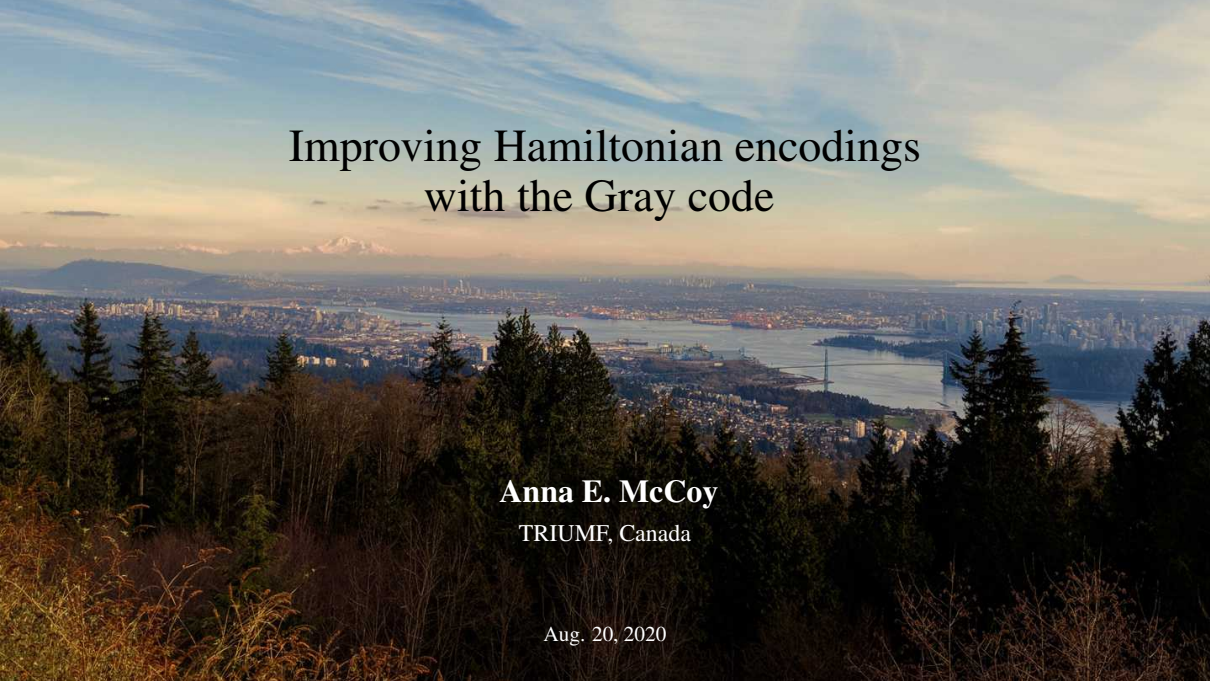


Improving Hamiltonian encodings with the Gray code

Anna E. McCoy
TRIUMF, Canada

Aug. 20, 2020

Outline

- Introduction to mapping fermionic many-body problems onto quantum computers
- Our alternative approach (Gray code encoding)
- Simulation results for deuteron

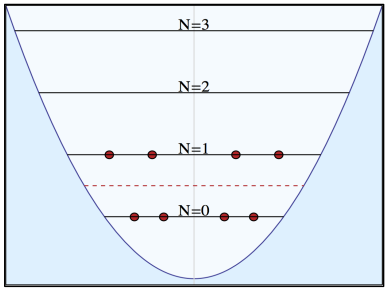
Solving quantum many-body problems

– Hamiltonian expressed in terms of creation and annihilation operators

$$H = \sum_{ab} \langle a|H|b\rangle \, a_a^\dagger a_b + \sum_{cdef} \langle cd|H|ef\rangle \, a_c^\dagger a_d^\dagger a_e a_f + \ldots$$

– Basis states are configurations, i.e., distributions particles over single particle states (harmonic oscillator *nlj* states).

– States represented in occupation representation $|0100101\ldots\rangle$



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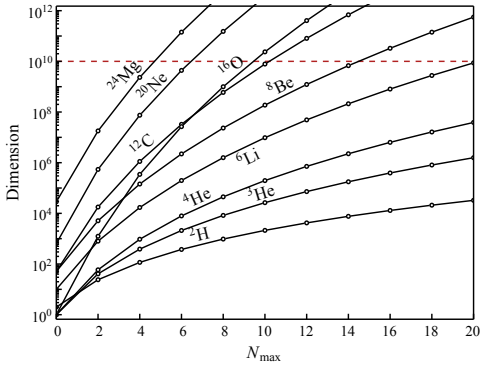
– Basis states are configurations, i.e., distributions particles over single particle states (harmonic oscillator *nlj* states).

– States represented in occupation representation $|0100101\ldots\rangle$

– *Calculations in configuration basis often limited by rapid growth of the basis*



Solving quantum many-body problems on a quantum computer

- On a quantum computer, the problem is expressed in terms of Pauli operators $\{X_n, Y_n, Z_n\}$ acting on the nth qubit

- A qubits can be spin up $|0\rangle$, spin down $|1\rangle$, or some linear combination $\alpha|0\rangle + \beta|1\rangle$

- If each qubit represents a single particle state and we map unoccupied states to spin up and occupied states to spin down, then

$$\underbrace{|0100101\ldots\rangle}_{\text{Occupation}} \quad \rightarrow \quad \underbrace{|0100101\ldots\rangle}_{\text{Qubit}}$$

Solving quantum many-body problems on a quantum computer

– We need to define operators which act on the qubit the same way $a^\dagger$ and a act on the occupation basis.

– Common choice is to use the Jordan-Wigner (JW) transformation:

$$a_n^\dagger \to \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n - iY_n) \qquad a_n \to \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n + iY_n)$$

$$\underbrace{a_1 |01\rangle = |00\rangle}_{\textit{occupation}} \quad \to \quad \underbrace{-\frac{1}{2} Z_0 (X_1 + iY_1)|01\rangle = |00\rangle}_{\textit{qubit}}$$

Example: deuteron

E. F. Dumitrescu et al. Phys. Rev. Lett. **120** *21 (2018).*
O. Shehab et al. (2019) arxiv:1904.04338v2.

To leading order, the Hamiltonian of the deuteron is given by:

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

where $a^\dagger_n$ and a_n create or annihilate a deuteron in the relative state $|n\rangle$, and

$$\langle n'|V|n\rangle = V_0 \delta^0_n \delta^{n'}_n$$

$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}[(2n+3/2)\delta^{n'}_n - \sqrt{n(n+1/2)}\delta^{n'+1}_n - \sqrt{(n+1)(n+3/2)}\delta^{n'-1}_n]$$

Example: deuteron

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

For $N = 2$, the Hamiltonian in second quantized form is

$$H_2 = -0.4366 \cdot a^\dagger_1 a_1 - 4.2867 \cdot (a^\dagger_1 a_2 + a^\dagger_2 a_1) + 12.25 \cdot a^\dagger_2 a_2$$

After Jordan-Wigner, the Hamiltonian is given by :

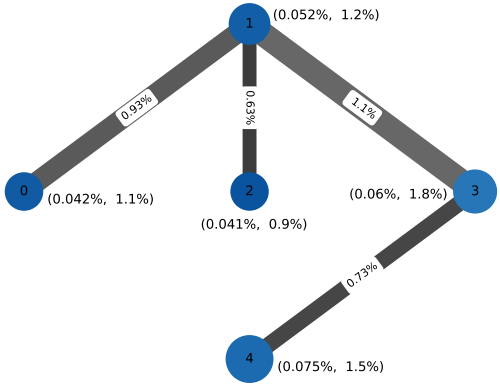
$$H_2 = 5.9067 \cdot \mathbb{1}\mathbb{1} + 0.2183 \cdot Z\mathbb{1} - 6.125 \cdot \mathbb{1}Z - 2.143 \cdot (XX + YY)$$

Noisy, intermediate-scale quantum computing (NISQ)

Ideally we would directly solve the Hamiltonian eigenproblem on a quantum computer

However, quantum computers today have ...

- Limited number of qubits
- Limited qubit connectivity
- Noise, high error rates
- Etc.



IBMQ Vigo machine

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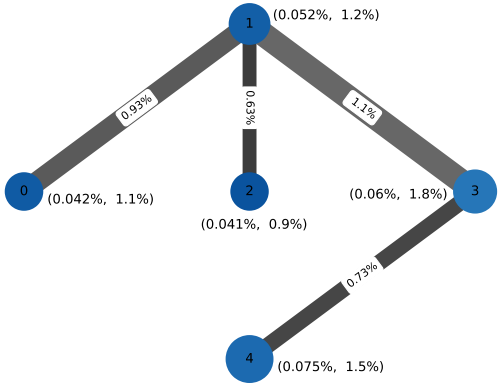
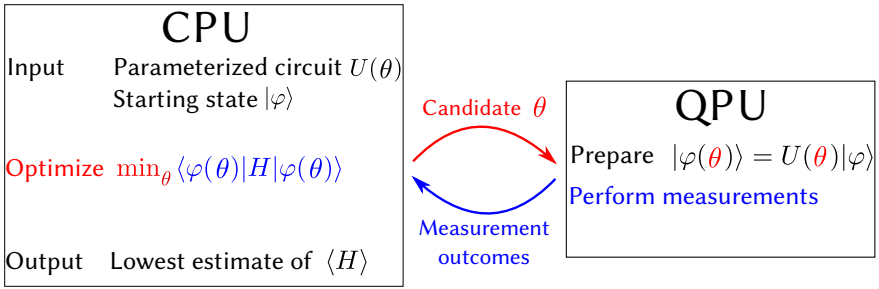
Hybrid algorithms!



IBMQ Vigo machine

Variational quantum eigensolver (VQE)

- Write down a Hamiltonian
- Convert the Hamiltonian to a qubit Hamiltonian
- Choose a variational ansatz (parameterize the wavefunction $\varphi(\theta)$)
- Find θ which minimizes $\langle\varphi(\theta)|H|\varphi(\theta)\rangle$.



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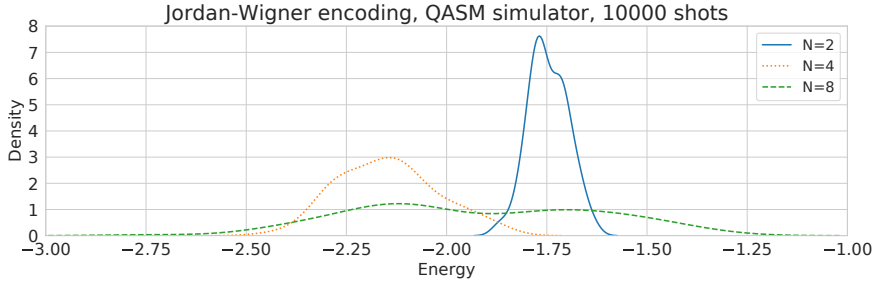
- *Get distribution of lowest energy from repeated trials*



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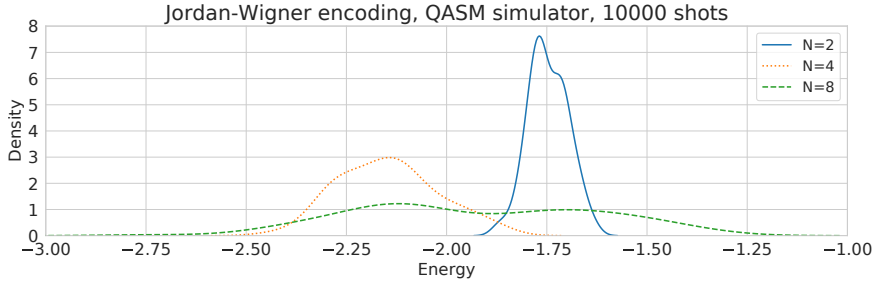

Inefficiency of Jordan Wigner

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

JW requires N qubits for N single particle states:

$$|0\rangle \to |1000\rangle, \quad |1\rangle \to |0100\rangle, \quad |2\rangle \to |0010\rangle, \quad |3\rangle \to |0001\rangle.$$

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But the space of N qubits contains 2^N states!

$\|0000\rangle$	$\|0001\rangle$	$\|0010\rangle$	$\|0011\rangle$
$\|0100\rangle$	$\|0101\rangle$	$\|0110\rangle$	$\|0111\rangle$
$\|1000\rangle$	$\|1001\rangle$	$\|1010\rangle$	$\|1011\rangle$
$\|1100\rangle$	$\|1101\rangle$	$\|1110\rangle$	$\|1111\rangle$

Can we use the rest?

Gray code encoding for qubit Hamiltonians

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

States assigned according to Gray code ordering

A Gray code cycles over bitstrings by changing one bit each time:

$$00 \rightarrow 01 \rightarrow 11 \rightarrow 10 \rightarrow 00$$

Use N qubits to represent 2^N states (4 states $\rightarrow$ 2 qubits).

$$|0\rangle \rightarrow |00\rangle, \quad |1\rangle \rightarrow |01\rangle, \quad |2\rangle \rightarrow |11\rangle, \quad |3\rangle \rightarrow |10\rangle$$

Gray code Hamiltonian

- Need qubit representation of Hamiltonian $H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n$
- Two types of terms appear:
  - Number operators: $a_n^\dagger a_n |n\rangle = n|n\rangle$
  - Ladder operators: $a_{n\pm1}^\dagger a_n |n\rangle = |n \pm 1\rangle$
- Both terms are effectively projection operators
- Define single qubit projection operators

$$P_0 = \frac{1}{2}(\mathbb{1} + Z) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P_1 = \frac{1}{2}(\mathbb{1} - Z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Gray code operators

Example: 4 states (2 qubits) with gray-code ordering:

Number operators

Initial state	Final state	Operator
$\|00\rangle$	$\|00\rangle$	0 $P_0 \otimes P_0$
$\|01\rangle$	$\|01\rangle$	1 $P_0 \otimes P_1$
$\|11\rangle$	$\|11\rangle$	2 $P_1 \otimes P_1$
$\|10\rangle$	$\|10\rangle$	3 $P_1 \otimes P_0$

Ladder operators

Initial state	Final state	Operator
$\|00\rangle$	$\|01\rangle$	$P_0 \otimes X$
$\|01\rangle$	$\|11\rangle$	$X \otimes P_1$
$\|11\rangle$	$\|10\rangle$	$P_1 \otimes X$

Note: $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ acts as a NOT gate

Simulation details

We implemented our methods using Qiskit and OpenFermion.

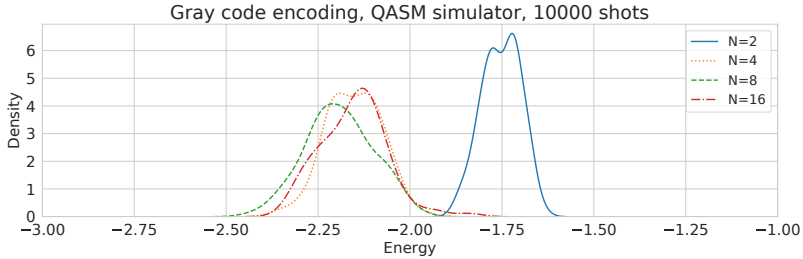
Encoding for any number of qubits is automated for

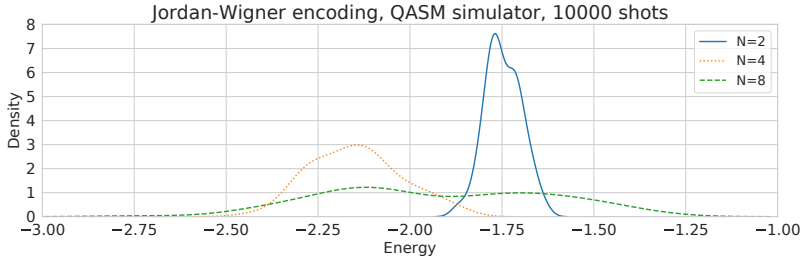
- Gray code
- Jordan-Wigner

Ran VQE with both encodings using :

- The QASM simulator (ideal quantum computer)
- The QASM simulator with simulated hardware noise based on IBMQ data

Simulation results for Gray code and Jordan Wigner encodings





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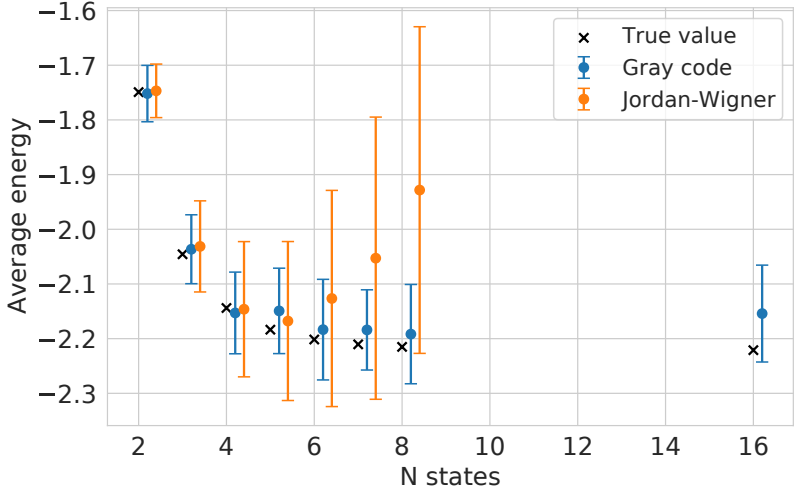

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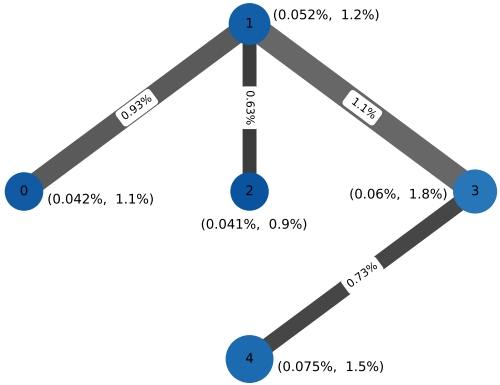
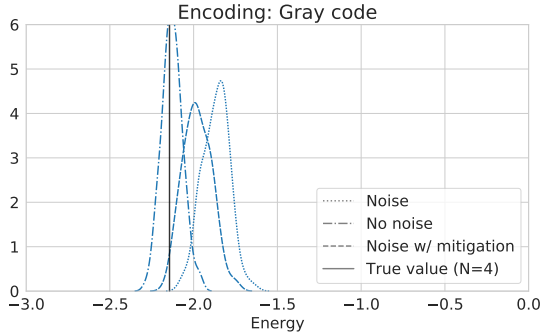


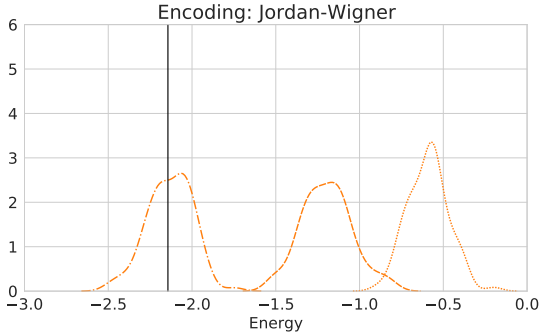
IBMQ Vigo machine

Simulation with Vigo noise model

- With noise (simulating results on current IBMQ machines)
- Mitigating noise with Qiskit measurement error mitigation
- No noise (ideal quantum computer)

Gray code more resilient against noise than Jordan-Wigner





Summary

Advantages of the Gray code encoding:

- Exponentially fewer qubits than Jordan-Wigner encoding
- Lower variance of solutions in QASM simulations
- Greater resilience to presence of (simulated) hardware noise

Future work:

- Testing on actual quantum device
- Moving beyond the deuteron
- Further exploration of Hamiltonian simulation

Collaborators

Olivia Di Matteo
Peter Gysbers
Takayuki Miyagi
Richard Woloshyn
Petr Navrátil

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Merci!

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