Fermionic Hamiltonians

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

- $t_{ij} = t_{ji}^*$, $u_{ijkl} = u_{lkji}^*$
- used to study: hopping, chemical potential, two particle interaction
- not used to study: superconductivity, relativistic effects
- M ~ number of (fermionic) modes present
- H acts on $\bigoplus_{k=0}^{M} \Lambda^k \mathbb{C}^M$ $\equiv$ hilbert space of dimension 2^M $\equiv \mathcal{H}_{nature}$
- (for later use): number operator $N = \sum_{k=0}^{M} a_k^\dagger a_k$ commutes with H_{nature}.
- fermionic operators satisfy commutation rules:

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

Hubbard model

graph $G = (V, E)$, spin ½ particle at vertices

$$H_{hubbard} = -t \sum_{(i,j) \in E} \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(a^{\dagger}_{i\sigma} a_{j\sigma} + a^{\dagger}_{j\sigma} a_{i\sigma} \right)$$

$$+ u \sum_{i \in V} n_{i\uparrow} n_{i\downarrow}$$

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

u ~ potential for finding two electrons at same site

Representation on quantum computer

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

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

our goal today is to study encodings of nature onto QC

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

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

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

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

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

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

Jordan-Wigner transformation

- $\dim(\mathcal{H}_{nature}) = 2^M$ 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))

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

example : 3 modes : $|n_1, n_2, n_3\rangle$, $|1\,0\,1\rangle$

$\equiv$ 2 fermionic modes present, present in 1^{st}, 3^{rd} modes

- annihilation operators : $(a_k, a_k^\dagger)_{simulator}$

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

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

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

creation operators given by hermitian conjugates

<u>exercise</u> : calculate $a_1^\dagger a_3 |001\rangle$

$a_1^\dagger a_3 |011\rangle$

Jordan-Wigner transformation

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

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

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

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

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

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

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

  leads to fermionic operators which scale <u>linearly</u> 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

- 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 : $\mathrm{span}_{\mathbb{C}} \{ |n_1, \dots, n_M\rangle \}_{n_k \in \{0,1\}}$

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

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

  encoding $\mathcal{E}$ sends $|\psi\rangle_{nature}$ to $|p_1, \dots, p_m\rangle$

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

  example $\qquad |000\rangle_{JW} \longmapsto |000\rangle_P$

  $\qquad\qquad\quad |010\rangle_{JW} \longmapsto |011\rangle_P$

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

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

Parity mapping tranformation

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

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

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 wrt Pauli notation

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

Binary-tree transformation

- 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

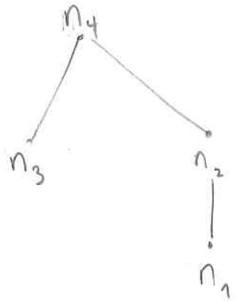
- leads to creation/annihilation operators of weight $\mathcal{O}(\log(M))$.

- reference: 2012 Seeley, Richard, Love - The BK transformation for quantum computation of electronic structure

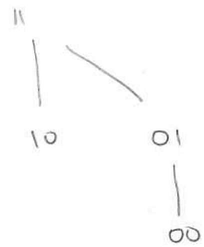
- morally is the JW transformation under conjugation by Fourier transform

Binary-tree transformation

well look at an example with $M=4$ modes
(this is easy since 4 is a power of 2)
we give a mapping $T: \mathcal{H}_{JW} \longrightarrow \mathcal{H}_{BK}$



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



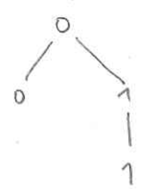
there is a partial order on binary strings pictured above $\leq$

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

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

e.g. $|1100\rangle_{JW} \longmapsto |1\ 0\ 0\ 0\rangle_{BK}$

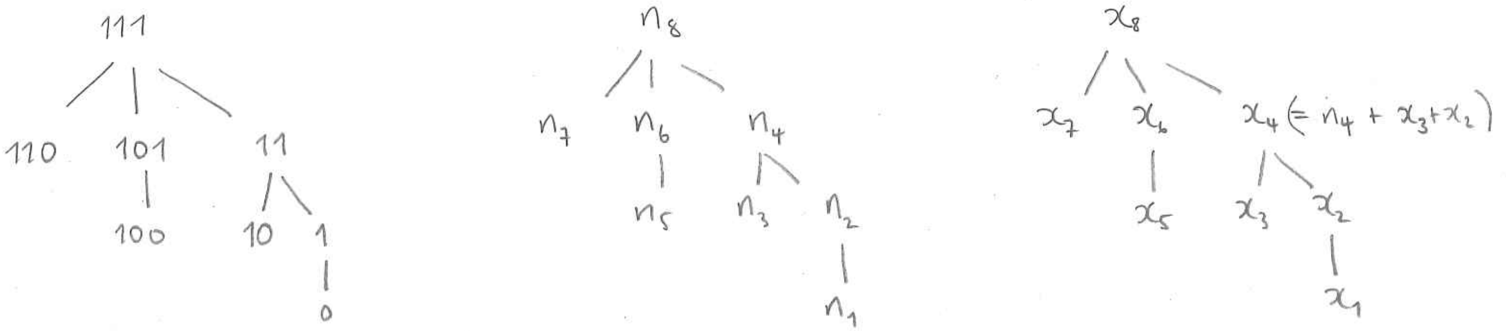
is



Binary-tree transformation

require knowledge of parity/update/flip sets

- parity $P(k)$ ~ qubits storing parity of orbitals in index less than k
- update $U(k)$ qubits which store a partial sum including qubit k
- flip $F(k)$ qubits which determine if qubit k has same parity as orb k.



k	1	2	3	4	5	6	7	8
$P(k)$	$\emptyset$	1	2	2,3	4	4,5	4,6	4,6,7

k	1	2	3	4	5	6	7	8
$U(k)$	2,4,8	4,8	4,8	8	6,8	8	8	$\emptyset$

k	1	2	3	4	5	6	7	8
$F(k)$	$\emptyset$	1	$\emptyset$	2,3	$\emptyset$	5	$\emptyset$	4,6,7

$R(k) = P(k) \setminus F(k)$	$\emptyset$	$\emptyset$	2	$\emptyset$	4	4	4,6	$\emptyset$

Binary-tree transformation

let's actually (and finally) write BK operators

- "even/odd" operators are projections onto kets with even/odd 1s in bit-string associated with indexing set

  if S is indexing set $\quad E_S = \frac{1}{2}(I + Z_S)$

  $\quad O_S = \frac{1}{2}(I - Z_S)$

- $\Pi_k^{\pm}$ are creation/annihilation which check if parity is flipped

$$\Pi_k^{-} = E_{F(k)} \otimes |0\rangle\langle 1|_k - O_{F(k)} \otimes |1\rangle\langle 0|_k$$

$$\Pi_k^{+} = E_{F(k)} \otimes |1\rangle\langle 0|_k - O_{F(k)} \otimes |0\rangle\langle 1|_k$$

(look back at first part of $(a_k)_P$, $(a_k^\dagger)_P$)

(think about how easy these look when k is odd)

- finally

$$(a_k)_{BK} = Z_{R(k)} \otimes \Pi_k^{-} \otimes X_{U(j)}$$

$$(a_k^\dagger)_{BK} = Z_{R(k)} \otimes \Pi_k^{+} \otimes X_{U(j)}$$

Superfast encoding

"one can speculate that, in principle, electron might not be fundamental particles but, rather, excitations in a non perturbative system of bosons"

an encoding for when modes interact locally, giving graph $G=(V,E)$ with $|V|=M \sim$ modes, and $H = \sum_{(i,j)\in E} H_{ij}$.

rather than encode $a_k, a_k^\dagger$, we encode $2M$ Majorana modes

$$c_{2k} = a_k + a_k^\dagger$$

$$c_{2k+1} = -i(a_k - a_k^\dagger)$$

- we can easily recover $a_k, a_k^\dagger$
- Majoranas possess a very nice algebraic structure : $c_i c_j + c_j c_i = 2\delta_{ij}$ which in a (complexified) Clifford algebra

our H_{nature} only possessed "even" weight terms, so don't need to encode the whole algebra of second quantised operators, but rather just the even part

$$B_k = -i\, c_{2k}\, c_{2k+1} \qquad \text{(to each vertex)}$$

$$A_{ij} = -i\, c_{2i}\, c_{2j} \qquad \text{(to each edge)}$$

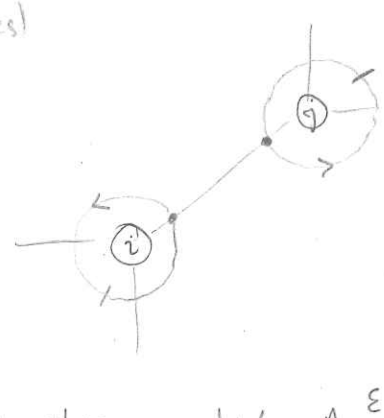
- these satisfy a whole lot of obvious relations plus a non-obvious "loop" relation.

Superfast encoding:

- place qubit on edge of graph (morally more edges than vertices)

$$B_j \longmapsto B_j^{\varepsilon} = \prod_{i|(i,j)\in E} Z_{ij}$$

$$A_{ij} \longmapsto A_{ij}^{\varepsilon} = \varepsilon_{ij}\, X_{ij} \prod_{a|ia <_i ij} Z_{ia} \prod_{b|bj <_j ij} Z_{bj}$$



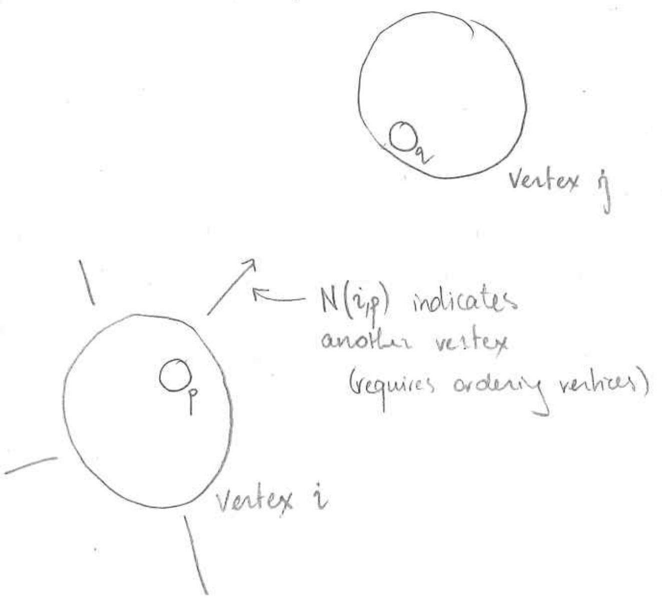
- codespace (image$_\varepsilon$ H_{nature}) is obtained by restricting qubits to subspace on which A_{ij}^{ε} satisfy the non-local "loop" relation.

Generalised superfast encoding

- same setup as before $G = (V, E)$ with d_k even for all $v_k \in V$
- place $d_k/2$ qubits at each vertex giving d_k local Majorana modes

$$\gamma_{k,p}^{\dagger} = \gamma_{k,p} \qquad \gamma_{k,p}\gamma_{k,q} + \gamma_{k,q}\gamma_{k,p} = 2\delta_{pq}$$

- local Majorana modes at different vertices commute.



$$B_j^{\varepsilon} = (-i)^{d_j/2} \; \gamma_{j,1} \cdot \gamma_{j,2} \cdot \, — \, \cdot \gamma_{j,d_j}$$

$$A_{ij}^{\varepsilon} = \varepsilon_{ij} \; \gamma_{ip} \cdot \gamma_{jq}$$

where $j = N(i,p)$
$i = N(j,q)$

- similar to original superfast encoding, need to declare codespace as $+1$ subspace corresponding to stabilizer subgroup generated by loops of A_{ij}^{ε}.

Tapering off qubits

- we have mostly looked at H_{nature} acting on $\Lambda^\bullet \mathbb{C}^M = \bigoplus_{k=0}^{M} \Lambda^k \mathbb{C}^M$ and thought about how to fully encode $\Lambda^\bullet \mathbb{C}^M$.
- but our problems of interest (non-relativistic quantum chemistry) possess many symmetries that we should take advantage of.
  - particle conservation
  - spin conservation
- eg. if we knew that N= number of modes then we should only care about encoding $\Lambda^N \mathbb{C}^M \subset \Lambda^\bullet \mathbb{C}^M$ which is of dimension ${}^M C_N = \frac{M!}{N!(M-N)!} \ll 2^M$
- imagine $\exists Q$ with ${}^M C_N \ll 2^Q \ll 2^M$ (then could encode into only Q-qubits)
- one idea comes from error correction encoding ideas, but we will look at a discrete idea. A systematic way to remove 1 qubit per each $\mathbb{Z}_2$ symmetry.

- start with J.W. transformation

$$H_{simulator} = \sum_{j=1}^{r} h_j \sigma_j \qquad \sigma_j \text{ is an } M\text{-qubit Pauli operator}$$

of every term in H_{sim}

- imagine there is a stabiliser symmetry $S \leq P_M$, then (theorem) we can write $S = \langle \tau_1, \ldots, \tau_k \rangle$ with $\tau_i = U \sigma_i^x U^\dagger$, $U \in C_M$.

$$H_{sim}' := U H_{sim} U^\dagger = \sum_{j=1}^{r} h_j \eta_j \qquad \eta_j = U \sigma_j U^\dagger$$

- this implies $\{\sigma_i^x\}_{i=1}^{r}$ commute with H_{sim}' so first r-qubits can be tapered off and replaced with ± 1 associated evalue.

- this procedure might increase weight of Pauli terms (η_j)
- there is also an efficient procedure to find generators of the symmetry group.