

Fermionic Hamiltonians

①

$$H_{\text{nature}} = \sum_{i,j} t_{ij} a_i^\dagger a_j + \sum_{i,j,k,l} u_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

- $t_{ij} = t_{ji}^*$, $u_{ijkl} = u_{kji}^*$

- used to study: hopping, chemical potential, two particle interaction

- not used to study: superconductivity, relativistic effects

- $M \sim$ number of (fermionic) modes present

- H acts on $\bigoplus_{k=0}^M \wedge^k \mathbb{C}^M \equiv$ hilbert space of dimension 2^M
 $\equiv \mathcal{H}_{\text{nature}}$

- (for later use): number operator $N = \sum_{k=0}^M a_k^\dagger a_k$ commutes with H_{nature} .

- fermionic operators satisfy commutation rules:

$$\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0, \quad \{a_i, a_j^\dagger\} = \delta_{ij}$$

Hubbard model

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graph $G = (V, E)$, spin $1/2$ fermion at vertices

$$H_{\text{Hubbard}} = -t \sum_{(i,j) \in E} \sum_{\sigma \in \{\uparrow, \downarrow\}} (a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) \\ + u \sum_{i \in V} n_{i\uparrow} n_{i\downarrow}$$

t \sim hopping of arbitrary spin from one site to
same spin at a neighbouring site

u \sim potential for finding two electrons at same site

Representation on quantum computer

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at our disposal, we have a QC of Q -qubits, each qubit giving \mathbb{C}^2

- QC gives access to Hilbert space $\mathcal{H}_{\text{simulator}} = (\mathbb{C}^2)^{\otimes Q}$

our goal today is to study encodings of nature into QC

- an encoding is an isometry $\mathcal{E} : \mathcal{H}_{\text{nature}} \longrightarrow \mathcal{H}_{\text{simulator}}$

(where \mathcal{H}_{sim} may have dimension larger than $\mathcal{H}_{\text{nature}}$)

- a simulator hamiltonian H_{sim} "simulates" H_{nature} if

$$H_{\text{sim}} \circ \mathcal{E} = \mathcal{E} \circ H_{\text{nature}}$$

(if $\dim \mathcal{H}_{\text{sim}} > \dim \mathcal{H}_{\text{nature}}$ then we don't mind what H_{sim} does away from $\text{image}_{\mathcal{E}}(\mathcal{H}_{\text{nature}})$)

intuition : it is much nicer to think of QC structure of H_{sim} rather than \mathcal{E}

Jordan-Wigner transformation

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- $\dim(\mathcal{H}_{\text{nature}}) = 2^M$ so seems easy to use M -qubits ($Q=M$)

- occupation of mode k indicated by $|0\rangle, |1\rangle$ state of k^{th} qubit

(intuitively super easy. see: 2000 Bravyi, Kitaev - Fermionic quantum computation (section 2))

- $\mathcal{H}_{\text{sim}} = \text{span}_{\mathbb{C}} \{ |n_1, \dots, n_M\rangle \}_{n_k \in \{0,1\}}$

example: 3 modes: $|n_1, n_2, n_3\rangle$, $|101\rangle$
 $\equiv 2$ fermionic modes present,
present in 1st, 3rd modes

- annihilation operators: $(a_k, a_k^+)_{\text{simulation}}$

$$a_k | \text{---} 0_k \text{---} \rangle = 0$$

$$a_k | \text{---} 1_k \text{---} \rangle = (-1)^{\sum_{i=1}^{k-1} n_i} | \text{---} 0_k \text{---} \rangle$$

(depends on the order you put on your M fermionic modes)

creation operators given by hermitian conjugates

exercise: calculate $a_1^+ a_3 |001\rangle$
 $a_1^+ a_3 |011\rangle$

Jordan-Wigner transformation

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it's very easy to see how to represent creation/annihilation as terms familiar to a QC.

use notation: X_k, Y_k, Z_k & $|0\rangle\langle 1|_k, |1\rangle\langle 0|_k$


$$\text{where } |0\rangle\langle 1| = \frac{1}{2} (X - iY) \\ |1\rangle\langle 0| = \frac{1}{2} (X + iY)$$

$$- (a_k)_{\text{naive}} \mapsto (a_k)_{\text{sim}} = \left(\prod_{i=1}^{k-1} Z_i \right) |0\rangle\langle 1|_k$$

$$(a_k^\dagger)_{\text{naive}} \mapsto (a_k^\dagger)_{\text{sim}} = \left(\prod_{i=1}^{k-1} Z_i \right) |1\rangle\langle 0|_k$$

- occupation of mode is stored locally in \mathcal{H}_{sim}
parity of system is stored non-locally in \mathcal{H}_{mem}

leads to fermionic operators which scale linearly with respect to number of modes considered.

- exercise: think about Hubbard model on a lattice.
order qubits by snake 

and now consider a swap between two qubits in adjacent rows.

Parity mapping transformation

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- morally the complete dual to J-W
- parity of system is stored locally in \mathcal{H}_{sim}
occupation of mode is stored non-locally in \mathcal{H}_{sim}
(still leads to linear scaling for weight of fermionic operators)

- \mathcal{H}_{sim} is still M -qubits: $\text{span}_{\mathbb{C}} \{ |n_1, \dots, n_M\rangle \}_{n_k \in \{0,1\}}$

order the modes given in "nature"-problem: m_1, m_2, \dots, m_k

define parity $p_k = \sum_{i=1}^k m_i$ $m_i \in \{0,1\}$ depending on presence of fermion in i^{th} mode

encoding \mathcal{E} sends $|k\rangle_{\text{nature}}$ to $|p_1, \dots, p_M\rangle$

- rather than understanding \mathcal{E} it is easier to understand the map $T: \mathcal{H}_{\text{JW}} \rightarrow \mathcal{H}_{\text{PARITY}}$

example

$$\begin{aligned} |000\rangle_{\text{JW}} &\longmapsto |000\rangle_{\text{P}} \\ |010\rangle_{\text{JW}} &\longmapsto |011\rangle_{\text{P}} \end{aligned}$$

in general $T = \begin{bmatrix} 1 & & \\ & \ddots & \\ 1 & & 1 \end{bmatrix}$ $T^{-1} = \begin{bmatrix} 1 & & \\ & \ddots & \\ 0 & 1 & 1 \end{bmatrix}$

$$(a_k)_{\text{parity}} = T \circ (a_k)_{\text{JW}} \circ T^{-1}$$

Parity mapping transformation

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exercise: calculate $(a_k)_{\text{parity}}$ explicitly via

- take $\psi_P = |n_1, \dots, n_M\rangle_P$
- calculate $T^{-1}\psi_P$ which gives JW rep ψ_{JW}
- calculate $(a_k)_J \psi_J$
- calculate $T(a_k)_J \psi_J$ which gives $(a_k)_P \psi_P$
- deduce formula

$$\text{answer: } (a_k)_P = |0\rangle\langle 0|_{k-1} \otimes |0\rangle\langle 1|_k \otimes \prod_{i=k+1}^M X_i \\ - |1\rangle\langle 1|_{k-1} \otimes |1\rangle\langle 0|_k \otimes \prod_{i=k+1}^M X_i$$

$$(a_k^\dagger)_P = |0\rangle\langle 0|_{k-1} \otimes |1\rangle\langle 0|_k \otimes \prod_{i=k+1}^M X_i \\ - |1\rangle\langle 1|_{k-1} \otimes |0\rangle\langle 1|_k \otimes \prod_{i=k+1}^M X_i$$

remark: can rewrite above terms w/ Pauli notation

$$\text{eg } |0\rangle\langle 0|_{k-1} \otimes |0\rangle\langle 1|_k - |1\rangle\langle 1|_{k-1} \otimes |1\rangle\langle 0|_k = \frac{1}{2} (Z_{k-1} X_k - i Y_k)$$

Binary-tree transformation

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- due to Bravyi-Kitaev
- idea can be traced to "Fenwick trees" in classical computer science (which offers a slight generalization to what I present below)
- basic idea is to find middle ground between locality of storing
 - occupation of mode
 - parity of system
- leads to creation/annihilation operators of weight $O(\log(M))$.
- reference: 2012 Seeley, Richard, Love - The BK transformation for quantum computation of electronic structure
- morally is the JW transformation under conjugation by Fourier transform

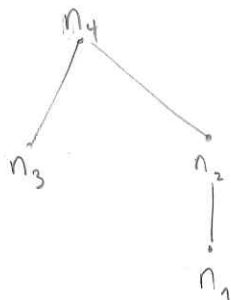
Binary-tree transformation

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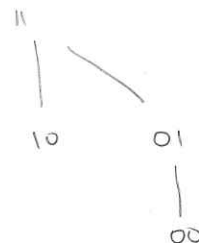
we'll look at an example with $M=4$ modes

(this is easy since 4 is a power of 2)

we give a mapping $T: \mathcal{H}_{\text{JW}} \rightarrow \mathcal{H}_{\text{BK}}$



comes from writing $k-1$ (in n_k) in binary



there is a partial order on binary strings pictured above \leq

$$T: |n_1 n_2 n_3 n_4\rangle_{\text{JW}} \longmapsto |x_1 x_2 x_3 x_4\rangle_{\text{BK}}$$

where $x_k = \sum_{i \leq k} n_i$.

e.g. $|1100\rangle_{\text{JW}} \longmapsto |11000\rangle_{\text{BK}}$

