A bird's eye view of quantum simulation

Qiskit Global Summer School 2022

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Part I

What is quantum simulation?

What models do we want to simulate?

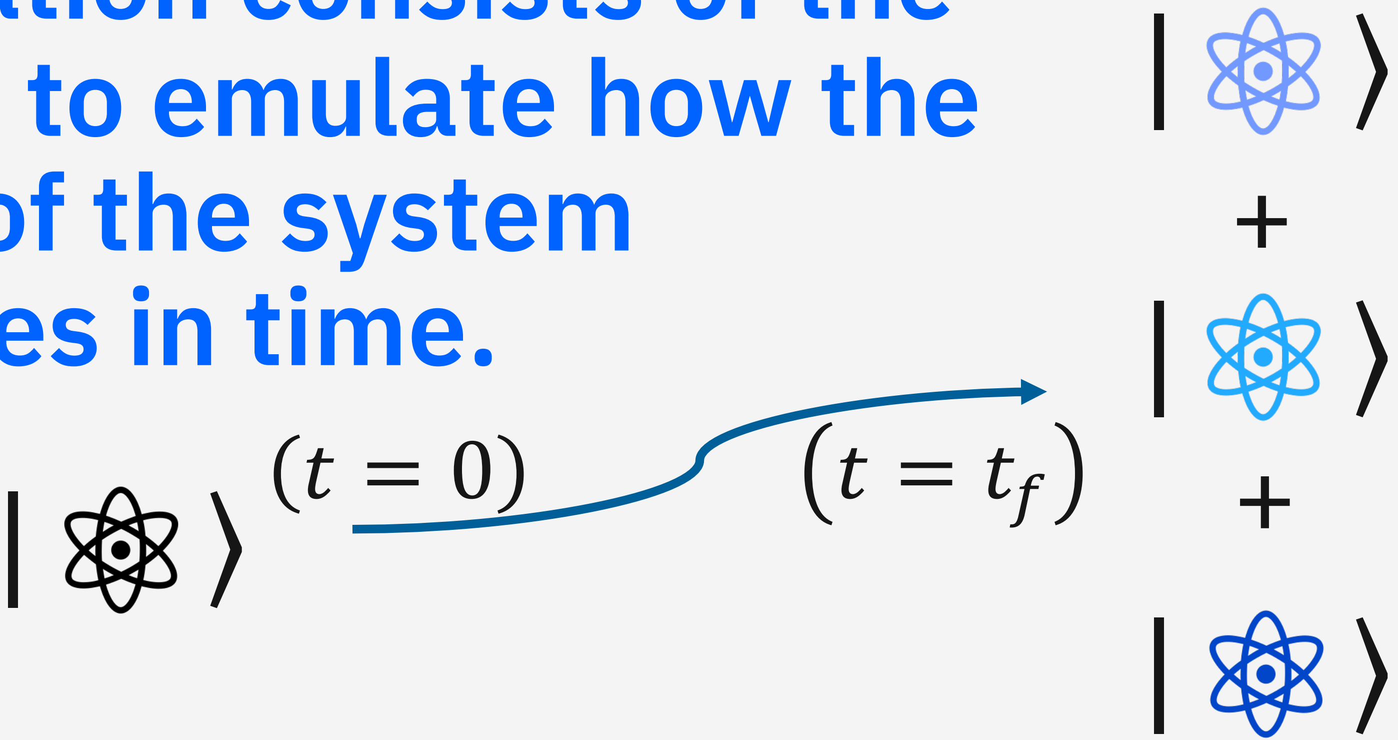
Brief look at classical Methods

Part II

Broad overview of modern methods used for quantum simulation on quantum computers

What is quantum Simulation?

For a particular model of a quantum system its simulation consists of the ability to emulate how the state of the system changes in time.



A simulation with the ability to track $|⚛(t)\rangle$ precisely can also estimate observables:

$$\langle ⚛(t)|\hat{O}|⚛(t)\rangle$$

The models we examine will be described by a Hamiltonian as long as our systems are closed.

$$H = H^\dagger$$

If H is time-independent then its propagator is given by:

$$|\psi(t)\rangle = U(t,0)|\psi_0\rangle = e^{-iHt}|\psi(0)\rangle$$

If $H(t)$ is time-dependent then the propagator is given by:

$$|\psi(t)\rangle = \mathcal{T} \exp\left[\int_0^t dt'\, H(t')\right]$$

$$= 1 - i\int_0^t dt_1\, H(t_1) + (-i)^2 \int_0^t \int_0^{t_1} dt_1 dt_2\; H(t_1)H(t_2) + \cdots$$

Why simulation?

1. **Model validation with experiment**

2. **Model to Model validation**
   - Emergent effective models

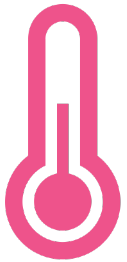
3. **Savings in terms of time and resources compared to running experiments.**

4. **Emergence of states and phases**
   - Equilibrium/steady state properties

Statics

- Under certain conditions we know what type of states a system will reach in equilibrium…

- System is weakly coupled to a bath at inverse temperature $\beta \rightarrow \frac{e^{-\beta H}}{Tr\left[e^{-\beta H}\right]}$
  - $= Z^{-1}(\beta) \sum_n e^{-\beta E_n} |E_n\rangle \langle E_n|$



- If: $\frac{1}{\beta} \ll (E_1 - E_0)$ or under relaxation properties:
  - $|\psi\rangle \rightarrow |E_0\rangle \;\coloneqq \min_{|\phi\rangle} \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}$
  - Behavior is dominated by ground state properties

Dynamics

Quench

$$|\psi_0\rangle = G.S.\,of\ H_0$$

$$At\ t = 0{:}\ \ H_0 \rightarrow H$$

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

Interested in certain observables vs. time:

$$\langle\psi(t)|O|\psi(t)\rangle$$

Un-equal time correlators

$$C_{ab}(t_1, t_2) = \langle\psi_0|O_a(t_1)O_b(t_2)|\psi_0\rangle$$

$$= \langle\psi_0\big|e^{iHt_1}O_a e^{iH(t_2-t_1)}O_b e^{-iHt_2}\big|\psi_0\rangle$$

$$k - point\ correlators:$$

$$C_{a_1,a_2,\ldots,a_k}(t_1, t_2, \ldots, t_k)$$
$$= \langle O_{a_1}(t_1)O_{a_2}(t_2)\ldots O_{a_k}(t_k)\rangle$$

What models are we interested in simulating?

Coulomb Hamiltonian

$$H = T_e + T_n + U_{ee} + U_{nn} + U_{en}$$

Coulomb Hamiltonian

$$H = \boldsymbol{T_e} + T_n + U_{ee} + U_{nn} + U_{en}$$

$$\boldsymbol{T_e = \sum_i \frac{1}{2m_i} \nabla_{r_i}^2}$$

Coulomb Hamiltonian

$$H = T_e + \boldsymbol{T_n} + U_{ee} + U_{nn} + U_{en}$$

$$\boldsymbol{T_n = \sum_i \frac{1}{2M_i} \nabla^2_{R_i}}$$

Coulomb Hamiltonian

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$$H = T_e + T_n + U_{ee} + U_{nn} + U_{en}$$

$$U_{ee} = \frac{1}{2} \sum_{i} \sum_{j \neq i} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

Coulomb Hamiltonian

$$H = T_e + T_n + U_{ee} + U_{nn} + U_{en}$$

$$U_{nn} = \frac{1}{2}\sum_{i}\sum_{j\neq i}\frac{Z_i Z_j}{|\vec{R}_i - \vec{R}_j|}$$

Coulomb Hamiltonian

IBM **Quantum**

$$H = T_e + T_n + U_{ee} + U_{nn} + U_{en}$$

$$U_{en} = -\sum_i \sum_j \frac{Z_i}{|\vec{R}_i - \vec{r}_j|}$$

Born-Oppenheimer Approximation

$$H\Psi(r,R) = E\Psi(r,R)$$

$$\Psi(r,R) = \psi_e(r,R)\phi_n(R)$$

$$\boldsymbol{Clamped\ Nuclei}:$$

$$H_e = T_e(r) + U_{en}(r,R) + \underbrace{\boxed{U_{nn}(R)}}_{\text{const}} + U_{ee}(r)$$

$$H_e\psi_e(r,R) = E_e\psi(r,R)$$

(anti)-symmetric wave functions

- For Fermionic wavefunction we have the pauli exclusion principle requiring the wavefunction to be anti-symmetric under the exchange of 2 particles:

  - $\psi(r_1, r_2, \dots r_i, \dots, r_j, \dots, r_N) = -\psi(r_1, r_2, \dots r_j, \dots, r_i, \dots, r_N)$

- Where as for Boson we have symmetry under exchange:

  - $\psi(r_1, r_2, \dots r_i, \dots, r_j, \dots, r_N) = +\psi(r_1, r_2, \dots r_j, \dots, r_i, \dots, r_N)$

Slater Determinate

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- Simplest way to approximate wavefunctions is to express them as products of single particle wavefunctions:
  - $\psi(r_1, r_2, \ldots, r_N) = \phi_1(r_1)\phi_2(r_2) \ldots \phi_N(r_n)$
- But this wavefunction is not anti-symmetric…
- Anti-symmetrize via Slater determinate:
  - $\psi(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N}} \begin{vmatrix} \phi_1(r_1) & \phi_2(r_1) & \cdots & \phi_N(r_1) \\ \phi_1(r_2) & \phi_2(r_2) & \cdots & \phi_N(r_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(r_N) & \phi_2(r_N) & \ldots & \phi_N(r_N) \end{vmatrix}$

2^{nd} Quantization (Fermions)

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- $For\ M\ modes\ and\ N\ particles$:
- $Define\ creation\ and\ annihilation\ operators$:
    - $|n_1 n_2 \ldots n_M\rangle = \left(c_1^\dagger\right)^{n_1}\left(c_2^\dagger\right)^{n_2} \ldots \left(c_M^\dagger\right)^{n_M}|0\rangle\ , n_j \in \{0,1\}$
    - $\left\{c_i, c_j\right\} = c_i c_j + c_j c_i = \left\{c_i^\dagger, c_j^\dagger\right\} = 0\quad ,\quad \left\{c_i, c_j^\dagger\right\} = \delta_{ij}$
- $General\ wavefunction$:
    - $\sum_{n_1,n_2,\ldots,n_M} \alpha_{n_1,n_2,\ldots,n_M} |n_1 n_2 \ldots n_M\rangle$
- $|0100111\rangle$ $represents\ a\ Slater\ determinate\ of\ 4\ particles\ that\ fills\ modes\ 2{,}5{,}6{,}7$

2^{nd} Quantized Hamiltonian

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- The electronic Hamiltonian will now have a structure that looks like:

- $H_e = \sum_{pq} t_{pq} \; c_p^\dagger c_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} \; c_p^\dagger c_r^\dagger c_s c_q$

- $t_{pq} = \int dr \;\; \phi_p^*(r)\, f(r) \phi_p(r)$

- $v_{pqrs} = \int \int dr_1 \, dr_2 \;\; \phi_p^*(r_1) \phi_r^*\,(r_2) g(r_1, r_2) \phi_q(r_1) \phi_s(r_2)$

Effective Models

Band Models:

$$\sum_{i,k} \epsilon_{i,\vec{k}} \; c^\dagger_{i,\vec{k}} \, c_{i}, \vec{k}$$

Hubbard like Models:

$$t \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{j,\downarrow}$$

Electron-Phonon Models

$$t \sum_{<ij>} c^\dagger_i c_j + \omega a^\dagger_i a_i + \lambda\left(a^\dagger_i + a_i\right) c^\dagger_j c_k$$

BSC Type Models:

$$\sum_{ij} t \, c^\dagger_i c_j + \left(\Delta \, c^\dagger_i c^\dagger_j + \Delta^* \, \mathrm{c_i c_j}\right)$$

Impurity Models

$$\sum_{k,\sigma} \epsilon_k \, c^\dagger_k c_k + \sum_{\sigma} \epsilon_d \, d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow$$

$$+ \sum_{k,\sigma} V_k \left(d^\dagger_\sigma c_{k,\sigma} + c^\dagger_{k,\sigma} d_\sigma\right)$$

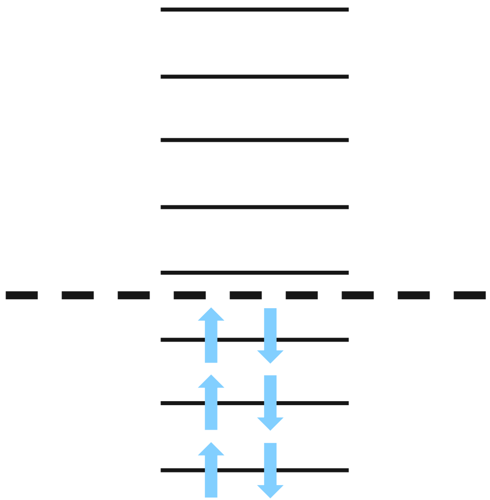
Heisenberg Models

$$\sum_{ij} J_{ij} \, \vec{S_i} \cdot \vec{S_j}$$

Classical Methods

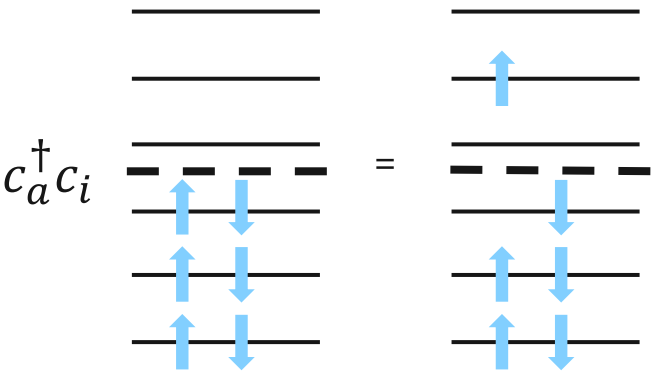
Hartree-Fock

- Minimal energy for single determinate
- Define an Orbital rotation as : $e^{-\kappa}$, $\kappa = \sum_{pq} \theta_{pq}\, c_p^\dagger c_q - c_q^\dagger c_p$
    - Single particle change of basis: $e^{\kappa} c_p e^{-\kappa} = \sum_q \alpha_q\, c_q$
- Determinate of configuration $C \coloneqq |C\rangle$
- $E_0^{HF} = \min_{\kappa} \langle C| e^{\kappa} H e^{-\kappa} |C\rangle$, $\left|\Phi_0^{HF}\right\rangle = e^{-\kappa}|C\rangle$



Configuration Interaction

- $|\Psi_0\rangle = \alpha_0 \left|\Phi_0^{HF}\right\rangle + \sum_{ia} \alpha_i^a | \Phi_i^a\rangle + \sum_{i<j,a<b} \alpha_{ij}^{ab} \left|\Phi_{ij}^{ab}\right\rangle + \sum_{i<j<k,a<b<c} \alpha_{ijk}^{abc} |\Phi_{ijk}^{abc}\rangle + \cdots$
- $\left|\Phi_{i_1,i_2,\ldots i_k}^{a_1 a_2 \ldots a_k}\right\rangle = c_{a_1}^\dagger c_{a_2}^\dagger \ldots c_{a_k}^\dagger c_{i_1} c_{i_2} \ldots c_{i_k} |\Phi_0^{HF}\rangle$
- Vary α coefficients to minimize energy



Coupled Cluster

Define cluster operator: $T = T_1 + T_2 + \cdots$

$$T_1 = \sum_{ia} \tau_i^a \; c_a^\dagger c_i$$

$$T_2 = \sum_{ab,ij} \tau_{ij}^{ab} \; c_a^\dagger c_i c_b^\dagger c_j$$

Solve coupled cluster equations:

$$\left\langle \Phi_0^{HF} \middle| e^{-T} H e^{T} \middle| \Phi_0^{HF} \right\rangle = E_{CC}$$
$$\left\langle \mu \middle| e^{-T} H e^{T} \middle| \Phi_0^{HF} \right\rangle = 0$$

$$\langle \mu | \in \left\{ \langle \Phi_i^a |, \langle \Phi_{ij}^{ab} |, \ldots \right\}$$

FCI Method

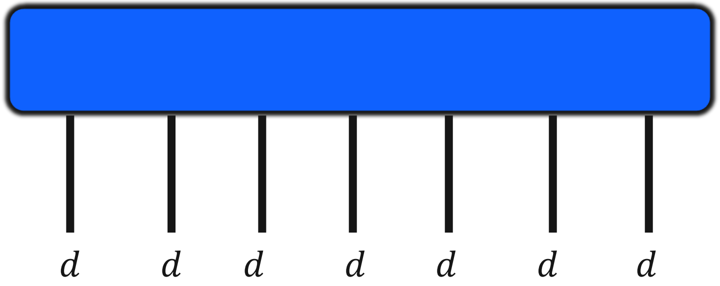
- Krylov space methods: $\{|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, \ldots H^k|\psi\rangle\}$
  - Power iteration, Lanczos, Davidson
  - Convergence : $\sim C\left(\frac{1}{|\langle\psi|E_0\rangle|^2}\right)\rho^{-2(k-1)}$, $\rho = \frac{(E_1 - E_0)}{(E_n - E_1)}$

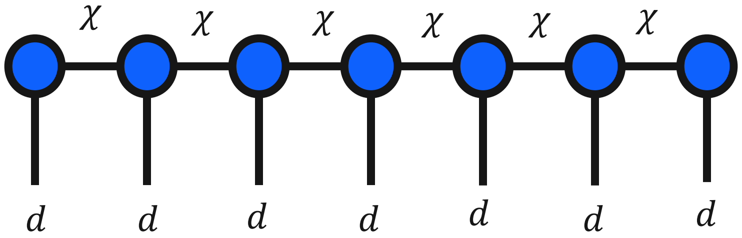
- Sparsity of basis functions will become exponentially dense with k.

Matrix Product States

The density-matrix renormalization group in the age of matrix product states

Ulrich Schollwöck



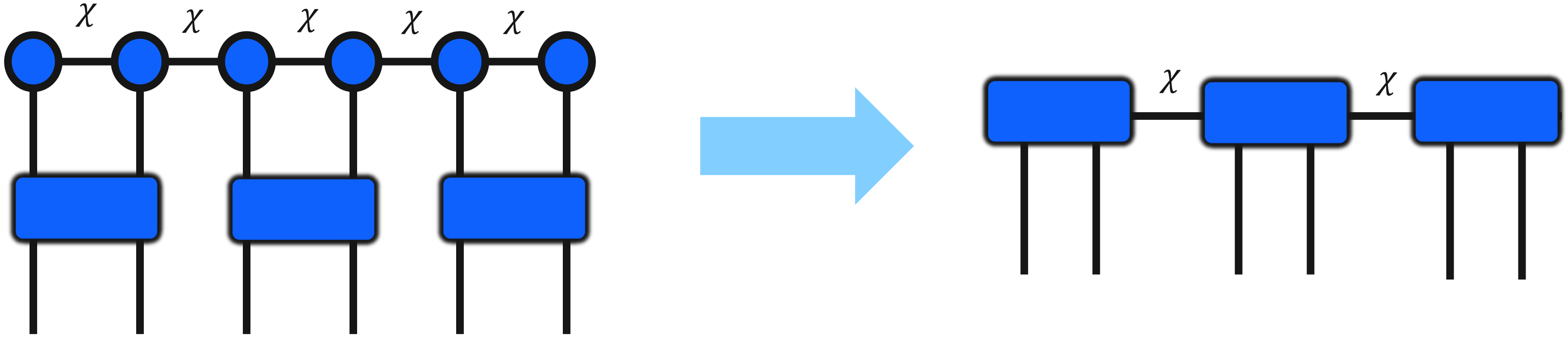


d^N

$$|\psi\rangle = \sum_{n_1,n_2,\ldots n_N} \alpha_{n_1,n_2,\ldots,n_N} |n_1 n_2 \ldots n_N\rangle$$

$N d \chi^2$

χ is controlled by the amount of entanglement/correlations in the system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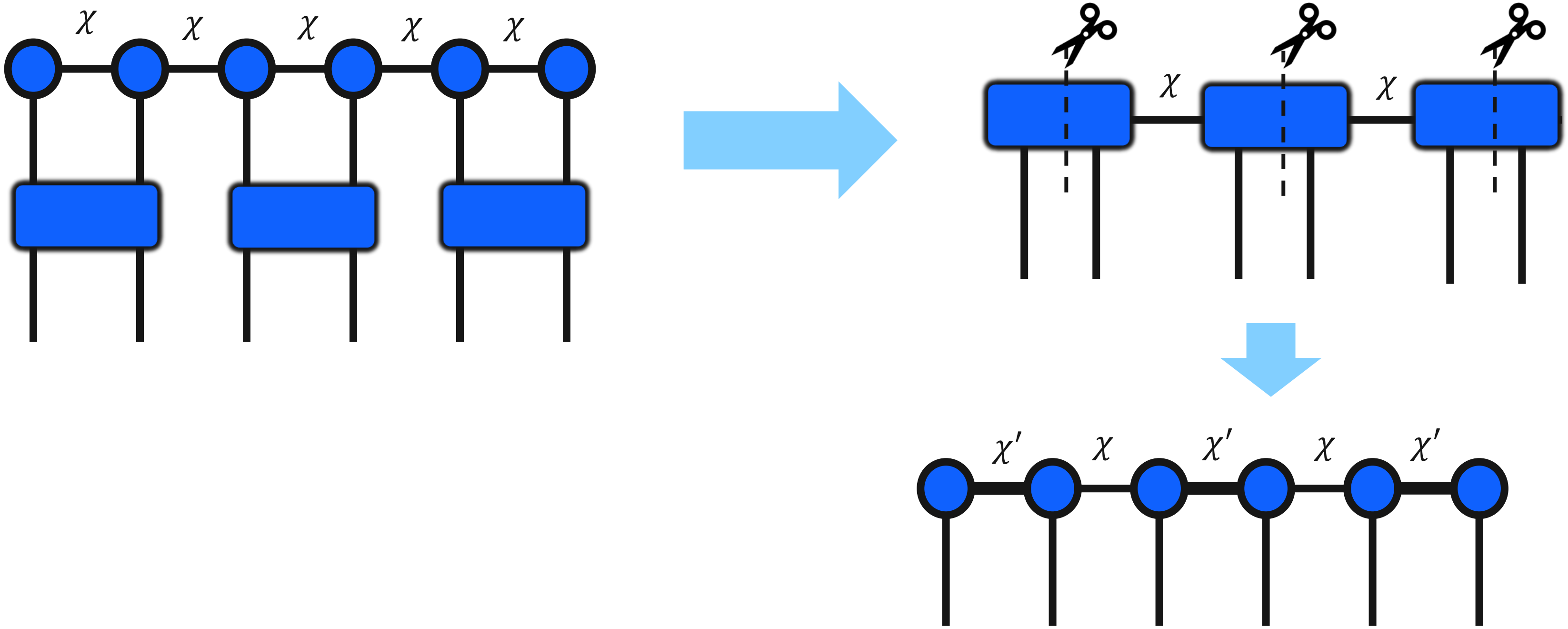

Applying 2 − qubit gates will generally increase the entanglement which increases χ.

Other Common Methods not mentioned

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- Density functional Theory
- Quantum Monte Carlo
- Dynamical Mean Field Theory
- Density Matrix Embedding Theory
- Green’s Function Methods

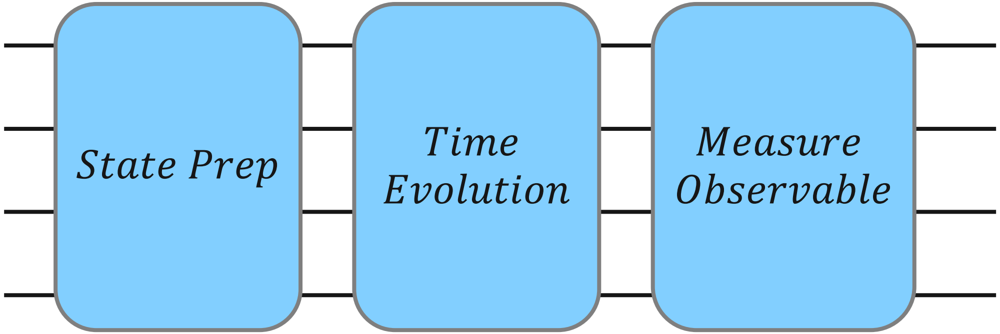
- All struggle in different manner eventually
- Each has their advantages for certain properties or types of problems

Part II: Quantum Simulation Methods

Digital Quantum Simulation

1) *Map degrees of freedom onto qubits*

2)



Jordan Wigner Mapping

Qubits can naturally store the orbital occupations in the computational basis:

- $c_j^\dagger = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \frac{X_j - iY_j}{2}$
- $c_j = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \frac{X_j + iY_j}{2}$
- $c_j^\dagger c_j = \frac{I - Z_j}{2} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = |1\rangle\langle 1|$

- But this does not obey the anti-commutation relations:
  - $c_j c_k = -c_k c_j$
- $\left(\frac{X_j + iY_j}{2}\right)\left(\frac{X_k + iY_k}{2}\right) = \frac{1}{4}\left(X_j X_k + iX_j Y_k + iY_j X_k + Y_j Y_k\right) = \frac{1}{4}\left(X_k X_j + iX_k Y_j + iY_k X_j + Y_k Y_j\right) = + \left(\frac{X_k + iY_k}{2}\right)\left(\frac{X_j + iY_j}{2}\right)$

JW Mapping

- Note that the Pauli operators anti-commute: $ZX = -XZ$
- We can fix our original construction by tracking the parity before each c_j operator:

  - » $c_1^\dagger = \frac{X_1 - iY_1}{2}$
  - » $c_2^\dagger = Z_1 \left(\frac{X_2 - iY_2}{2}\right)$
  - » $c_3^\dagger = Z_1 Z_2 \left(\frac{X_3 - iY_3}{2}\right)$
  - » $c_N^\dagger = Z_1 Z_2 \ldots Z_{N-1} \left(\frac{X_N - iY_N}{2}\right)$

JW Mapping of ES Hamiltonian

$$H_e = \sum_{pq} t_{pq}\ c_p^\dagger c_q + \frac{1}{2}\sum_{pqrs} v_{pqrs}\ c_p^\dagger c_r^\dagger c_s c_q$$

- $c_p^\dagger c_p = \left(\frac{1-Z_p}{2}\right)$, $c_p^\dagger c_q + c_q^\dagger c_p = \frac{1}{2}\prod_{j=q+1}^{p-1} Z_j \left(X_p X_q + Y_p Y_q\right)$

- $n_p n_q = \frac{1}{4}\left(I - Z_p - Z_q + Z_p Z_q\right)$
- $c_p^\dagger c_q^\dagger c_q c_r = \frac{1}{2}\prod_{j=r+1}^{p-1} Z_j \left(X_p X_r + Y_p Y_r\right)\left(\frac{1-Z_s}{2}\right)$
- $c_p^\dagger c_q^\dagger c_r c_s = (XXXX - XXYY + XYXY + YXXY + YXYX - YYXX + XYYX + YYYY)$

First order Totter

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$$H = \sum_{j=1}^{L} h_j$$

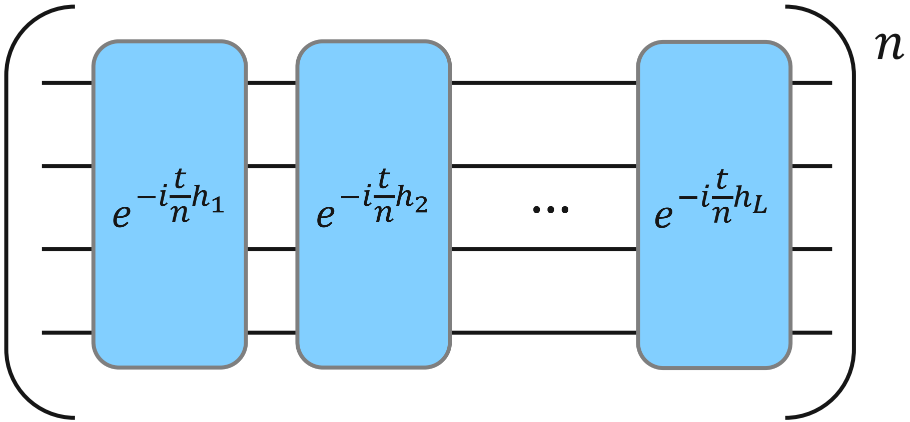
$Exact: e^{-itH}$

$Trotter: \mathcal{S}_1(t;n) = \left[\prod_{j=1}^{L} e^{-i\frac{t}{n}h_j}\right]^n$

$$\epsilon = \left|e^{-itH} - \mathcal{S}_1(t)\right| = \frac{t^2}{2n}\sum_{j>i}\left|\left[h_i, h_j\right]\right| + \mathcal{O}(t^3) \leq \frac{t^2L^2\Lambda^2}{n} + \mathcal{O}(t^3) \rightarrow n = \frac{(tL\Lambda)^2}{\epsilon}\ Totter\ steps\ , \Lambda = \max(h_j)$$

$$1\ step = L\ gates\ \left(e^{-i\Delta t h_j}\right)$$

$$Total\ gates\ \left(e^{-i\Delta t h_j}\right)\ to\ simulate\ e^{-itH}\ to\ precision\ \epsilon = \frac{L^3(\Lambda t)^2}{\epsilon}$$


$e^{-i\frac{t}{n}h_1}$
$e^{-i\frac{t}{n}h_2}$
…
$e^{-i\frac{t}{n}h_L}$
n

Trotter Suzuki

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$$\mathcal{S}_2(t\colon n) = \left[\prod_{j=1}^{L} e^{-i\frac{t}{2n}h_j} \prod_{j=L}^{1} e^{-i\frac{t}{2n}h_j}\right]^n$$

$$\epsilon = \left|e^{-itH} - \mathcal{S}_2(t;n)\right| \leq \frac{(L\Lambda t)^3}{n^2} + \mathcal{O}(t^4) \rightarrow n = \frac{(L\Lambda t)^{3/2}}{\sqrt{\epsilon}} \quad steps$$

$$\#\ of\ \ gates\ \left(e^{-i\Delta t h_j}\right) = \frac{L^{5/2}(\Lambda t)^{3/2}}{\sqrt{\epsilon}}$$

Trotter Suzuki

$$\mathcal{S}_{2k}(t;n) = \left[\mathcal{S}_{2k-2}^2\left(u_k\frac{t}{n}\right)\mathcal{S}_{2k-2}\left(\frac{(1-4u_k)t}{n}\right)\mathcal{S}_{2k-2}^2\left(u_k\frac{t}{n}\right)\right]^n$$

$$u_k = \frac{1}{\left(4-4^{\frac{1}{2k-1}}\right)}$$

$$\#\ of\ gates\left(e^{-i\Delta t h_j}\right) = \frac{L^{2+\frac{1}{2k}}(\Lambda t)^{1+\frac{1}{2k}}}{\epsilon^{\frac{1}{2k}}}$$

QDRIFT

A random compiler for fast Hamiltonian simulation

Earl Campbell[1]

IBM **Quantum**

Randomized product formula (qDRIFT)

Inputs: Hamiltonian $H = \sum_{j=1}^{L} h_j$ with interaction strength $\lambda = \sum_j \|h_j\|$, evolution time t, and number of steps N.

At each t/N interval: evolve a random term in Hamiltonian

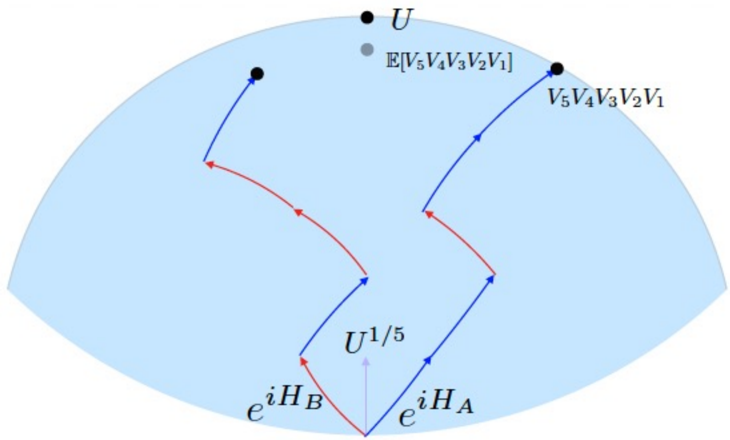
$$V_k = \exp(-\mathrm{i}(t/N)X_k) \tag{4}$$

according to its importance

$$X_k \overset{i.i.d.}{\sim} X = \begin{cases} \frac{\lambda}{\|h_1\|} h_1 & \text{with prob. } p_1 = \frac{\|h_1\|}{\lambda} \\ \vdots & \\ \frac{\lambda}{\|h_L\|} h_L & \text{with prob. } p_L = \frac{\|h_L\|}{\lambda} \end{cases}.$$

Output: the unstructured (randomly generated) product formula

$$V^{(N)} = V_N \cdots V_1.$$



Concentration for random product formulas

Chi-Fang Chen,[1,*] Hsin-Yuan Huang,[2,3,*] Richard Kueng,[2,3,4] and Joel A. Tropp[3]

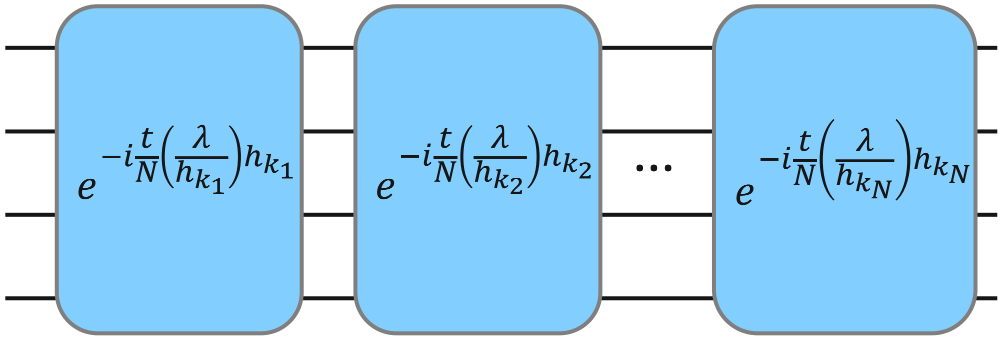
QDRIFT

A random compiler for fast Hamiltonian simulation

Earl Campbell[1]

Protocol	**Gate count** (upper bound)
1^{st} order Trotter DET	$O(L^3(\Lambda t)^2/\epsilon)$
2^{nd} order Trotter DET	$O(L^{5/2}(\Lambda t)^{3/2}/\epsilon^{1/2})$
$(2k)^{th}$ order Trotter DET	$O(L^{2+\frac{1}{2k}}(\Lambda t)^{1+\frac{1}{2k}}/\epsilon^{1/2k})$
$(2k)^{th}$ order Trotter RANDOM	$O(L^2(\Lambda t)^{1+\frac{1}{2k}}/\epsilon^{1/2k})$
qDRIFT (general result)	$O((\lambda t)^2/\epsilon)$
qDRIFT (when $\lambda = \Lambda L$)	$O(L^2(\Lambda t)^2/\epsilon)$
qDRIFT (when $\lambda = \Lambda\sqrt{L}$)	$O(L(\Lambda t)^2/\epsilon)$

sample:



$$with\ propability = p_{k_1} p_{k_2} \dots p_{k_N}$$

Linear Combination of Unitaries (LCU)

IBM **Quantum**

Simulating Hamiltonian dynamics with a truncated Taylor series

Dominic W. Berry[1], Andrew M. Childs[2,3,4,5], Richard Cleve[2,5,6], Robin Kothari[2,6,7], and Rolando D. Somma[8]

$$H = \sum_{j=1}^{L} \alpha_j h_j \text{ , each } h_j \text{ is unitary}$$

$$e^{itH} = \sum_{k=0}^{\infty} \frac{(itH)^k}{k!} \approx \sum_{k=0}^{K} \frac{(itH)^k}{k!}$$

$$e^{itH} \approx \sum_{k=0}^{K} \sum_{l_1, l_2, \ldots, l_k} \alpha_{l_1} \alpha_{l_2} \ldots \alpha_{l_k} \; h_{l_1} h_{l_2} \ldots h_{l_k} = \sum_j \beta_j V_j = \widetilde{U}(t)$$

$$B|0\rangle = \frac{1}{\sqrt{s}} \sum_j \sqrt{\beta_j}\, |j\rangle \;, \qquad s = \sum_j |\beta_j|$$

$$select(V)|j\rangle = V_j|j\rangle$$

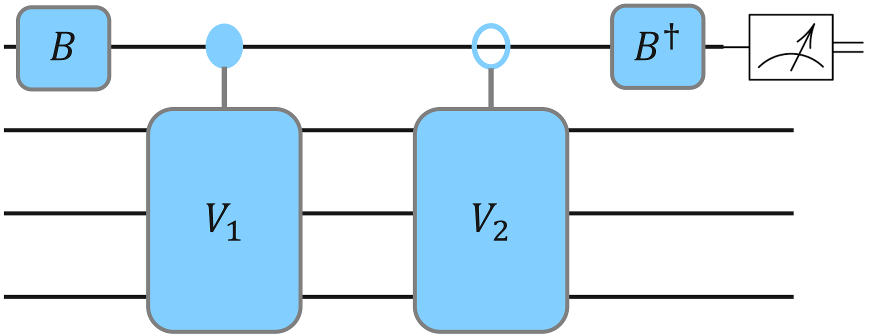
$$W = B^{\dagger} select(V) B$$

LCU

$$W|0\rangle|\psi\rangle = \frac{1}{s}\sum_j \beta_j |0\rangle V_j |\psi\rangle + \sqrt{1-\frac{1}{s^2}}|\perp\rangle$$

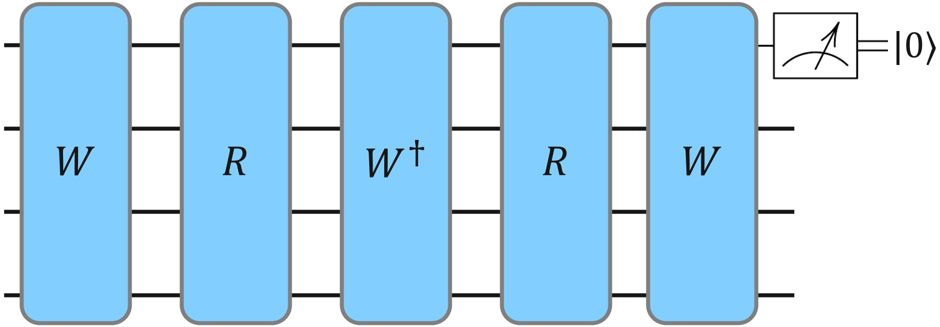
$$The\ |0\rangle\ state\ is\ measured\ withpropability\ \frac{1}{s^2}$$

$$whcih\ returns\ the\ state\colon \frac{1}{s}\widetilde{U}(t)$$



LCU

$$Now\ define\ reflection\ operator:\ \ R = (1 - 2|0\rangle\langle 0|) \otimes I$$



$$= -\frac{3}{s}\widetilde{U}(t) + \frac{4}{s^3}\widetilde{U}(t)\widetilde{U}^\dagger(t)\widetilde{U}(t)$$

$$If\ \widetilde{U}(t)\ is\ close\ to\ unitary\ then\ we\ have: -\left(\frac{1}{s} - \frac{4}{s^3}\right)\widetilde{U}(t)$$

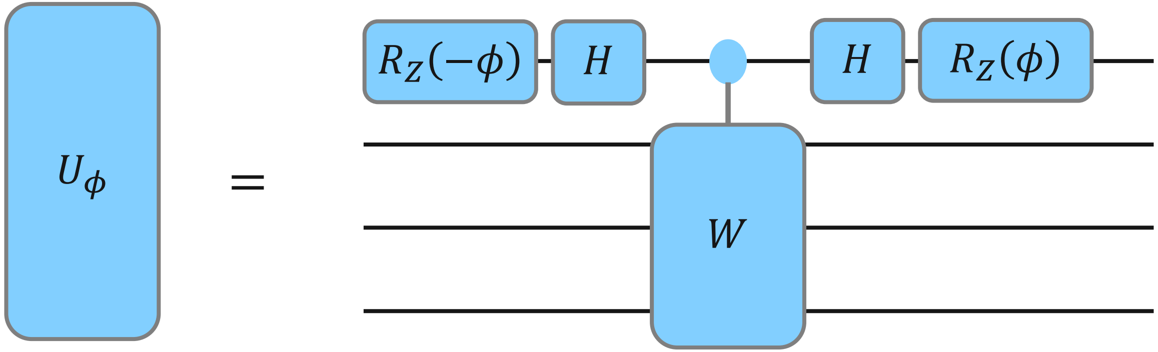
$$whose\ amplitude\ can\ be\ boosted\ to\ 1\ if\ we\ set\ s = 2!$$

Block Encoding + Quantum Signal Processing

$$W = \begin{pmatrix} H/s & \cdot \\ \cdot & \cdot \end{pmatrix}$$

Optimal Hamiltonian Simulation by Quantum Signal Processing

Guang Hao Low, Isaac L. Chuang



$$V_N = U_{\phi_1} U_{\phi_2} \cdots U_{\phi_N} = \begin{pmatrix} P_N(H/s) & \cdot \\ \cdot & \cdot \end{pmatrix}$$

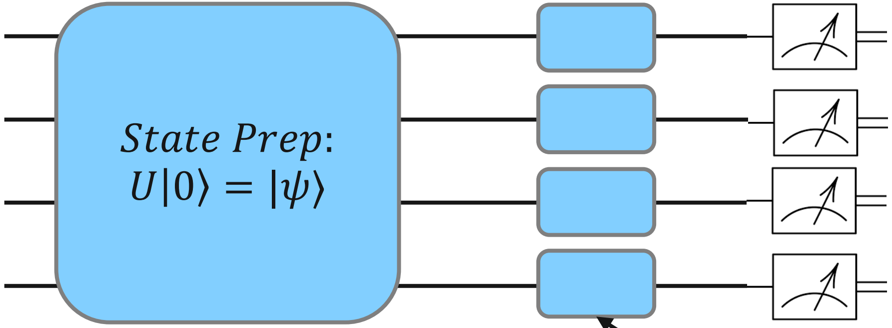
Measuring H

$$H = sum\ of\ Pauli's = \sum_{j=1}^{L} \alpha_j\ P_j$$

$Measure\ \langle\psi|H|\psi\rangle\ to\ precision\ \epsilon$:

$We\ can\ measure\ in\ the\ basis\ of\ each\ Pauli\ string$:

$$Var(P_j) = \langle\psi|P_j^2|\psi\rangle - (\langle\psi|P_j|\psi\rangle)^2 = 1 - \langle P_j\rangle^2$$



$\{I, H, HS\}$

$I = Z\ basis$
$H = X\ basis$
$HS = Y\ basis$

$$\epsilon = \sum_j \sqrt{\frac{\alpha_j^2 Var(P_j)}{S_j}} = \sum_j \sqrt{\frac{\alpha_j^2 \left(1 - \langle\psi|P_j|\psi\rangle^2\right)}{S_j}}\ ,\qquad S_j = number\ of\ shots\ for\ P_j$$

Measurements

$$If\ S_j = \frac{S}{L}\ where\ S\ is\ total\ number\ of\ shots:$$

$$\epsilon = \sum_j \sqrt{\frac{\alpha_j^2 Var(P_j)}{S_j}} = \sqrt{\frac{L}{S}\sum_j \alpha_j^2 Var\left(P_j\right)}$$

$$S = L\sum_j \frac{\alpha_j^2 Var(P_j)}{\epsilon^2}$$

$$If\ H\ is\ a\ generic\ Fermionic\ Hamiltonian:$$

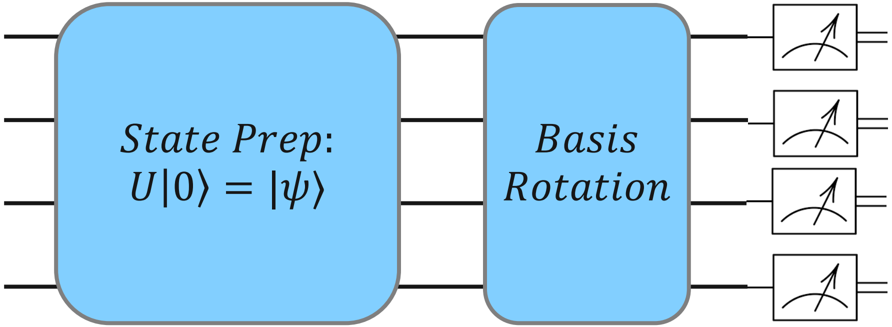
$$L \sim N^4 \rightarrow S \sim \frac{N^4}{\epsilon^2}$$

- $Set\ S_j \sim |\alpha_j|$
- $Trucate\ terms\ with\ |\alpha_j| \leq \epsilon$
- Qubit wise Commuting
- Rotate to mutually commuting basis

Group Commuting Terms

$$H = \sum_j h_j \quad , \qquad h_j = \sum_i \alpha P_i \ , such\ that\ \forall ij\ [P_i, P_j] = 0$$

Rotate to diagonal basis of grouped Pauli terms with a Clifford circuit

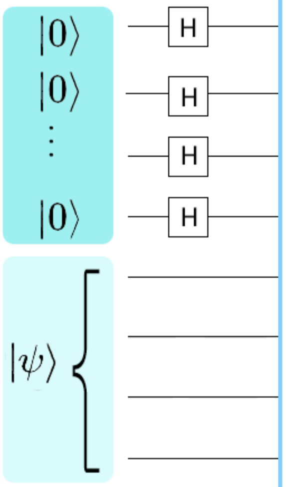


Quantum Phase Estimation

IBM **Quantum**

m-qubits

n-qubits

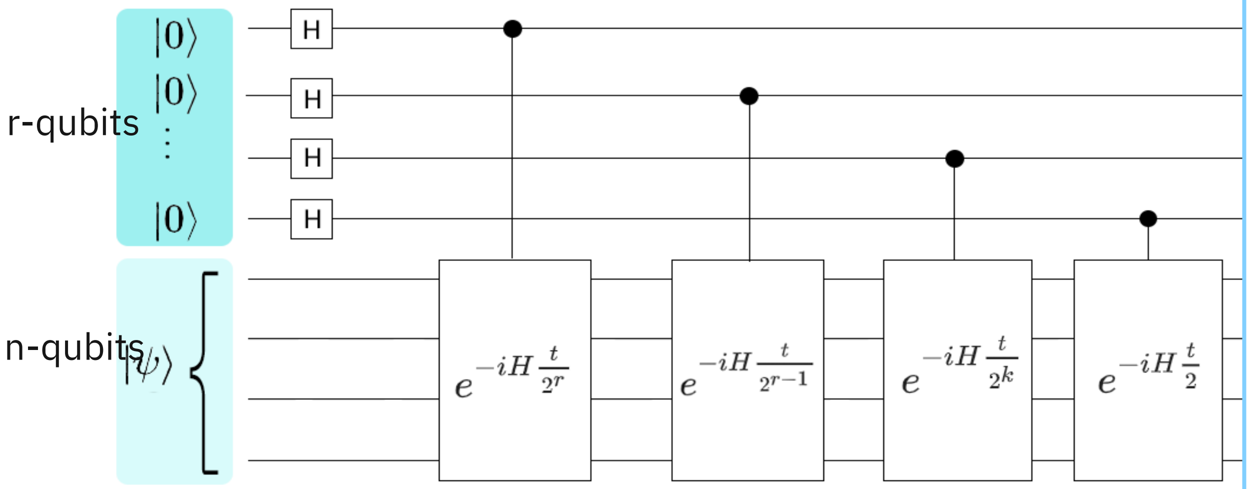


$$|\psi\rangle = \sum_n c_n |E_n\rangle$$

$$|00\ldots 0\rangle|\psi\rangle$$

$$\rightarrow \frac{1}{\sqrt{2^m}} \sum_j |j\rangle|\psi\rangle$$

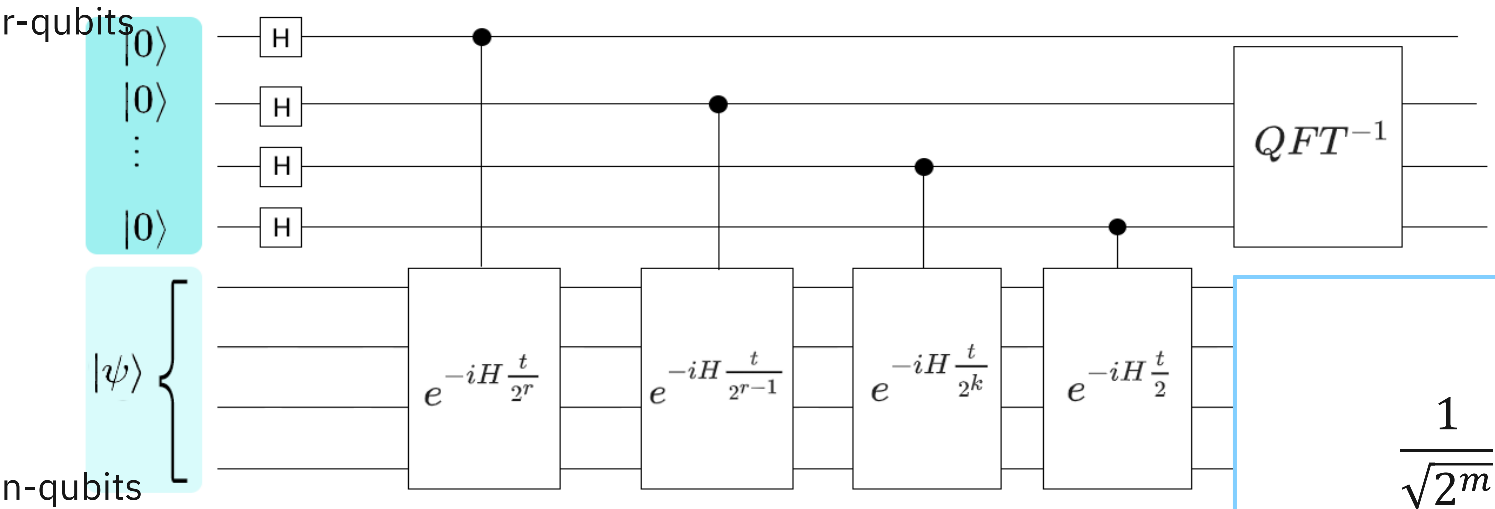
Quantum Phase Estimation



$$\frac{1}{\sqrt{2^m}}\sum_j |j\rangle|\psi\rangle$$

$$\rightarrow \frac{1}{2^{\frac{m}{2}}}\sum_{j,n} c_n\, e^{-\frac{ijE_j t}{2^r}}$$

Quantum Phase Estimation



$$\frac{1}{\sqrt{2^m}}\sum_j |j\rangle|\psi\rangle$$

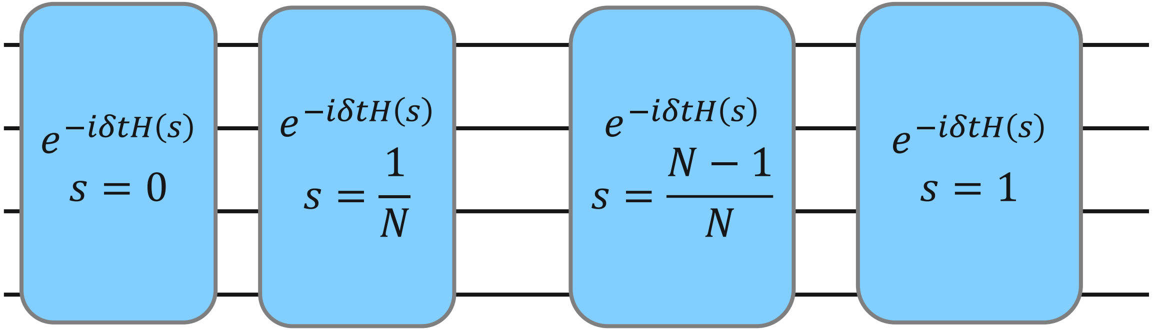
$$\rightarrow \frac{1}{\sqrt{2^m}}\sum_j\sum_n c_n e^{\frac{2\pi i j}{r^2}\left(x - E_j\frac{t}{2\pi}\right)}$$

Adiabatic State Preparation

$$Define:\ H(s) = (1-s)H_{easy} + sH_{hard}\ , \qquad s \in [0,1]$$

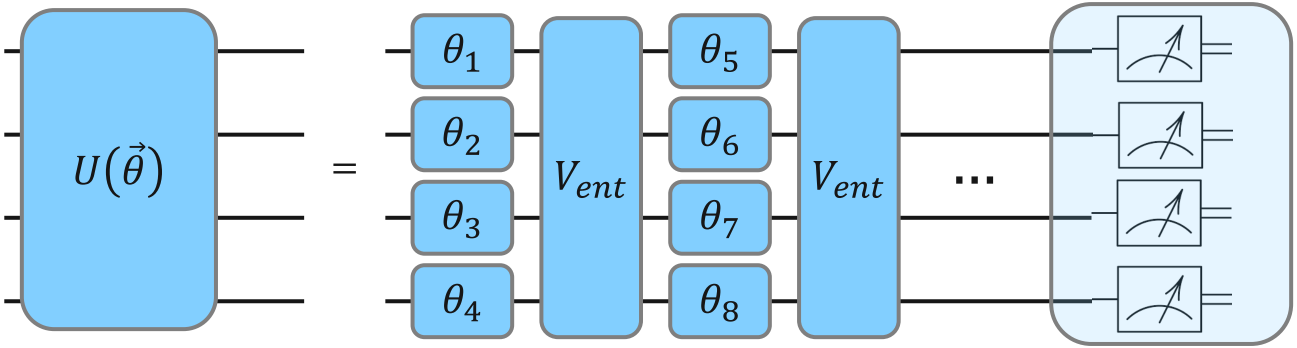
1. Prepare GS of H_{easy} on QC

2. Evolve $|\psi_0\rangle = |GS\rangle_{easy}\ under\ H(s)\ slowly\ changing\ s\ from\ 0\ to\ 1$:



3. $\frac{ds}{dt}\ is\ upper\ bounded\ buy\ \Delta = \min_s\big(E_1(s) - E_0(s)\big)$

Variational Quantum Eigensolver (VQE)



$$E(\theta) = \langle\psi_0|U^\dagger(\vec{\theta})HU(\vec{\theta})|\psi_0\rangle$$

$$\frac{dE(\vec{\theta})}{d\theta_j} = \left\langle\psi_0\left|\left(\frac{dU^\dagger(\vec{\theta})}{d\theta_j}\right)HU(\vec{\theta})\right|\psi_0\right\rangle + \left\langle\psi_0\left|U^\dagger(\vec{\theta})H\left(\frac{U(\vec{\theta})}{d\theta_j}\right)\right|\psi_0\right\rangle$$

Gradients

$$\boxed{\theta_j} = e^{-i\theta_j G}$$

$$U(\vec{\theta}) = \prod_{l=L}^{1}\left[\left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\right]$$

$$\frac{\partial U(\vec{\theta})}{\partial\theta_{k,l'}} = \prod_{l=L}^{l'-1}\left[\left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\right]\left(G_k\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\prod_{l=l'+1}^{1}\left[\left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\right]$$

$$U_R = \left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\prod_{l=l'+1}^{1}\left[\left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\right]$$

$$U_L = \prod_{l=L}^{l'-1}\left[\left(\prod_{j=N}^{1} e^{-i\theta_{j+l-1}G}\right)V_{ent}\right]$$

$$\frac{\partial E(\vec{\theta})}{\partial\theta_{k,l'}} = i\langle\psi_0|U_R^{\dagger}[G_k, U_L^{\dagger}HU_L\,]U_R|\psi_0\rangle$$

VQE Notes

IBM **Quantum**

- Requires many measurements and circuits to converge to minimum energy state
- Construct circuit ansatz and initial states and initial parameter wisely

Subspace Methods (1)

Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states

Jarrod R. McClean,[1,*] Mollie E. Kimchi-Schwartz,[2] Jonathan Carter,[1] and Wibe A. de Jong[1]

1. Prepare an initial estimate of the G.S. : $|\psi\rangle$
2. Define subspace states: $\mathcal{B}^k = \left\{ c_{i_1}^\dagger c_{j_1} c_{i_2}^\dagger c_{j_2} \dots c_{i_k}^\dagger c_{j_k} |\psi\rangle \right\}$, $i_l \in [1, M]$
3. Measure subspace Hamiltonian : $\widetilde{H}_{ij} = \langle\psi|O_i H O_j|\psi\rangle$and overlap matrix: $S_{ij} = \langle\psi|O_i O_j|\psi\rangle$, $O_i \in \mathcal{B}^k$
4. Classically solve the generalized Eigen problem: $\widetilde{H}\mathcal{C} = \epsilon S\mathcal{C}$

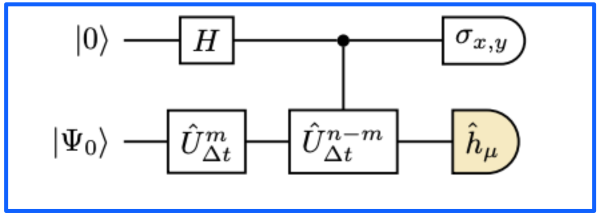
- ❖ Polynomial overhead of extra Pauli strings to measure.
- ❖ Measuring a symmetry operator in the subspace O_S allows one to project the subspace Hamiltonian to the proper symmetry sector.
- ❖ Can extract excited state energies. Also see:

Quantum equation of motion for computing molecular excitation energies on a noisy quantum processor

Pauline J. Ollitrault,[1,2] Abhinav Kandala,[3] Chun-Fu Chen,[3] Panagiotis Kl. Barkoutsos,[1] Antonio Mezzacapo,[3] Marco Pistoia,[3,4] Sarah Sheldon,[3] Stefan Woerner,[1] Jay M. Gambetta,[3] and Ivano Tavernelli[1,*]

Subspace Methods (2)

- Build subspace with reference state $|\psi\rangle$ as : $\{e^{-in\delta tH}|\psi\rangle\}$, $n \in 0,1,2,\dots,k$
- K-time steps span the k-dimensional Krylov space if δt is small.
- Construct $\widetilde{H}_{ij}$ and S_{ij} and solve: $\widetilde{H}\mathcal{C} = \epsilon S\mathcal{C}$
  - $\widetilde{H}_{nm} = \langle\psi|e^{im\delta tH}He^{-in\delta tH}|\psi\rangle \xrightarrow{?} \langle e^{i(m-n)\delta tH}H\rangle$
  - $S_{nm} = \langle\psi|e^{im\delta tH}\mathrm{e}^{-in\delta tH}|\psi\rangle \xrightarrow{?} \langle e^{i(m-n)\delta t}\rangle$



Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware

Katherine Klymko,[1,2,*] Carlos Mejuto-Zaera,[1,3,†] Stephen J. Cotton,[4,5] Filip Wudarski,[4,6] Miroslav Urbanek,[1] Diptarka Hait,[3,7] Martin Head-Gordon,[3,7] K. Birgitta Whaley,[3] Jonathan Moussa,[8] Nathan Wiebe,[9] Wibe A. de Jong,[1,‡] and Norm M. Tubman[4,§]

A Multireference Quantum Krylov Algorithm for Strongly Correlated Electrons

Nicholas H. Stair, Renke Huang, and Francesco A. Evangelista*

Quantum Krylov subspace algorithms for ground- and excited-state energy estimation

Cristian L. Cortes and Stephen K. Gray

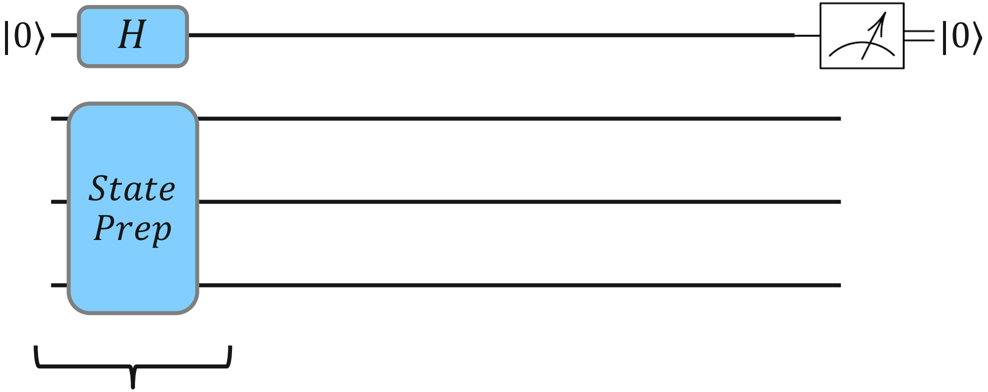
Quantum Filter Diagonalization: Quantum Eigendecomposition without Full Quantum Phase Estimation

Robert M. Parrish[1,*] and Peter L. McMahon[1,2]

Quantum Filter Diagonalization with Compressed Double-Factorized Hamiltonians

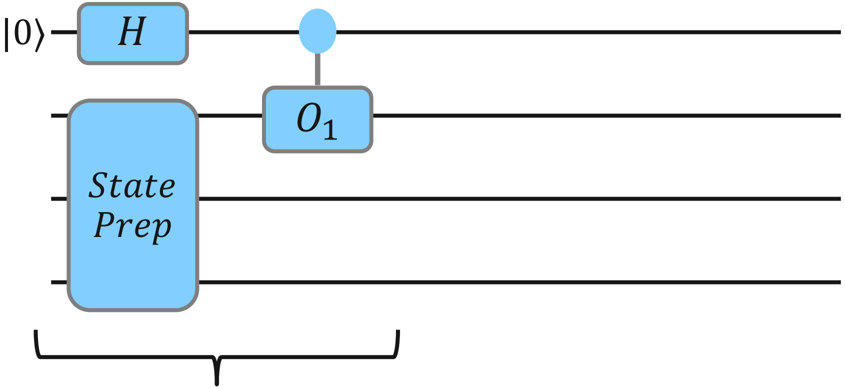
Jeffrey Cohn,[1,*] Mario Motta,[1,†] and Robert M. Parrish[2,‡]

Dynamic Correlation Functions



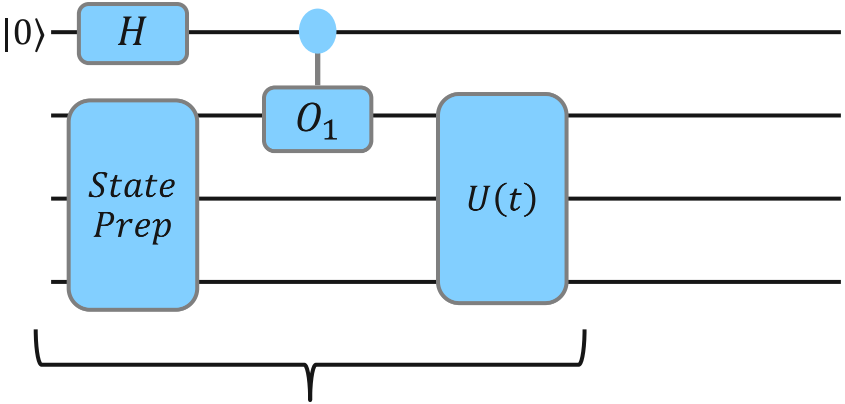
$$\frac{1}{\sqrt{2}}[|0\rangle|\psi\rangle + |1\rangle|\psi\rangle]$$

Dynamic Correlation Functions



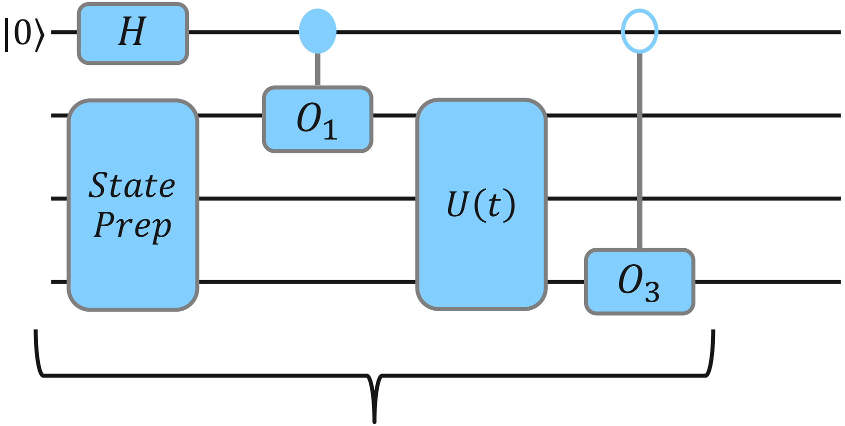
$$\frac{1}{\sqrt{2}}\left[|0\rangle|\psi\rangle + |1\rangle O_1|\psi\rangle\right]$$

Dynamic Correlation Functions



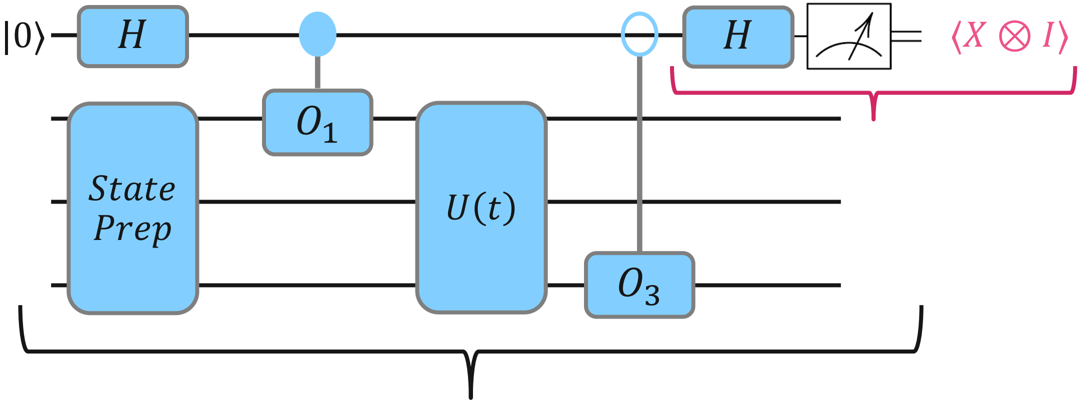
$$\frac{1}{\sqrt{2}}\left[|0\rangle U(t)|\psi\rangle + |1\rangle U(t) O_1 |\psi\rangle\right]$$

Dynamic Correlation Functions



$$\frac{1}{\sqrt{2}}\left[|0\rangle O_3 U(t)|\psi\rangle + |1\rangle U(t) O_1 |\psi\rangle\right]$$

Dynamic Correlation Functions



$$\frac{1}{2}[\langle\psi|O_1^\dagger U^\dagger(t)\langle 1| + \langle\psi|U^\dagger(t)O_3^\dagger\langle 0|][|0\rangle\langle 1| \otimes I + |1\rangle\langle 0| \otimes I][|0\rangle O_3 U(t)|\psi\rangle + |1\rangle U(t)O_1|\psi\rangle]$$

$$= \frac{1}{2}\langle\psi|O_1^\dagger U^\dagger(t)O_3 U(t)|\psi\rangle + \frac{1}{2}\langle\psi|U^\dagger(t)O_3^\dagger U(t)O_1\rangle = Re\{\langle\psi|O_1^\dagger(0)O_3(t)|\psi\rangle\} = Re\{C_{1,3}(0,t)\}$$

Gibbs State Preparation

IBM **Quantum**

- $We\ want\ to\ sample\ eigenstates\ \{|E_n\rangle\}\ of\ H\ with\ probability$: $\mathrm{p_n}(\beta) = \frac{\mathrm{e}^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$

Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution

Mario Motta,[1,*] Chong Sun,[1] Adrian T. K. Tan,[2] Matthew J. O'Rourke,[1] Erika Ye,[2] Austin J. Minnich,[2] Fernando G. S. L. Brandão,[3] and Garnet Kin-Lic Chan[1,†]

QITE:

$H = \sum_m h[m]$., where each h$[m]$ $act\ on\ at\ most\ k\ neighboring\ qubits$

$$e^{-\beta H} = \left[e^{-\Delta\tau h[1]} e^{-\Delta\tau h[2]} \dots e^{-\Delta\tau h[m]}\right]^n , \qquad \Delta\tau = \frac{\beta}{n}$$

After a single Trotter step we have: $|\Psi'\rangle = c^{-1}\, e^{-\Delta\tau h[m]}|\Psi\rangle$

$$where\ c = \left\langle\Psi\middle|e^{-2\Delta\tau h[m]}\middle|\Psi\right\rangle = 1 - 2\Delta\tau\langle\Psi|h[m]|\Psi\rangle + \mathcal{O}(\Delta\tau^2)$$

We want to generate: $|\Psi'\rangle = e^{-i\Delta\tau A[m]}|\Psi\rangle$

$A[m]$ can be expanded into the Pauli basis on k qubits: $A[m] = \sum_{i_1,i_2,\dots,i_k} a_{i_1,i_2,\dots,i_k}\, \sigma_{i_1} \dots \sigma_{i_k} = \sum_I a[m]_I\, \sigma_I$

QITE

IBM **Quantum**

- $Now\ to\ 1st\ order\ in\ \Delta\tau\ the\ coefficients, a[m]_I, can\ be\ defined\ by\ the\ linear\ system$:
  - $\boldsymbol{S a}[m] = \boldsymbol{b}$
  - $S_{I,I'} = \langle\Psi|\sigma_I\sigma_{I'}|\Psi\rangle$, $b_I = -\frac{i}{\sqrt{c}}\langle\Psi|\sigma_I h[m]|\Psi\rangle$
- $The\ wavefunction\ is\ restricted\ to\ real\ values\ if\ the\ \sigma_I's\ are\ restricted\ to$
- $Pauli\ strinigs\ with\ an\ odd\ number\ of\ Y\ terms$.

- **QMETTS** (Quantum Minimally Entangled Typical Thermal States)

1. $Apply\ QITE\ to\ |\psi_0\rangle\ iterated\ to\ \beta\ and\ measure\ in\ the\ computational\ basis$
2. $Use\ most\ measured\ state\ as\ new\ inital\ state\ for\ QITE$.
3. $Iterate\ until\ convergence\ of\ \frac{1}{N}\sum_i\langle\psi_i|O|\psi_i\rangle$

Further Reading for Gibbs States

Quantum Metropolis Sampling

K. Temme [1], T.J. Osborne[2], K. Vollbrecht[3], D. Poulin[4], and F. Verstraete[1]

Variational ansatz-based quantum simulation of imaginary time evolution

Sam McArdle, Tyson Jones, Suguru Endo, Ying Li, Simon C. Benjamin & Xiao Yuan

Finite correlation length implies efficient preparation of quantum thermal states

Fernando G.S.L. Brandão[1] and Michael J. Kastoryano[2]