Quantum Simulation

1. Hamiltonian Simulation

- Hamiltonian : H

  Evolution equation: $\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$

  or $|\psi(T)\rangle = e^{-iHT}|\psi(0)\rangle$

- Trotterization

$H = \sum H_i$

$\delta t = T/N$

$$e^{-iHT} = \left(e^{-iHT/N}\right)^N \approx \left(\prod e^{-iH_i T/N}\right)^N$$

$$e^{-iH\delta t} = 1 - iH\delta t + O(\delta t^2)$$

$$\prod e^{-iH_i\delta t} = \prod\left(1 - iH_i\delta t + O(\delta t^2)\right)$$

$$= 1 - i\sum H_i\,\delta t + O(\delta t^2)$$

$$\Rightarrow e^{-iH\delta t} = \prod e^{-iH_i\delta t} + O(\delta t^2)$$

$$\Rightarrow e^{-iHT} = \left(\qquad\downarrow\qquad\right)^N$$

$$= \left(\prod e^{-iH_i\delta t}\right)^N + O(N\cdot\delta t^2)$$

$$= O(T^2/N)$$

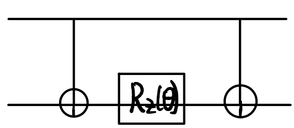
- ex. $H = a(x_1 + x_2 + x_3) + b(z_1 z_2 + z_2 z_3)$

$$e^{-iHT} \approx \left[e^{-ia(x_1+x_2+x_3)\cdot\delta t}\cdot e^{-ib(z_1z_2+z_2z_3)\cdot\delta t}\right]^N$$

$$e^{-ia(x_1+x_2+x_3)\cdot\delta t} = e^{-iax_1\delta t}\cdot e^{-iax_2\cdot\delta t}\cdot e^{-iax_3\cdot\delta t}$$

$$e^{-ib(z_1z_2+z_2z_3)\cdot\delta t} = e^{-ibz_1z_2\cdot\delta t}\cdot e^{-ibz_2z_3\cdot\delta t}$$

$$e^{-i\theta z_1 z_2/2} =$$



- Higher order Trotter.

$$e^{-iH\cdot\delta t} = 1 - i\delta t\cdot\sum H_i + \frac{(-i\delta t)^2}{2}\underbrace{\left(\sum H_i\right)^2}_{=\sum H_i H_j} + \cdots$$

$$\overrightarrow{\prod_i} e^{-iH_i\delta t} = \overrightarrow{\prod_i}\left(1 - i\delta t H_i + \frac{(-i\delta t)^2}{2}H_i^2 + \cdots\right)$$

$$= 1 - i\delta t\sum H_i + \frac{(-i\delta t)^2}{2}\left(\sum_{i=j} H_i H_j + 2\sum_{i<j} H_i H_j\right) + \cdots$$

$$T_{\rightarrow} e^{-iH\cdot\delta t} = \overrightarrow{\prod_i} e^{-iH_i\delta t} = 1 - i\delta t\sum H_i + \frac{(-i\delta t)^2}{2}\overrightarrow{\sum_{ij}} H_i H_j + \frac{(-i\delta t)^3}{3!}\overrightarrow{\sum_{ijk}} H_i H_j H_k$$

$$T_{\leftarrow} e^{-iH\cdot\delta t} = \overleftarrow{\prod_i} e^{-iH_i\delta t} = \sim$$

$$\delta t^2: \quad \overrightarrow{\prod_i} e^{-iH_i\delta t}\cdot\overleftarrow{\prod_i} e^{-iH_i\delta t} = 1 - i2\delta t\cdot\sum H_i + (-i\delta t)^2\left(\sum H_i\right)^2 + \frac{(-i\delta t)^2}{2}\left(\overrightarrow{\sum_{ij}} + \overleftarrow{\sum_{ij}}\right)H_i H_j$$

$$= 1 - i(2\delta t)\cdot\sum H_i + \underline{(-i2\delta t)^2\left(\sum H_i\right)^2}$$

$$S_2(\delta t) = \overrightarrow{\prod} e^{-iH_i\delta t/2}\,\overleftarrow{\prod} e^{-iH_i\delta t/2}$$

$$S_{2k}(\delta t) = \left[S_{2k-2}(p_k\cdot\delta t)\right]^2 S_{2k-2}((1-4p_k)\delta t)\left[S_{2k-2}(p_k\cdot\delta t)\right]^2$$

$$p_k = 1/\left(4 - 4^{1/2k-1}\right)$$

- Time-dependent H

$$\mathcal{T} e^{-i\int_0^{\delta t} H(t)\cdot dt} = \mathcal{T} e^{-i\int_0^{\delta t}\sum H_i(t)\cdot dt}$$

$$\simeq \prod_i \mathcal{T} e^{-i\int_0^{\delta t} H_i(t)\cdot dt}$$

We need a very small δt if $H(t)$ has high frequency

$$\mathcal{T} e^{-i\int_0^{\delta t} H(t)\cdot dt} \approx e^{-i\int_0^{\delta t} H(t)\cdot dt}$$

$$\approx e^{-i\frac{\sum H_n(t)}{N}\cdot dt}$$

2. Adiabatic evolution

- $H_i \longrightarrow H_f$

$$H_t = \frac{t}{T} \cdot H_f + \left(1 - \frac{t}{T}\right) \cdot H_i \qquad t: 0 \to T$$

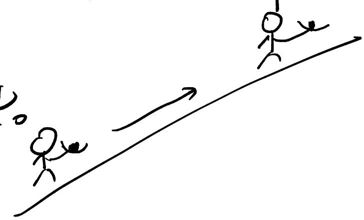
Suppose H_t is non-degenerate.

and $|\psi_i(t)\rangle$ is the ith eigenstate of H_t

Then $|\psi_i(t)\rangle = T e^{\int -i H_t \cdot dt} |\psi_i(0)\rangle + O\left(\frac{1}{T}\right)$

- $H = H_0 + V$

$\psi_0 \quad \phi_0 \qquad \phi_0 \xrightarrow{AE} \psi_0$



- AE is universal

$U = U_k U_{k-1} \cdots U_1$

$H_F = \sum_{j=1}^{k} H_j \qquad H_j = \underset{\substack{\uparrow \\ n\text{-qubits}}}{U_j} \otimes |j\rangle\langle j-1| + U_j^{\dagger} \otimes |j-1\rangle\langle j|$

$|\psi_j\rangle = U_j U_{j-1} \cdots U_1 |\bar{0}\rangle \otimes |j\rangle$

$H_F |\psi_j\rangle = |\psi_{j+1}\rangle + |\psi_{j-1}\rangle$

$|\eta\rangle = \frac{1}{\sqrt{k+1}} \sum_{j=0}^{k} |\psi_j\rangle$ is the ground state of $-H_F$

$H_i = -|\bar{0}\rangle\langle\bar{0}| \otimes |0\rangle\langle 0|$

$H_f = H_i - H_F$

We can get $U_j U_{j-1} \cdots U_1 |\bar{0}\rangle$ with prob. $\frac{1}{k+1}$

3. Eigenstate / Eigenvalue of H.

— suppose $H = H_0 + V$.

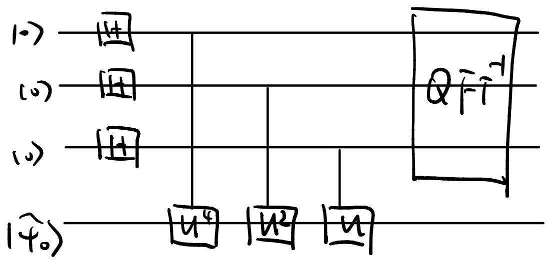
step 1. solve H_0 and get its ground state ϕ_0

step 2. Apply AE from H_0 to H

$$\phi_0 \to \tilde{\varphi}_0$$

step 3. Apply QPE to $\tilde{\varphi}_0$

suppose $H = \sum E_i |\varphi_i\rangle\langle\varphi_i|$ $\qquad \tilde{\varphi}_0 = \sum \alpha_i |\varphi_i\rangle$



$$\sum \alpha_i |\varphi_i\rangle|0\rangle \longrightarrow \sum \alpha_i |\tilde{\varphi}_i\rangle|\tilde{E}_i\rangle$$

— VQE