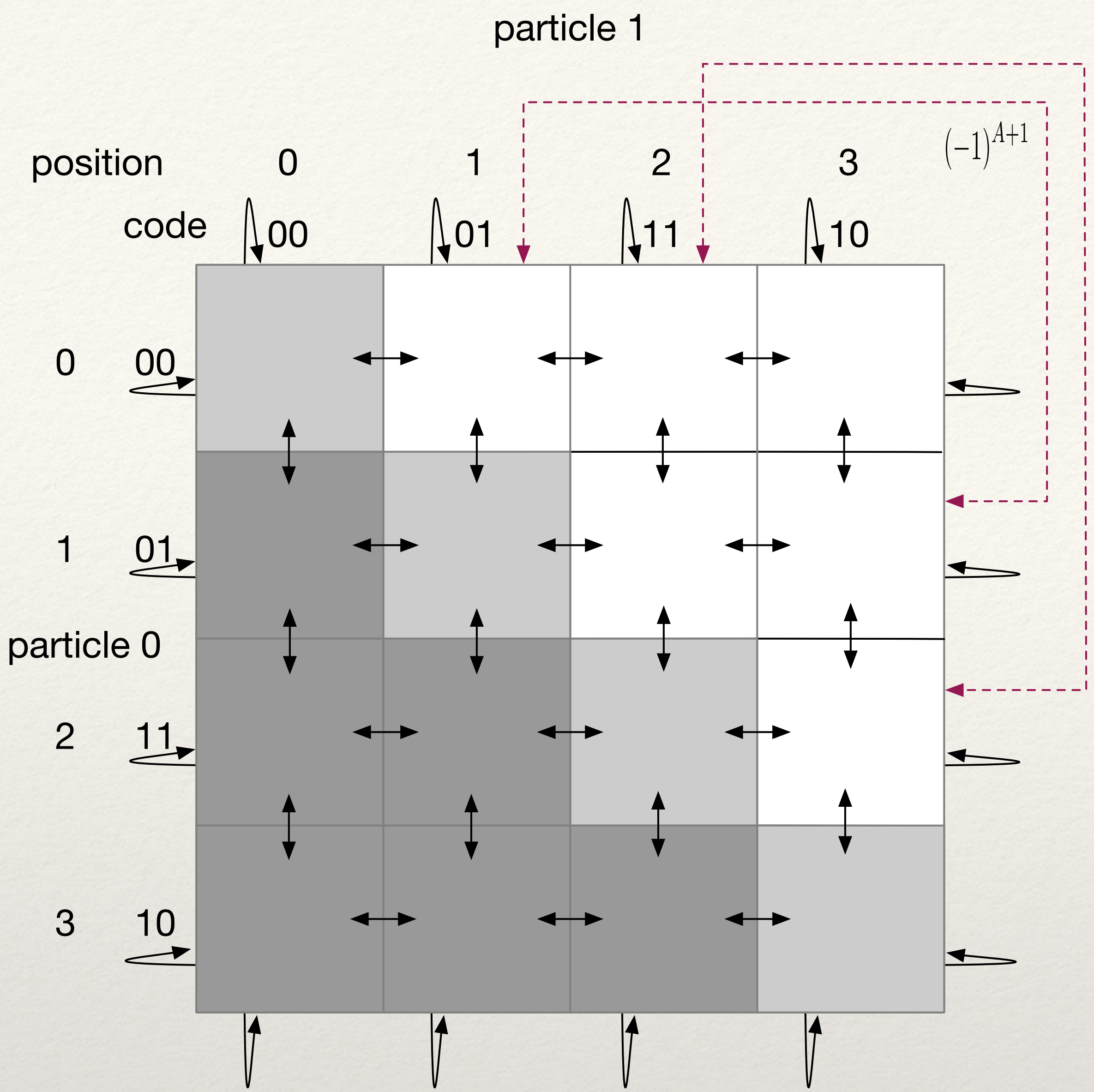

The Fermionic Schrödinger Equation in AQC

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Objective: Find Ground State of H

- Goal is to put the circuit in the ground state of a target Hamiltonian $H = T + V$ where T is the kinetic energy operator and V is a local potential
- The Hamiltonian will be discretized over a finite volume periodic lattice in first quantization.
- Example Target Problems:
  - 2D: Fractional Quantum Hall
  - 3D: Nuclei (May be simpler than encoding shell model)

Focus on Laplacian

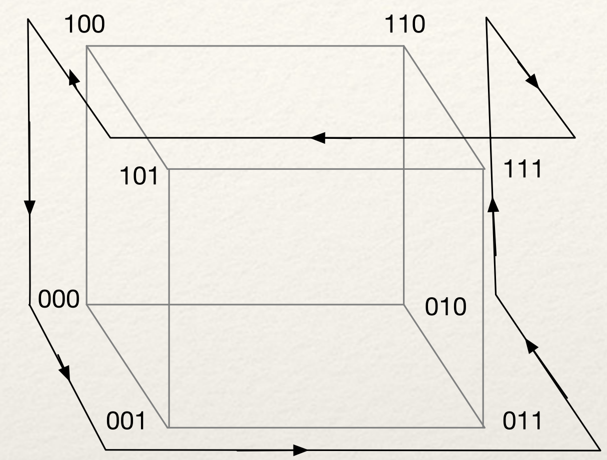
- The challenge is to efficiently implement the Laplacian. The one particle discrete version being:

$$\nabla^2\psi(a\vec{n}) \approx L\psi(\vec{n}) = \frac{1}{h^2}\sum_{d=0}^{D-1} \psi\left(\vec{n} - \hat{e}_d\right) - 2\psi\left(\vec{n}\right) + \psi\left(\vec{n} + \hat{e}_d\right)$$

- The difficulty over the distinguishable particle case is that the references to neighboring lattice sites are essentially motions of the particles that interact with exchange symmetry.

BRGC Code

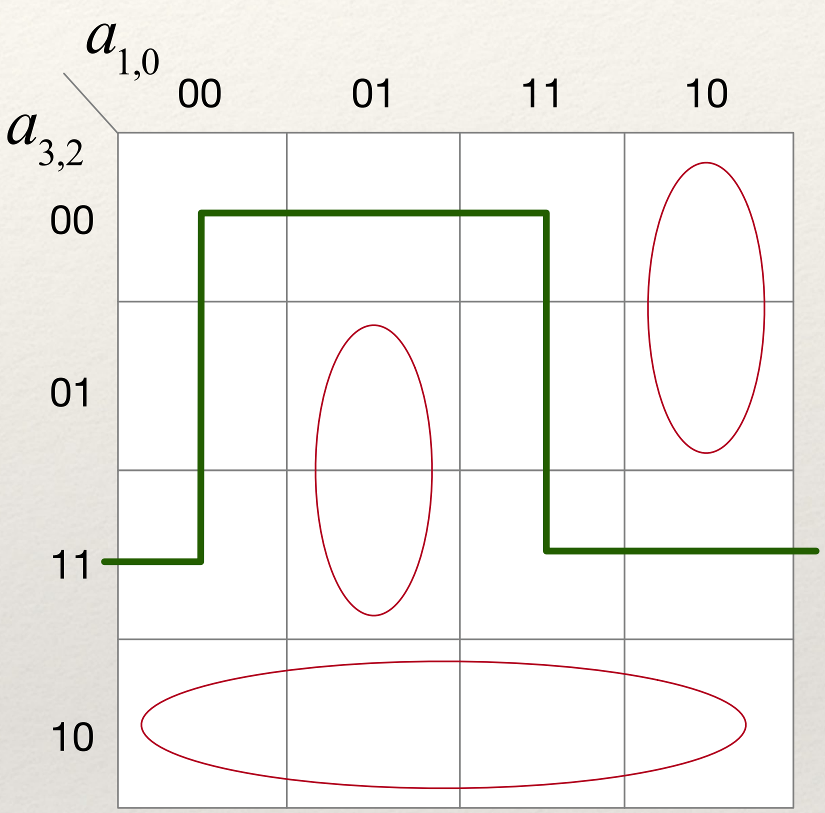
- Gray code is an encoding of the integers $0 \;\ldots\; 2^n - 1$ such that neighboring integers have codes differing in a single bit. It is a Hamiltonian Path on a D=n dimension binary hyper-cube.
- Binary Reflected Gray Code is constructed recursively by reflecting the code from one fewer bits, and adding a leading sunblock bit.
- We are interested because neighboring codes automatically share all but one spin state in their corresponding basis elements. This simplifies the operator structure of the Laplacian.



num	gray
0	000
1	001
2	011
3	010

Distinguishable Particles

- I am building on top of [1], which implements the Laplacian for distinguishable particles

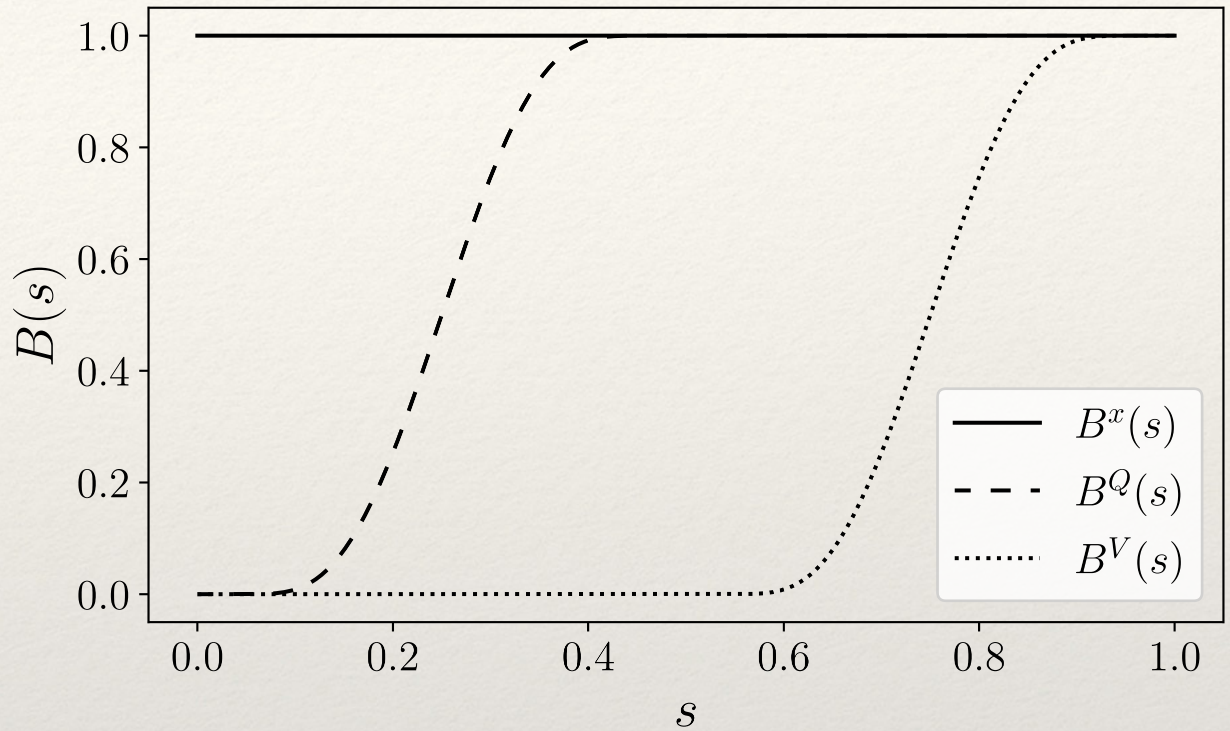


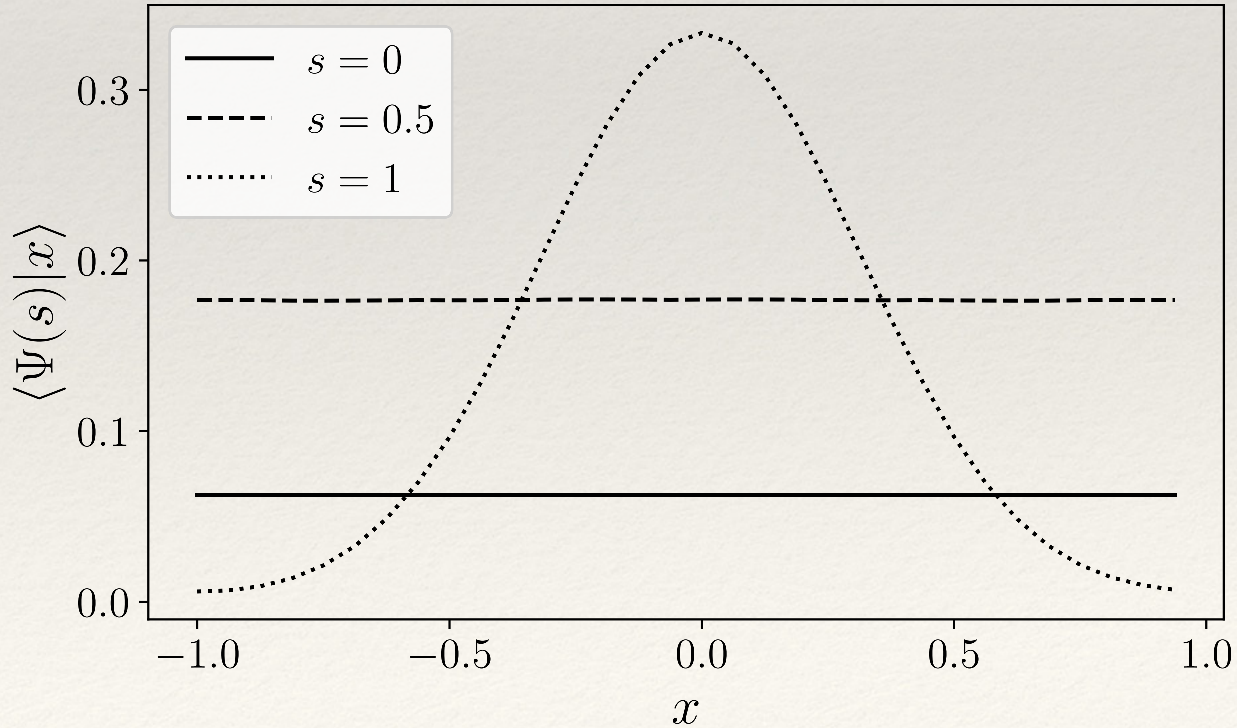
- Hamming-distance-2 Gray code encoding of 1D position
- Red ovals are penalized states
- The 1D laplacian is simply $\mathscr{L} \propto L = -2 + \sum \sigma^x_{a,i}$, generating all neighbor contributions. Off path contributions are filtered away by penalties

[1] Chang, McElvain, Rrapaj, Wu, PRX Quantum 3, 020356 2022

HO Example with H2GC encoding

- 32 Lattice positions, 8 qubits
- Off path penalty B^Q enabled first, potential V last.
- At $s = 0.0$ $H = \sum \sigma_i^x$. The GS wave function is constant with amplitude $\sqrt{1/256}$
- At $s = 0.5$, the GS wave function is now only along the path with amplitude $\sqrt{1/32}$
- At $s = 1$ the wave function takes on the familiar harmonic oscillator GS form





Indistinguishable Fermions

- A single fermionic product state is a sum of distinguishable particle product states (4 particle case):

$$\Phi(x_0, x_1, x_2, x_2) = \frac{1}{\sqrt{4!}} \begin{vmatrix} \phi_a(x_0) & \phi_b(x_0) & \phi_c(x_0) & \phi_d(x_0) \\ \phi_a(x_1) & \phi_b(x_1) & \phi_c(x_1) & \phi_d(x_1) \\ \phi_a(x_2) & \phi_b(x_2) & \phi_c(x_2) & \phi_d(x_2) \\ \phi_a(x_3) & \phi_b(x_3) & \phi_c(x_3) & \phi_d(x_3) \end{vmatrix}$$

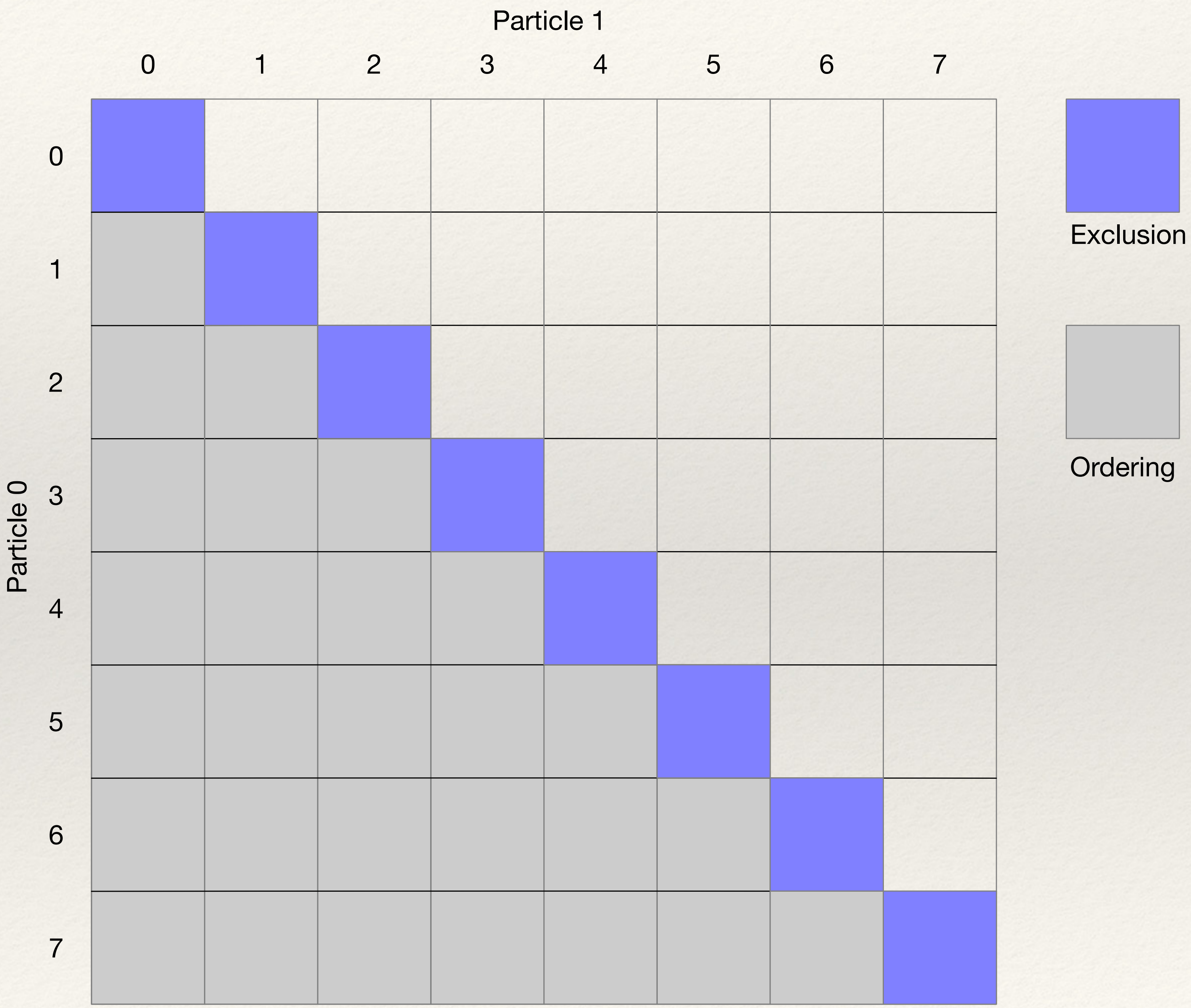
$$\equiv \left| a, b, c, d \right\rangle$$

where a, b, c, d are integer position labels on the lattice.

- There are 4! such terms that each naively corresponds to a product state. We choose the one satisfying $a < b < c < d$ to represent the fermionic state.

1D, 2 Particles

- Position labels ≡ 1D position index
- Shaded sites are suppressed by penalty
- Clear sites are associated with Slater determinants, AKA properly ordered states



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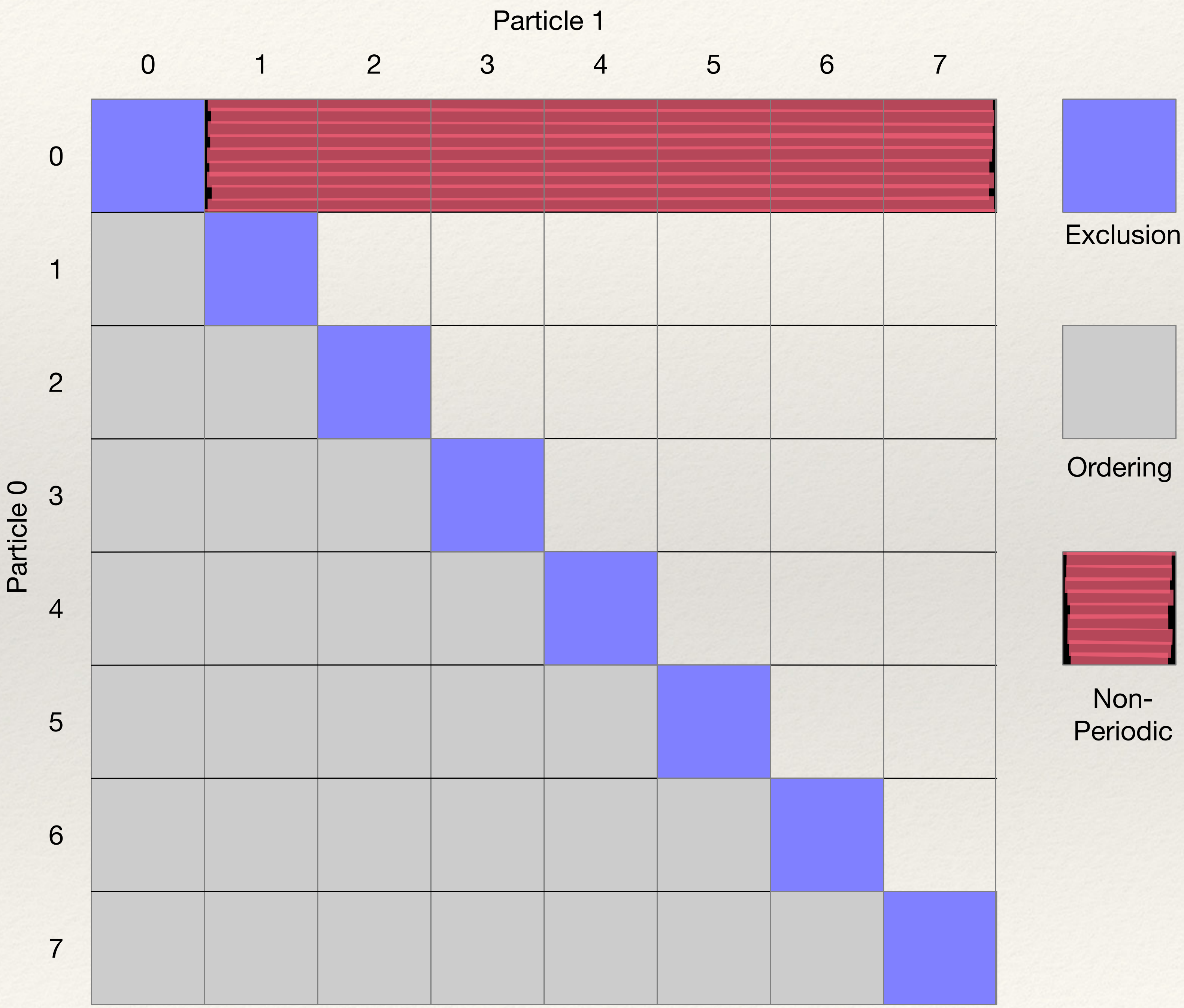
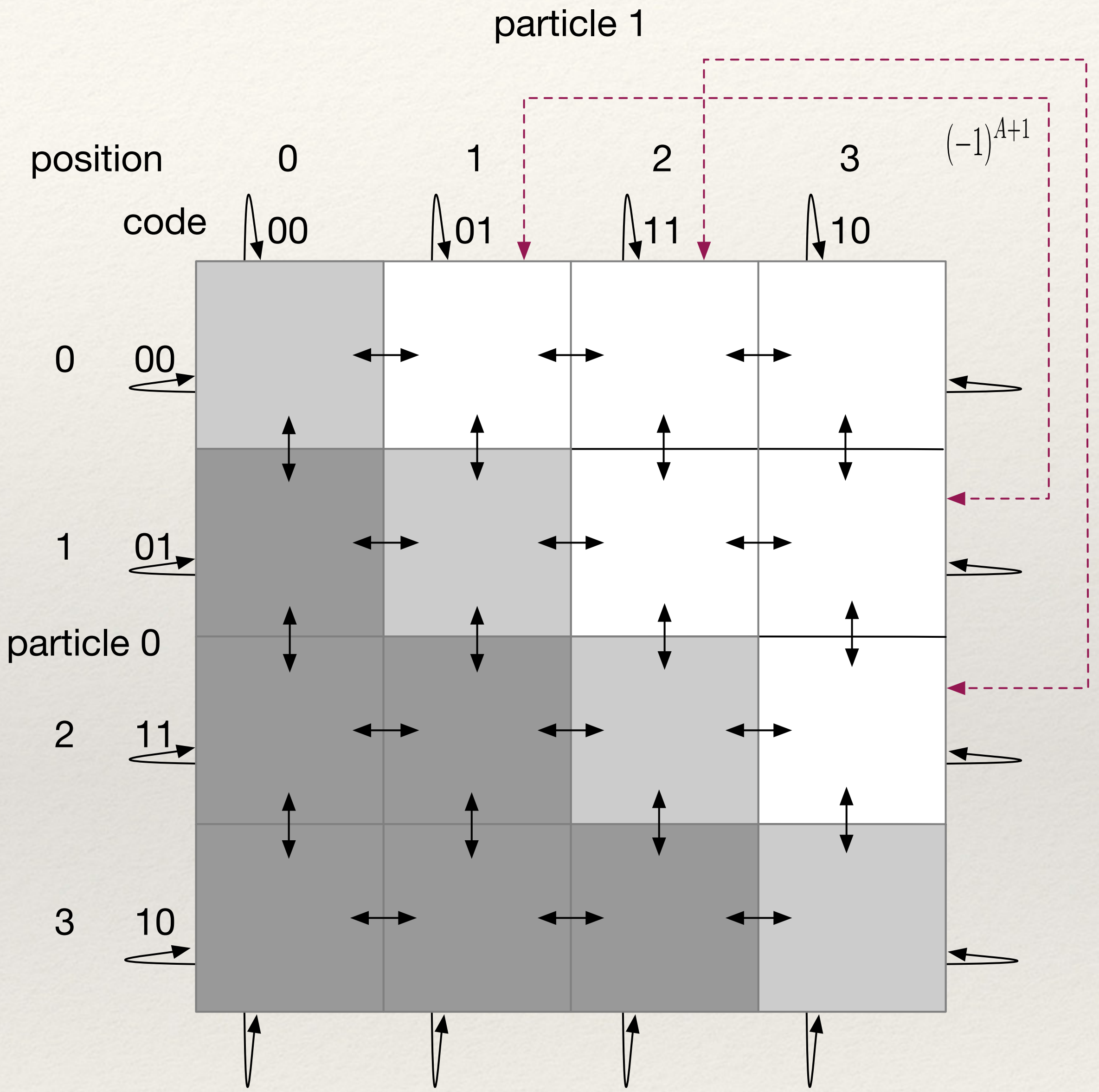


Distinguishable → Fermions

- Example: 1D with 2 particles
- Distinguishable L misses red dashed contributions and generates extra contributions (suppressed by penalties)
- How do we implement the red contributions? Periodic wrapping has violated the ordering constraint.



Entanglement Gadgets

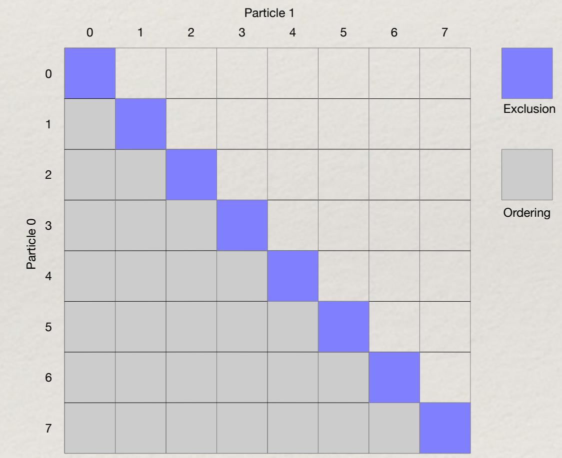
- Our first exposure to entanglement is often a 2 qubit wave function

$$|\uparrow\downarrow\rangle_{ab} + |\downarrow\uparrow\rangle_{ab}$$

- In this wave function the two qubits carry the same information, encoded differently.
- In an entanglement gadget we add $\Delta H = Q * P^{conflict}$ where $P^{conflict}$ projects out states that conflict with the desired entanglement. Q is the penalty value, ensuring that low lying states respect the desired entanglement. For the 2 qubit wave function above $P^{conflict} = |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| = P^{11}_{ab} + P^{00}_{ab}$
- Actions on spin a can be replaced by actions on spin b
- Optimization: The sum of projection operators can be allowed to overlap. The penalty may vary across the conflict subspace

Gray Code vs Binary

- We want Gray code positions for the Laplacian, but binary for the valid ordering projector $P^{ordering} = b_0 < b_1 < \cdots < b_{A-1}$
- Using the optimization (multiple terms may be on) $\tilde{P}_{unordered} = \left(b_0 \geq b_1\right) + \left(b_1 \geq b_2\right) + \cdots + \left(b_{A-2} \geq b_{A-1}\right)$
- This implements both the ordering and exchange penalties in diagram to right



- There are two remaining tasks
  - Implement binary / gray **entanglement gadget**
  - Implement binary $b \geq a \left(= a < b \right)$ projector

Binary/Gray Entanglement

- Boolean relationship:
  $g_{n-1} = b_{n-1}, \quad g_i = b_i \oplus b_{i+1}$
- Enforce bit by bit with
  $$\Delta H = QP_{g_i \oplus b_{i+1} \oplus b_i}$$
  $$\Delta H = Q\left(P^{100}_{g_i,b_i,b_{i+1}} + P^{111}_{g_i,b_i,b_{i+1}} + P^{010}_{g_i,b_i,b_{i+1}} + P^{001}_{g_i,b_i,b_{i+1}}\right)$$
- We will use g_i the for the Laplacian and the b_i for ordering

Binary	Gray
000	000
001	001
010	011
011	010
100	110
101	111
110	101
111	100

Less Than Projector

- Recursive boolean definition
  $x_i = a_i \oplus b_i$
  $a_{[n-1:0]} < b_{[n-1:0]} = x_{n-1}\, b_{n-1} \,|\, \bar{x}_{n-1} \left(a_{[n-2:0]} < b_{[n-2:0]} \right)$
- The x's can be implemented as additional qubits with penalties from the previous slide.
- A qubit is associated with each comparator size and a 4 qubit penalty expression is used to make the qubit match the required result
- Instead of the serial boolean form one can start with carry lookahead implementations, reducing the number of levels of ancillary qubits

Rotation Operators

- $\chi_{01} = (1/2)\left[I_0 I_1 + \sigma_0^x \sigma_1^x + \sigma_0^y \sigma_1^y + \sigma_0^z \sigma_1^z\right]$ is the swap operator
- For 2 qubits $R_{ij}^L = R_{ij}^R = \chi_{ij}, \quad R_i^R = I_i$
- $R_{012}^R = \chi_{01}\chi_{12} = \chi_{02}\chi_{01}, \quad R_{012}^L = \chi_{12}\chi_{01} = \chi_{02}\chi_{12}$
- Rotate sub-partitions, then rotate leftmost qubits $R_{0\ldots6}^R = R_{036}^R R_{012}^R R_{345}^R R_6^R$
- Will need multi-bit rotations - all pos bits of particles

Bloch-Horowitz Equation

- Used to make an effective Hamiltonian in a subspace P (with $Q = 1 - P$) of the full Hilbert Space

$$(P+Q)\,H\,|\psi_i\rangle = E_i\,|\psi_i\rangle \qquad \text{Schrodinger Eqn}$$

$$(E_i - QH)\,|\psi_i\rangle = E_i P\,|\psi_i\rangle \qquad \text{Rearrange}$$

$$|\psi_i\rangle = \frac{E_i}{E_i - QH} P\,|\psi_i\rangle \qquad \text{Reconstruct Wf}$$

$$E_i P\,|\psi_i\rangle = \boxed{PH\frac{E_i}{E_i - QH}P} P\,|\psi_i\rangle = H_{eff} P\,|\psi_i\rangle \qquad \text{BH Equation}$$

- The boxed expression is the BH Equation, forming an effective Hamiltonian acting in P with the same eigenvalues and projected eigenstates as H

Multi-Stage Decomposition

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

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

$\sigma^- = |1\rangle\langle 0|$

- Rotation by 3 in two layers

$$H = P_a^0 H_x P_a^0 + \sigma_a^- \chi_{1,2} + E\sigma_a^+ \chi_{0,1} \Rightarrow P_a^0 H_x P_a^0 + R_{0,1,2}^R$$

$$\begin{array}{cc|cc} & & \multicolumn{2}{c}{a} \\ & & 0 & 1 \\ a & 0 & H_x & \chi_{01} \\ & 1 & \chi_{12} & 0 \end{array}$$

- Analyze with BH eqn letting

$$P = P_a^0, \quad Q = 1 - P = P_a^1$$

project states with qubit $a = |1\rangle$

$$H_{eff} = P\left(PH_xP + \cancel{\sigma_a^- \chi_{12}} + E\sigma_a^+ \chi_{01}\right) \frac{E}{E - Q\left(\cancel{PH_xP} + \sigma_a^- \chi_{12} + \cancel{E\sigma_a^+ \chi_{01}}\right)} P$$

$$= P\left(PH_xP + E\sigma_a^+ \chi_{01}\right)(1 + \sigma_a^- \chi_{01}/E)P$$

higher powers in series are 0

$$= PH_xP + \chi_{01}\chi_{12}$$

- H^{eff} is energy dependent. Requires self consistent solution. Bound state solutions converge by simple iteration
- In the low lying model space we have generated a 3 bit rotation, without explicitly multiplying out the terms. Now we have a hammer …

All Rotations

- Generalize to all swaps, left and right rotations by 3

$$R^{(3)}_{order} = \sigma_a^- \sum_{i \in even}^{A-1} \chi_{i,i+1} + E\sigma_a^+ + E\sigma_a^+ \sum_{j \in odd}^{A-1} \chi_{j,j+1}$$

Interpret i,j as wrapping in $[0 \ldots A-1]$

$$+\sigma_b^- \sum_{i \in odd}^{A-1} \chi_{i,i+1} + E\sigma_b^+ + E\sigma_b^+ \sum_{j \in even}^{A-1} \chi_{j,j+1}$$

Singleton $\sigma^+_{a/b}$ results in effective $\chi_{i,i+1}$

$$\Rightarrow \sum_{i=0}^{A-1} \left(\chi_{i,i+1} + R^L_{i-1,i-1,i} + R^R_{i,i+1,i+2} \right) + Ignored$$

- Ignored is made of terms like $\chi_{1,2}\chi_{5,6}$. Applied to ordered states or states with one particle out of place they always produce an unordered and suppressed state

The Laplacian and Particle Order

- We act with the unscaled distinguishable Laplacian L on an ordered basis state:

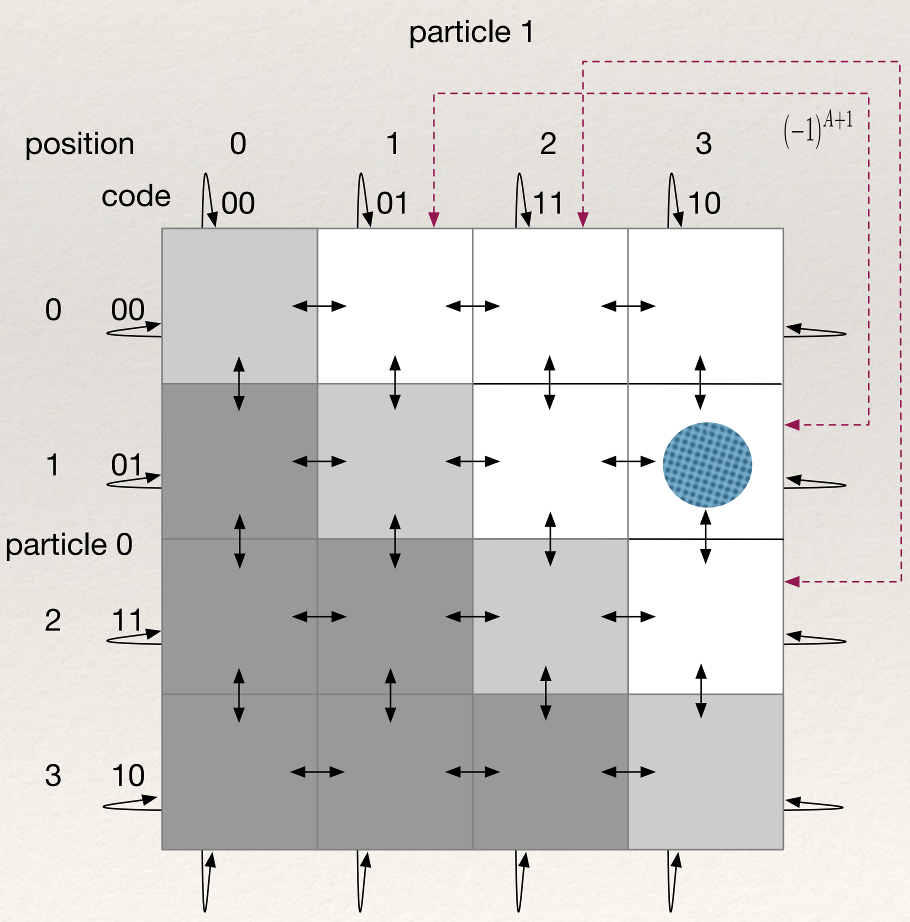
$$L\,|1,3\rangle = |0,3\rangle + |2,3\rangle + |1,2\rangle + |1,0\rangle$$

- Three of these states are properly ordered, but the last one is not! How do we recover?

$$L\left(1-\chi_{0,1}\right)|1,3\rangle = |0,3\rangle - |3,0\rangle + |2,3\rangle - |3,2\rangle + |1,2\rangle - |2,1\rangle + |1,0\rangle - |0,1\rangle$$

- Particle swapping operator $\chi_{0,1}$ generated three more improperly ordered states, but it recovered the proper order for $|1,0\rangle$ with corrected phase. The improperly ordered state contributions will be suppressed by the penalties on those states

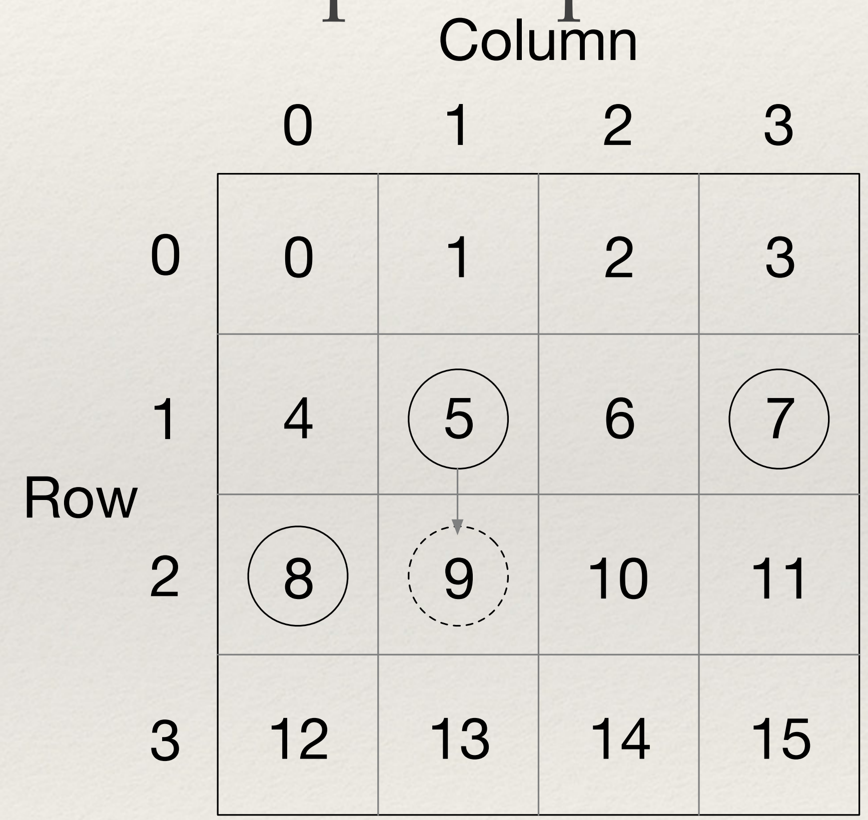
- The full operator to recover proper orderings is $\left(1+(-1)^{A+1}\left(R^R+R^L\right)\right)$. If we add the non-periodic penalty, then this operator is not needed



2^+D

- In 1D the increment or decrement of a particle position either finds an unoccupied and properly ordered position, or an occupied position blocked by exclusion principle

- In 2D, using a row first labeling, a vertical increment can hop over up to $A - 1$ particles.



$|5,7,8\rangle \rightarrow |9,7,8\rangle$

- Recovery of proper ordering requires

$$1 + \sum_{i=0}^{A} \sum_{j=1}^{A} (-1)^j \left(R^R_{[i:i+j]} + R^L_{[i-j:i]} \right)$$

- Assume that $A \ll 2^n$, limiting the size of required rotations

Summarizing H

- Components of H are penalties to define subspaces, penalties to establish entanglement, rotation operators to recover properly ordered states and application of the discrete particle Laplacian

$$H = V + Q\left(\tilde{P}_{H2GC} + \tilde{P}_{unordered} + \left[P_{nonperiodic}\right]\right) \quad \text{filtering}$$

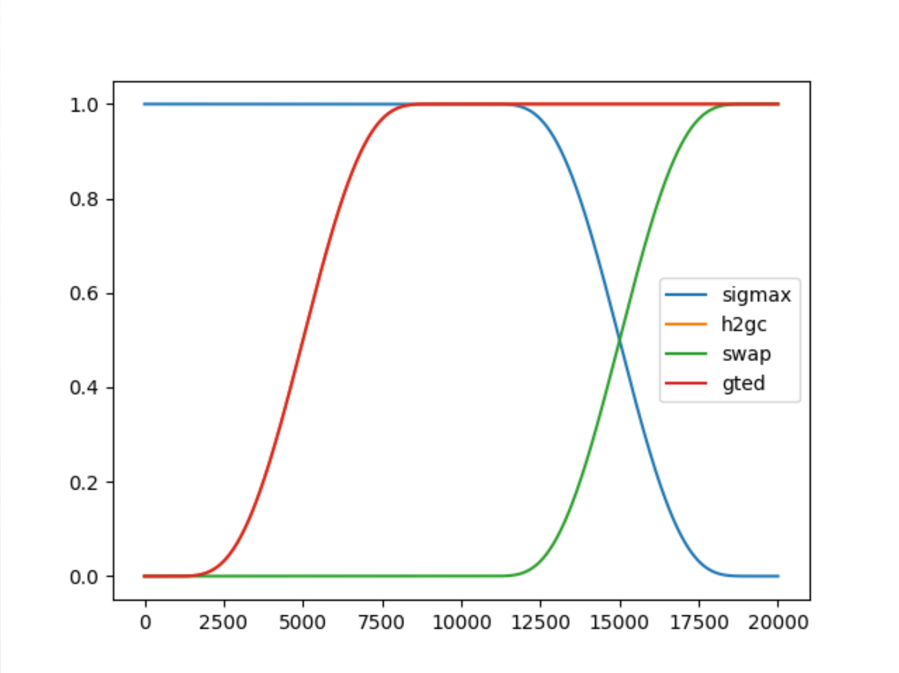
$$+Q\left(\sum \Delta H_{graybin} + \Delta H_{xor} + \Delta H_{<}\right) \quad \text{entanglement}$$

$$+\left(\sum_{i \in posbits} \sigma_i^x\right)\left(1 + \sum_{i=0}^{A} \sum_{j=1}^{B} (-1)^j \left(R^R_{[i:i+j]} + R^L_{[i-j:i]}\right)\right) \quad \text{L* ordering}$$

- $B = A$, or we can approximate with B a small fixed number . The approximation will improve with $N = 2^{n/2+1}$

Testing

- I ran an 8 qubit simulation of two particles in 2D, starting with a transverse H and ending with the fermionic Laplacian
  - Diagonalization of directly specified Laplacian yielded degenerate ground states
  - Adiabatic evolution of prior slide yielded a state that has the same energy and is a linear combination of the degenerate states
- Next step: Introducing a potential and simulate to find ground state - declare victory



Sequencing of H components

Conclusions

- Cost in qubits/pauli-operators is polynomial in A^D and n. The number of basis states we are solving in is $\mathcal{O}(2^n)$
- Penalties unwanted contributions from the distinguishable particle Laplacian that connected to improperly ordered states
- Entanglement gadgets were used to simplify a number of operations including maintaining position in both binary and gray encodings to minimize both the fermion ordering constraint implementation and the included distinguishable particle Laplacian
- As in the distinguishable particle case, the finite volume protects the gap between the GS and the first excited state, protecting the rate at which penalties and the potential are introduced

End