

$$U(\vec{\theta}) = \prod_{l=1}^{n} e^{-i\theta_l H_l} W_l$$

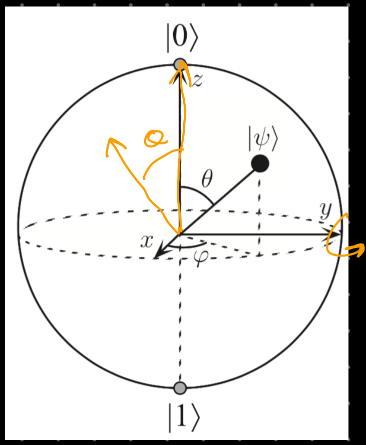
parametrized

unparametrized

:= $U(\vec{\theta})$ is built out of parametrized & unparametrized gates

Ex $|\psi_0\rangle = |0\rangle$

$|0\rangle - \boxed{R_y(\theta)} -$



3) Design a circuit that allows me to measure the cost function

$|0\rangle$ —[$R_y(\theta)$]—[↗]

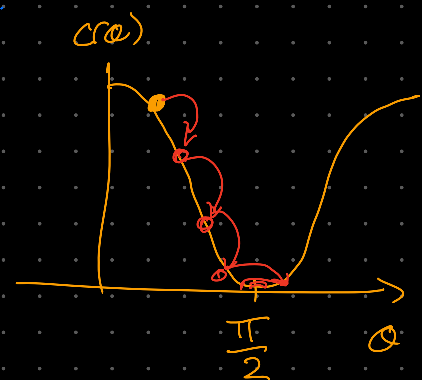
$$C(\theta) = \frac{N_0}{N} - \frac{N_1}{N}$$

$$p(0) \simeq \frac{N_0}{N} \underbrace{\pm \frac{1}{\sqrt{N}}}_{\Delta p(0)}$$

TIP # 5 Remember that the precision error due to finite measurements is $\frac{1}{\sqrt{N}}$ where N is the number of measurements shots.

4) Determine a parameter initialization strategy

5) Pick up an optimization method.



- gradient-based
- gradient-free → 'COBYLA'
  'Powell' → quantum-aware
  SPSA

VQE: Variational Quantum Eigensolver

Peruzzo et al Nat. Comm 5(1), 1-7 (2014), arXiv. 1304.3061

Quantum Chemistry

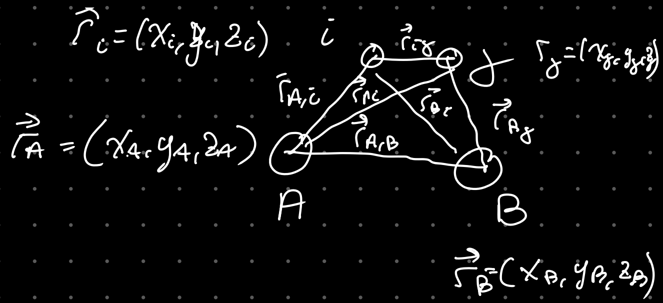
Task, Goal: find the ground-state of a given molecule.

$$i \frac{\partial |\psi(t)\rangle}{\partial t} = H |\psi(t)\rangle \longrightarrow H|\psi\rangle = E|\psi\rangle$$

molecular energy

1) N_e electrons $\vec{r}_i$ (i,j,w)

N_n nuclei $\vec{r}$ $(A,B,C\dots)$



(A) $\vec{r}_{12}=(x_1-x_2,\ y_1-y_2,\ z_1-z_2)$

$$\nabla_i^2=\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}$$

$$H = T + V = T_e + T_n + V_{ee} + V_{en} + V_{nn}$$

T: kinetic energy of the particles

V: potential energy of particle pairs

$$H = -\sum_{A=1}^{N_n}\frac{\hbar}{2M_A}\nabla_A^2-\sum_{i=1}^{N_e}\frac{\hbar}{2m_e}\nabla_i^2-\sum_{A=1}^{N_n}\sum_{i=1}^{n_e}\frac{Z_A e^2}{4\pi\varepsilon_0 \vec{r}_{Ai}}+\dots+ \dots$$

(A) H (position & momentum)

(B) Second Quantization $\quad H(x,p)\longrightarrow H$ fermionic operator

$$H=\sum_{IJ=1}^{N_{orbital}} h_{IJ}\, a_I^\dagger a_J+\sum_{IJKL} h_{IJKL}\, a_I^\dagger a_J^\dagger a_K a_L$$

$a^\dagger$ and a are creation & annihilation operators for electron excitations

$$H(x,p)\longrightarrow H(a^\dagger,a)$$

(C) Mapping to qubit & Pauli operators $\quad$ Jordan-Wigner, Bravyi-Kitaev

$$\begin{cases} a_j \rightarrow \sigma_-^{j}\otimes\sigma_z^{j-1}\otimes\dots\otimes\sigma_z^{1} \\ a_j^\dagger \rightarrow \sigma_+^{j}\otimes\sigma_z^{j-1}\otimes\dots\otimes\sigma_z^{1}\end{cases}$$

$\sigma_\pm$ ladder operators

$$\sigma_x=\frac{\sigma_+ + \sigma_-}{2}$$

$$H=\sum_{i\mu} h_i^{\mu}\,\sigma_\mu^{i}+\sum_{ij\mu\nu} h_{ij}^{\mu\nu}\,\underline{\sigma_\mu^{i}\otimes\sigma_\nu^{j}}\otimes\dots$$

A

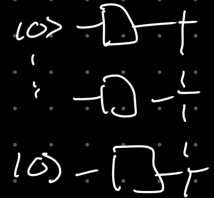
$$H(x,p) \xrightarrow[\text{Quantization}]{\text{2nd}} H(a^\dagger,a) \xrightarrow[\text{mapping}]{\text{JW}} H(\sigma_\mu)$$

$$C(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle = \sum_{i\mu} h_i^{\mu}\langle\underline{\sigma_\mu^{i}}\rangle + \sum_{ij\mu\nu} h_{ij}^{\mu\nu}\langle\underline{\sigma_\mu^{i}\sigma_\nu^{j}}\rangle + \cdots$$

2) Ansatz

$|\psi_0\rangle \to$ Hartree-Fock states as the solution to the mean field of the problem.

$|\psi_0\rangle \to$



$|\psi_{HF}\rangle$

$\boxed{U(\theta)}$ Unitary Coupled Cluster Ansatz

Anand arxiv 2019.15176

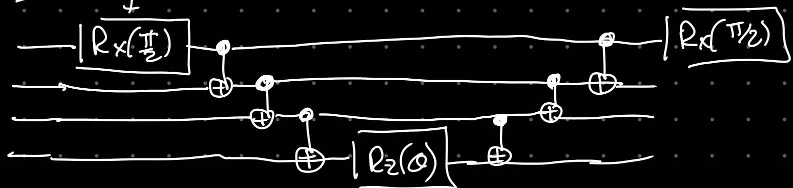
$$\underline{U(\theta) = e^{T-T^\dagger}} \qquad T = T_1 + T_2$$

1 body excitations, 2 body excitations

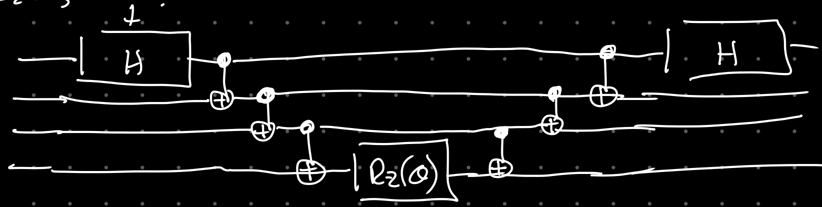
$$T_1 = \sum \theta_a^b a_a^\dagger a_b^\dagger$$

$$T_2 = \sum \theta_{ijab}\, a_a^\dagger a_b^\dagger a_j a_i$$

$$e^{i\frac{\theta}{2} Y_0 Z_1 Z_2 Z_3}$$

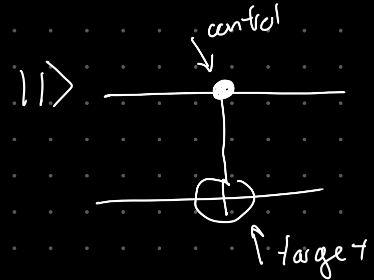


$e^{i\theta/2 \, X_0 Z_1 Z_2 Z_3}$



Depth(O(Leght pauli string?))

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$



if → this

$= \quad CNOT = |0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \otimes X$

$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$