Gray code implementation of the many-body Hamiltonian: Recent progress and future perspectives in quantum computing

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PRX Quantum 3, 020356 (2022), arxiv 2207.11647

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Binary Reflected Gray Code

Binary		
0	$\rightarrow$	000
1	$\rightarrow$	001
2	$\rightarrow$	010
3	$\rightarrow$	011
4	$\rightarrow$	100
5	$\rightarrow$	101
6	$\rightarrow$	110
7	$\rightarrow$	111

BRGC		
0	$\rightarrow$	000
1	$\rightarrow$	001
2	$\rightarrow$	011
3	$\rightarrow$	011
4	$\rightarrow$	110
5	$\rightarrow$	111
6	$\rightarrow$	101
7	$\rightarrow$	100

- Binary bit-string is also the base 2 integer
- Any 1:1 maping is a valid representation
- BRGC is an alternative mapping of bit-string to integer
- In BRGC consecutive integers differ by 1 bit-string

Quantum Computing

Power of Quantum Computing

- $|\Psi\rangle \equiv$ exponential number of states
- $e^{-i\hat{O}}\,|\Psi\rangle \rightarrow$ change all the amplitudes
  $\approxeq$ parallel computing
- Quantum Simulation

3 qubits

$$|\Psi\rangle = + \begin{array}{r|l} a_0 & |000\rangle \\ a_1 & |001\rangle \\ a_2 & |010\rangle \\ a_3 & |011\rangle \\ a_4 & |100\rangle \\ a_5 & |101\rangle \\ a_6 & |110\rangle \\ a_7 & |111\rangle \end{array}$$

Quantum Computing Paradigm

- Adiabatic QC
- Gate - based QC

Adiabatic Quantum Computing

- Start with ground state of solvable H_I
- Combine with target Hamiltonian: $H = A(t)H_I + B(t)H_F$
- Evolve slowly: $A(0) = B(t_F) = 1,\ A(t_F) = B(0) = 0$
- $H_I = -\sum_i \sigma_i^x,\ H_F = \sum_i \sigma_i^z + \sum_{i \neq j} \sigma_i^z \sigma_j^z$
- Measure

Schrodinger Equation

- $\frac{\partial^2}{\partial x^2} f(x) = \frac{1}{a^2}\left[f(x+a) + f(x-a) - 2f(x)\right]$
- $-\frac{\hbar^2}{2\mathrm{M}}\nabla^2\psi(\mathrm{x}) + \mathrm{V}(\mathrm{x})\psi(\mathrm{x}) = \mathrm{E}\psi(\mathrm{x}) \xrightarrow{\text{discretize}} -\frac{(\mathrm{L}\psi)(\mathrm{a}\mathbf{r})}{2\mathrm{Ma}^2} + (\mathrm{V}\psi)(\mathrm{a}\mathbf{r}) = \mathrm{E}\psi(\mathrm{a}\mathbf{r})$
- one lattice point $\leftrightarrow$ one qubit

Binary code:

- $L^{(n,\text{bin})}_{0\ldots n-1} = \sum_{l=1}^{n} \mathcal{B}_l,\ \mathcal{B}_l = (\sigma^x_{l-1} - 1)(\prod_{i=0}^{l-2} \sigma^x_i P^0_i + \prod_{i=0}^{l-2} \sigma^x_i P^1_i),\ \mathcal{B}_1 = L^{(1)}_0 = 2\sigma^x_0$
- 2^{n-2} n-local operators!

Gray code:

- $L^{(n,\text{BRGC})}_{0\ldots n-1} = \sum_{k=0}^{n-1} \mathcal{G}_k,\ \mathcal{G}_k = \left(\sigma^x_k - \sigma^x_{k-1}\right)\prod_{i=0}^{k-2} P^0_i,\ \mathcal{G}_0 = L^{(1)}_0 = 2\sigma^x_0$
- $L^{(n,\text{H2GC})}_{0\ldots n-1} = \sum_{i=0}^{n-1} \sigma^x_i + Q \sum_{p\in\text{penalty terms}} p,\ p \to$ 3-local σ^z, $Q = \mathcal{O}(1/a)$
- $\mathcal{O}(n)$ 2-local operators

Exponential gain in space complexity

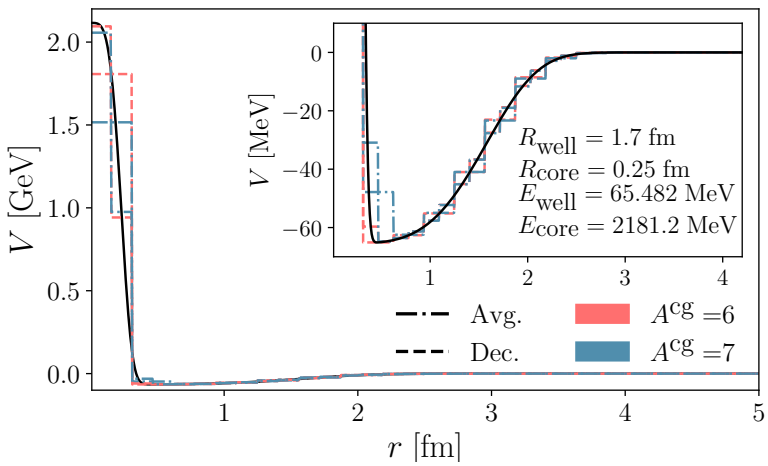
Jonathan Welch et al 2014 New J. Phys. 16 033040

Encoding the Potential

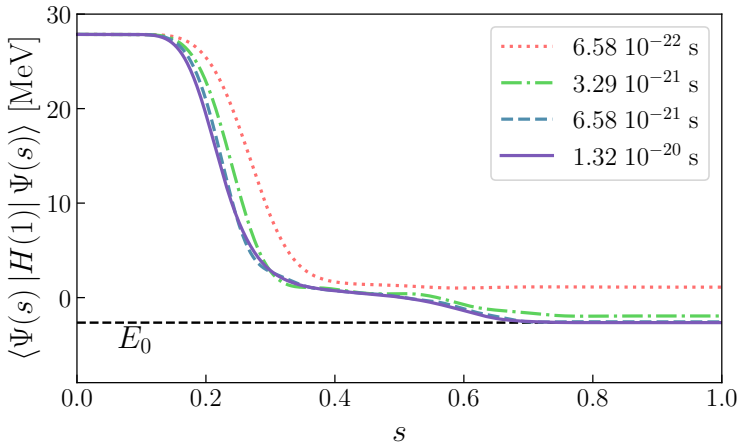
- Fast Walsh - Hadamard transform (FWHT) to get coefficients ($\mathcal{O}(\mathrm{N}\log(\mathrm{N}))$)
- However, $N = 2^n$
- Coarse-grain potential before FWHT
- Averaging decimation if known functional form
- Decimation coarse-graining as cheap alternative

C. C. Chang, K. S. McElvain, **E. Rrapaj**, Y. Wu PRX Quantum 3, 020356 (2022)

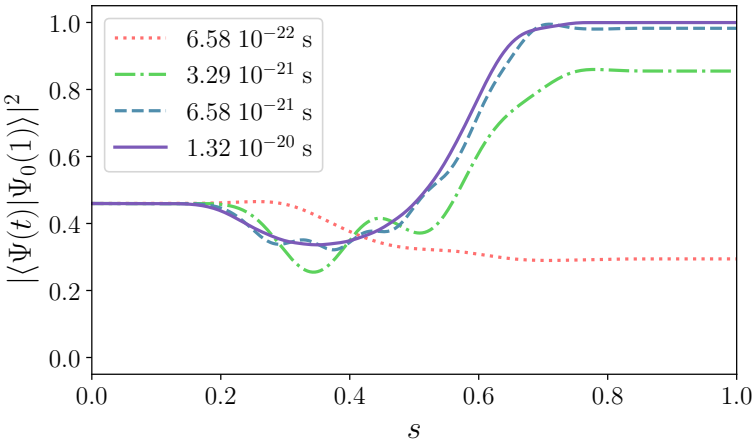
S-wave deuteron potential.



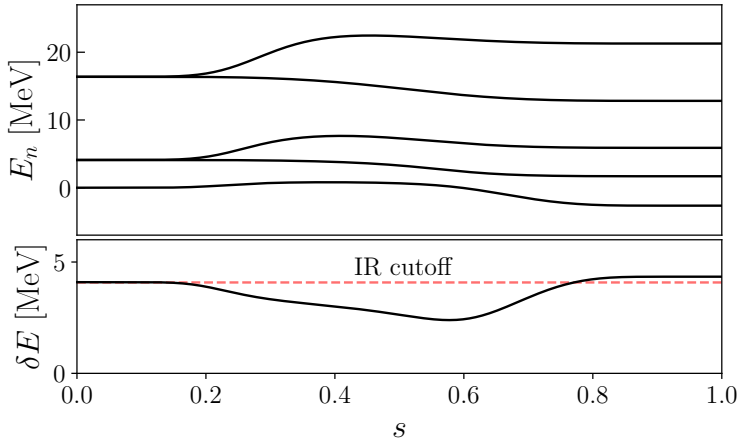
Target Hamiltonian



Overlap with ground state



Energy spectrum



Time complexity: Polynomial time to recover ground state

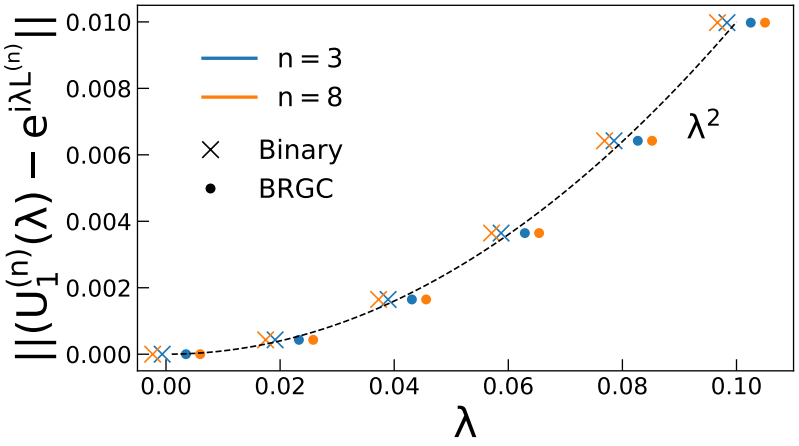
Gate Based Quantum Computing

- Start with $|0, 0....\rangle$
- Decompose the time-discretized unitary evolution operator $e^{-iH\delta t}$
  - Single qubit — rotation ($e^{-i\sigma^{x,y,z}\alpha}$)
  - Two qubit — controlled operation (CNOT)
- Apply the gates
- Measure
- 'Universal' computer

Time Evolution

E. Rrapaj, K. S. McElvain, C. C. Chang, Y. Wu, A. Walker-Loud, arXiv:2207.11647

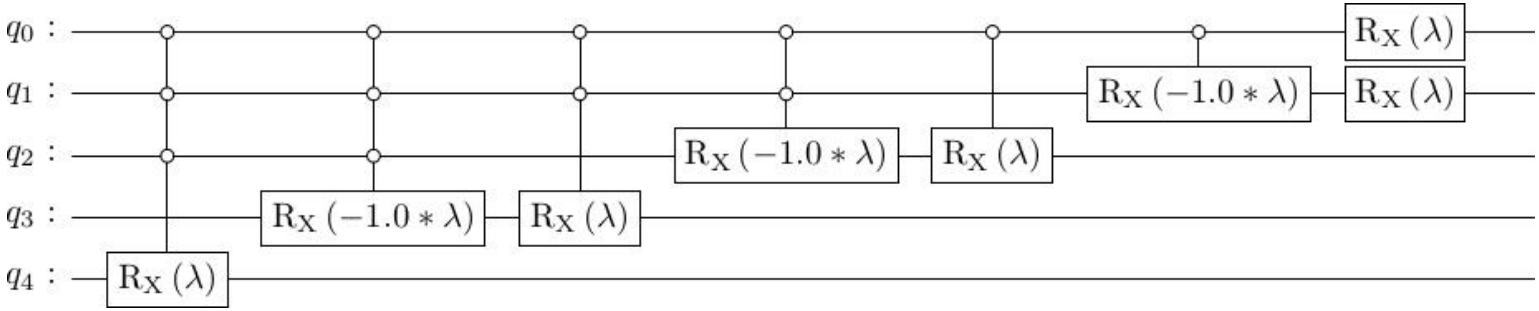
- $e^{-i\Delta t H} = e^{-i\Delta t V}\ e^{i\frac{\Delta t L}{2Ma^2}} + \mathcal{O}\left((\Delta t)^2\right)$
- $\exp\left(i\lambda L^{(n)}\right) = \prod_{k=0}^{n-1} \exp\left(i\lambda \mathcal{G}_k\right) + \mathcal{O}\left(\lambda^2\right) \equiv U_1^{(n)}(\lambda) + \mathcal{O}\left(\lambda^2\right)$
- $\left\| U_1^{(n)}(\lambda) - e^{i\lambda L^{(n)}_{0\ldots n-1}} \right\| \leq \frac{\lambda^2}{2} \sum_{j=2}^{n-1} \left\| \sum_{k=0}^{j-1} \left[\mathcal{G}_j, \mathcal{G}_k\right] \right\| = \frac{\lambda^2}{2} \sum_{j=2}^{n-1} 2 = (n-2)\lambda^2$
- $\left\| U_1^{(n)}(i\lambda) - e^{i\lambda L^{(n)}} \right\| = \frac{\lambda^2}{2} \left\| \sum_{b=2}^{n-1} \left[\mathcal{G}_b, \mathcal{L}^{(n)}_{0\ldots(b-1)}\right] \right\| + \ldots = \lambda^2 + \mathcal{O}(\lambda^3)$



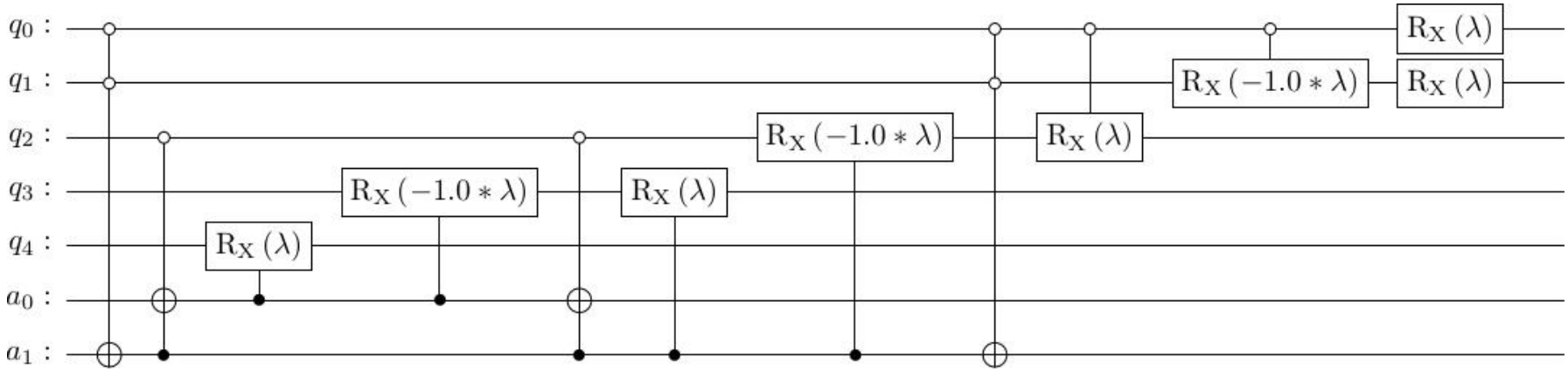
Gray Code circuit

E. Rrapaj, K. S. McElvain, C. C. Chang, Y. Wu, A. Walker-Loud, arXiv:2207.11647

Ideal Implementation

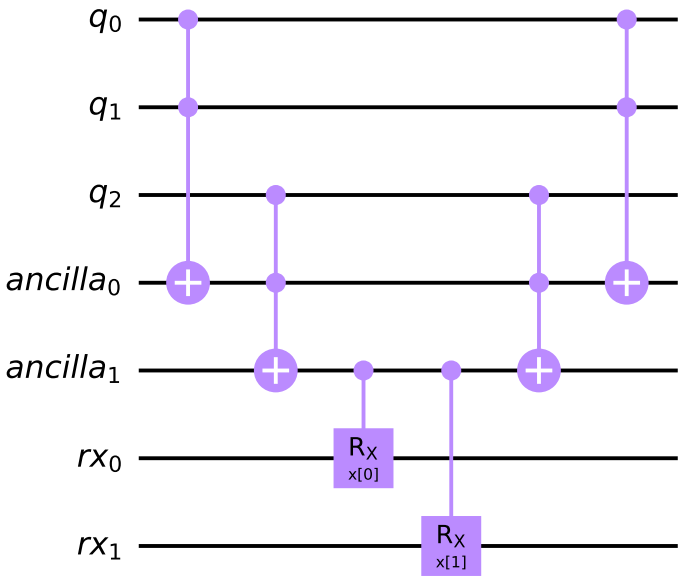


Proposed in this work



Proposed method: example

E. Rrapaj, K. S. McElvain, C. C. Chang, Y. Wu, A. Walker-Loud, arXiv:2207.11647



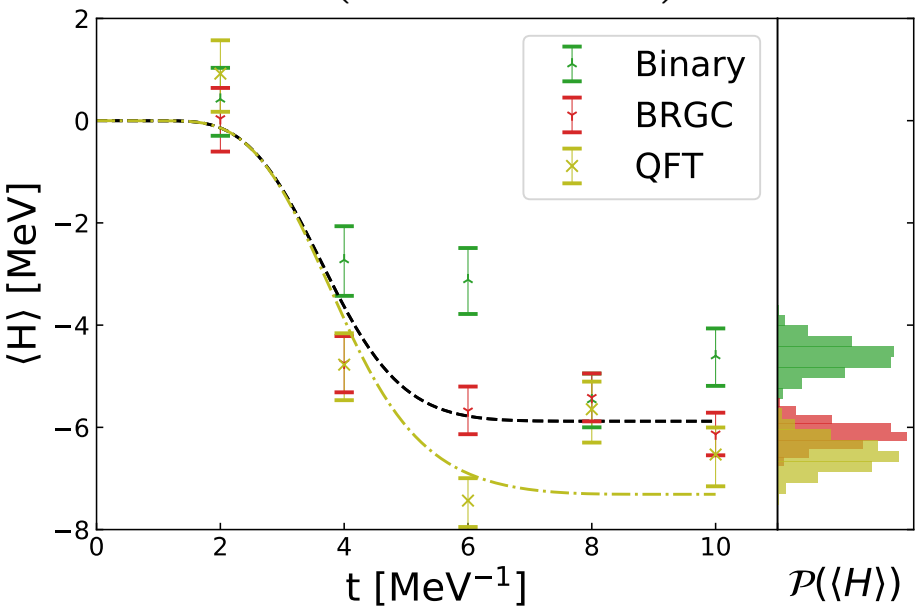
$n-3$ ancilla qubits

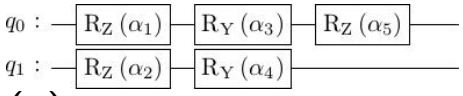
- $\mathrm{depth} = \mathcal{O}(\mathrm{n}),\ \mathrm{width} = \mathcal{O}(\mathrm{n})$
- $C^{\mathrm{BRGC}} = \mathcal{O}(T^2 nDA/\epsilon)$
- Quantum Fourier Transform: $\mathcal{C} = \mathcal{O}(n\log(n)DA),\ \mathrm{depth} = \mathcal{O}(\mathrm{n})$

Example: 2 qubit computation

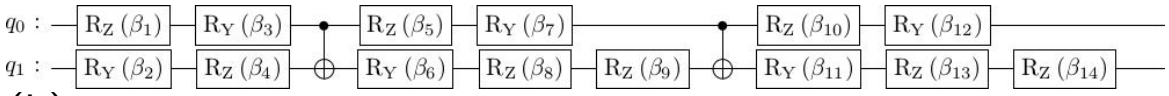
E. Rrapaj, K. S. McElvain, C. C. Chang, Y. Wu, A. Walker-Loud, arXiv:2207.11647

$$\mathrm{V} = \begin{pmatrix} V_0, & r < L/2 \\ -V_0, & r \geq L/2 \end{pmatrix}$$

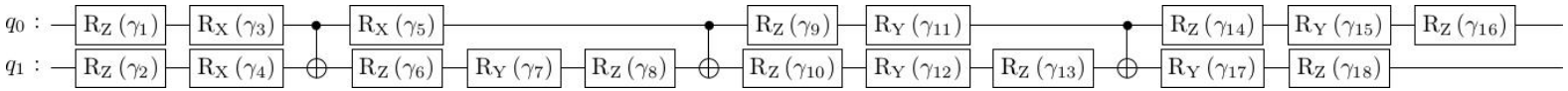




(a)BRGC



(b) Binary



(c) QFT

Summary

1. Exponential gain in space complexity
2. Reducible to polynomial number of 2-local operators
3. Universal quantum computers:
   - Circuit depth $= \mathcal{O}(n)$
   - Circuit width $= \mathcal{O}(n)$
   - Resulting circuit shallower than QFT and easier to implement

Next Steps

- Include Fermion / Boson statstics
- Gate decomposition

Thank you

Collaborators: Ken McKlevain, Chia Cheng Chang, Yantao Wu, André Walker-Loud

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Gates and Qubits: Introduction

- Qubit $\equiv$ spin $1/2$, two state system
- n qubits $\equiv$ 2^n states of n spin $1/2$ particle system
- Gate $\equiv$ unitary operator acting on qubits
- Only certain gates are available
  1. One qubit gates $\longrightarrow$ rotations in $SU(2)$
  2. Two qubit gates $\longrightarrow$ controlled rotations
- every other gate can be obtained from them

The state of one qubit

Generic State

$$|\Psi\rangle = \cos(\tfrac{\theta}{2})|0\rangle + e^{-i\phi}\sin(\tfrac{\theta}{2})|1\rangle$$

Z gate (phase flip)

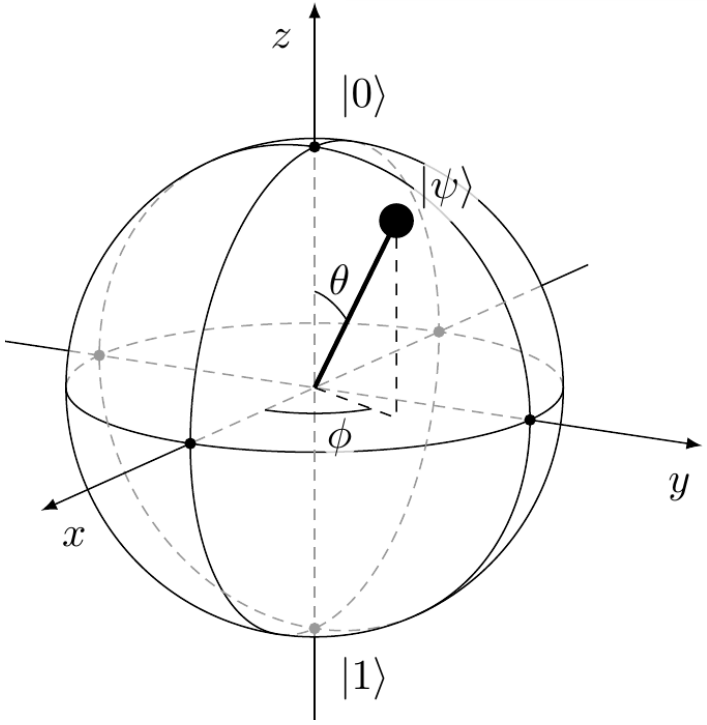
$$\hat{Z}\tfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \tfrac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

X gate (NOT)

$$\hat{X}|0\rangle = |1\rangle,\ \hat{X}|1\rangle = |0\rangle$$

RY gate

$$e^{-i\alpha/2\hat{Y}} = \cos(\tfrac{\alpha}{2})\hat{I} - i\sin(\tfrac{\alpha}{2})\hat{Y}$$



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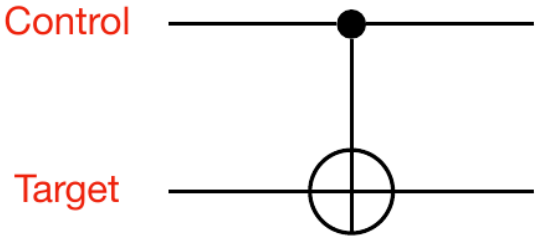
Modifying the state of two qubits

Controled X Gate (CNOT)



Target Control

$$|00\rangle \leftrightarrow |00\rangle$$

$$|01\rangle \leftrightarrow |11\rangle$$

$$|10\rangle \leftrightarrow |10\rangle$$

$$|11\rangle \leftrightarrow |01\rangle$$

back

Binary encoding of the Laplacian

I will talk more in detail about mapping of the kinetic energy operator

$$\frac{\partial^2}{\partial x^2}\Psi(x) \to \frac{1}{a^2}\left[\Psi(x+a)+\Psi(x-a)-2\Psi(x)\right]$$

A natural choice of a 1D lattice (with 8 sites) is labelled as

0	1	2	3	4	5	6	7

$$\frac{1}{a^2}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} - \frac{2}{a^2}\mathbb{1}$$

Yielding the following discrete derivative

can drop identity w/o loss of generality

back

Binary encoding of the Laplacian

$$\begin{array}{|c|c|c|c|c|c|c|c|}\hline 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline \end{array}$$

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

For this 3 qubit example

$0 \to 000$

1 bit difference

$1 \to 001$

2 bit difference

$2 \to 010$

1 bit difference

$3 \to 011$

3 bit difference

$4 \to 100$

1 bit difference

$5 \to 101$

2 bit difference

$6 \to 110$

1 bit difference

$7 \to 111$

The mapping of qubits to lattice site is complicated (but still has a pattern)

→

Interactions between spins to accomplish this is complicated (but still generalizable to A spins)

back

Binary encoding of the Laplacian

$$L^A = L^{A-1} - C^{A-1} + \sigma^x C^{A-1}$$
$$= L^{A-1} + (\sigma^x_{A-1} - 1) \prod_0^{A-1} \sigma^x_i (P^0_i + P^1_i)$$

$$C^A = \prod_0^{A-1} \sigma^+_i + \prod_0^{A-1} \sigma^-_i$$

$$P^0 = \frac{\mathbb{1} + \sigma^z}{2} \quad P^1 = \frac{\mathbb{1} - \sigma^z}{2}$$

$$\sigma^x_0 = \mathbb{1} \otimes \mathbb{1} \otimes \sigma^x$$
$$\sigma^x_0 \sigma^x_1 = \mathbb{1} \otimes \sigma^x \otimes \sigma^x$$
$$\sigma^x_0 \sigma^x_1 \sigma^x_2 \left(P^0_0 P^0_1 + P^1_0 P^1_1\right)$$
$$\sigma^x_0 \sigma^x_1 \left(P^0_0 P^0_1 + P^1_0 P^1_1\right)$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

back

Binary encoding of the Laplacian

Space complexity improvements

- Exponential number of lattice sites - Yes!
- Polynomial number of terms in the Hamiltonian - Yes!
- Fixed Pauli weight - Grows as order A
- Small Pauli support - Requires all 3 Pauli matrices and their products

We have “exponential space” improvement in a very restricted sense

back

Laplacian in binary reflected Gray code

Binary	BRGC
$0 \to 000$	$0 \to 000$
$1 \to 001$	$1 \to 001$
$2 \to 010$	$2 \to 011$
$3 \to 011$	$3 \to 010$
$4 \to 100$	$4 \to 110$
$5 \to 101$	$5 \to 111$
$6 \to 110$	$6 \to 101$
$7 \to 111$	$7 \to 100$

Karnaugh Map for BRGC

Visual way to see a valid Gray code

	00	01	11	10
0				
1				

back

Laplacian in binary reflected Gray code

Binary	BRGC
$0 \to 000$	$0 \to 000$
$1 \to 001$	$1 \to 001$
$2 \to 010$	$2 \to 011$
$3 \to 011$	$3 \to 010$
$4 \to 100$	$4 \to 110$
$5 \to 101$	$5 \to 111$
$6 \to 110$	$6 \to 101$
$7 \to 111$	$7 \to 100$

One way to visualize the simplification

1. Label site with bit-string
2. Convert to Int in BRGC
3. Reorder in increasing Int values

00 01 10 11

$$H^x = \sum_i \sigma_i^x = \begin{array}{c c} & \begin{array}{cccc} 0 & 1 & 3 & 2 \end{array} \\ \begin{array}{c} 0 \\ 1 \\ 3 \\ 2 \end{array} & \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array} \xrightarrow[\text{to bin}]{\text{brgc}} \begin{array}{c c} & \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\ \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array} & \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Maps transverse Hamiltonian to Laplacian
in the case of A=2
(previously we needed $\sigma^x\sigma^x$ as well)

back

Laplacian in binary reflected Gray code

$$L^2 = \sigma_0^x + \sigma_1^x$$

$$L^A = L^{A-1} + (\sigma_{A-1}^x - \sigma_{A-2}^x) \prod_i^{A-3} P_i^0$$

$$\sum_0^1 \sigma_i^x = \mathbb{1} \otimes \mathbb{1} \otimes \sigma^x + \mathbb{1} \otimes \sigma^x \otimes \mathbb{1}$$

$$\sigma_2^x P_0^0 = (\sigma^x \otimes \mathbb{1} \otimes \mathbb{1}) \times (\mathbb{1} \otimes \mathbb{1} \otimes P^0)$$

$$\sigma_1^x P_0^0 = \mathbb{1} \otimes \sigma^x \otimes \mathbb{1} \times \mathbb{1} \otimes \mathbb{1} \otimes P^0$$

$$\begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

back

Laplacian in binary reflected Gray code

Space complexity improvements

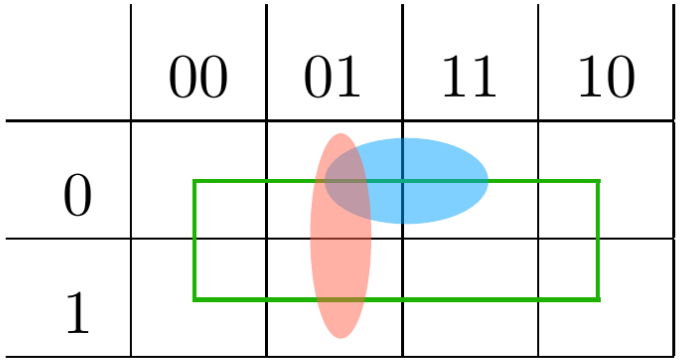
- Exponential number of lattice sites - Yes!
- Polynomial number of terms in the Hamiltonian - Yes!
- Fixed Pauli weight - Yes! (XZ^n is polynomially reducible to XZ and ZZ)
- Small Pauli support - Yes! (Only need X, XZ, and ZZ)

We have exponential space improvement

back

Hamming distance 2 Gray code

Why does BRGC need an XZ coupling?



Adjacent lattice sites are 1 bit different (Hamming distance = 1)

There are non-adjacent lattice sites that are also 1 bit different

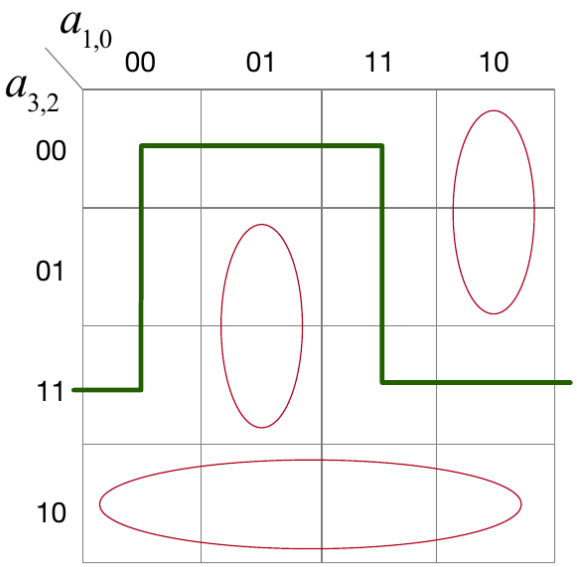
Pauli X will yield derivatives to both
XZ eliminates unwanted derivatives

Why not use a Gray code where non-adjacent codes are >= 2 bit different

back

Hamming distance 2 Gray code

4 qubits H2GC Karnaugh map



Only works with 2N qubits

If bit-strings are nulled

we can snake a path through wheren
non-adjacent site have
a Hamming distance of 2

Only Pauli X + Z and ZZ are needed

back

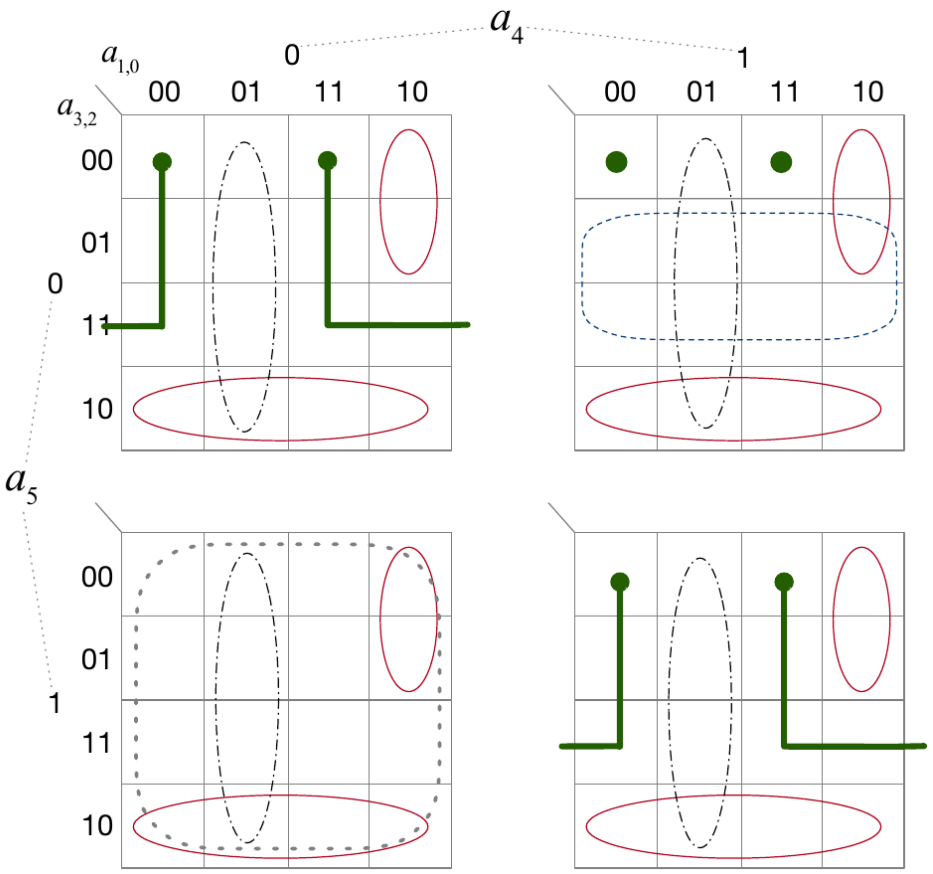
H2GC

6 qubit construction

The basic path is copied to a layer that is separated by a drill-through layer

Has $2^{A/2+1}$ valid sites
Exponential in number of qubits

The penalty terms are always at most a 3-body interaction



back

Hamming distance 2 Gray code

Space complexity improvements

- Exponential number of lattice sites - Yes!
- Polynomial number of terms in the Hamiltonian - Yes!
- Fixed Pauli weight - Yes!
- Small Pauli support - Yes! (Only need X, Z, and ZZ)

We have exponential space improvement

Can (almost) be implemented today!

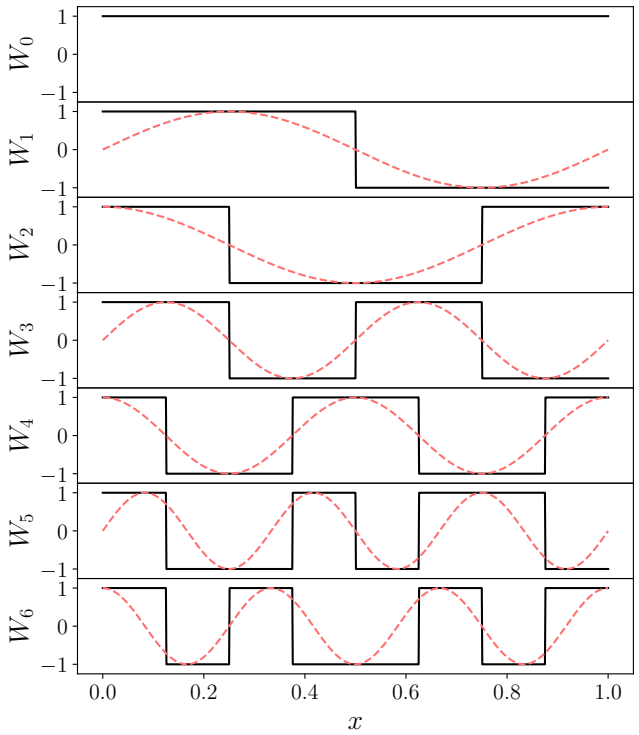
back

Fast Walsh - Hadamard transform (FWHT)

- divide-and-conquer algorithm
- recursively breaks down a WHT of size N into two smaller WHT of size $N/2$
- $H_N = \frac{1}{\sqrt{2}} \begin{pmatrix} H_{N-1} & H_{N-1} \\ H_{N-1} & -H_{N-1} \end{pmatrix}, \; H_1 = [1]$

Walsh series

- Complete basis
- Easily mapped to product of σ^z
- Sequency ordering
- Free of Gibbs phenomena



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Annealing Schedule

$$A(s) = 1, \;\; B(s) = \frac{\int_0^s \exp\left(\frac{-1}{s'(1-s')}\right) ds'}{\int_0^1 \exp\left(\frac{-1}{s'(1-s')}\right) ds'}$$

Dicretization effects

IR-cutoff, $\delta E \approxeq \frac{(2\pi)^2}{2mL^2} \gg 1/T$

UV-cutoff $\sim 1/a, \;\; a \approxeq (2\pi)/L$

back