Improving Schrodinger Equation Implementations with Gray code for Adiabatic Quantum Computers

Chia Cheng Chang

RIKEN iTHEMS
UC Berkeley

Problem and related works

Solve the Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t)$$

Can use {qubits} per lattice site (sol. is diag. in comp. basis, but expensive)
Phys. Rev. D 103, 016008 (2021)

Can use qubits to label positions on the lattice (exponentially less qubits)
arXiv: 2101.05821
In 2101.05821, the authors present a circuit QC algorithm.
In each trotter step, a QFT and inverse-QFT is performed.
The Laplacian and potential are diagonal in the respective spaces.

In this context, we present a new algorithm suitable for adiabatic quantum computing.

Adiabatic QC and quantum annealing

$$H(t) = A(t)H_0 + B(t)H_1$$

Solve eigenstate of final Hamiltonian by adiabatically evolving from initial H.

Hamiltonian are expressed as *k*-local (*A*-body) spin operators

$$H = \sigma^Z \otimes \sigma^Z = \sigma_0^Z \sigma_1^Z$$

Quantum annealing restricts Hamiltonians to 2-local transverse Ising Model

$$H_0 = \sum_i \sigma_i^X \qquad H_1 = \sum_i h_i \sigma_i^Z + \sum_{i>j} J_{ij} \sigma_i^Z \sigma_j^Z$$

Initial ground state is the maximal superposition state

$$\Psi(0) = (|\uparrow\rangle + |\downarrow\rangle)^{\otimes A}$$

Quantum annealing sets are our algorithm design considerations

Schrodinger equation w/ real potentials

$$\left[\nabla^2 + V(x,t)\right]\Psi(x,t)$$

Let us consider first time-independent real potentials.

Discretize the equation (e.g. with a periodic square well for now)

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} -10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \end{pmatrix}$$

Schrodinger equation w/ real potentials

$$\left[\nabla^2 + V(x,t)\right]\Psi(x,t)$$

Let us consider first time-independent real potentials.

Discretize the equation (e.g. with a periodic square well for now)

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} -10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \end{pmatrix}$$

This is a 3-qubit example (2^3 lattice sites in 1D)

Schrodinger equation w/ real potentials

$$\left[\nabla^2 + V(x,t)\right]\Psi(x,t)$$

Let us consider first time-independent real potentials.

Discretize the equation (e.g. with a periodic square well for now)

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} -10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \end{pmatrix}$$

This is a 3-qubit example (2^3 lattice sites in 1D)
Periodic boundary conditions

Schrodinger equation w/ real potentials

$$\left[\nabla^2 + V(x,t)\right]\Psi(x,t)$$

Let us consider first time-independent real potentials.

Discretize the equation (e.g. with a periodic square well for now)

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} -10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \end{pmatrix}$$

This is a 3-qubit example (2^3 lattice sites in 1D)
Periodic boundary conditions

Drop -2 global identity (constant energy shift)

$$\nabla^2 f(x) = f(x+1) + f(x-1) - 2f(x)$$

Schrodinger equation w/ real potentials

$$\left[\nabla^2 + V(x,t)\right]\Psi(x,t)$$

Let us consider first time-independent real potentials.

Discretize the equation (e.g. with a periodic square well for now)

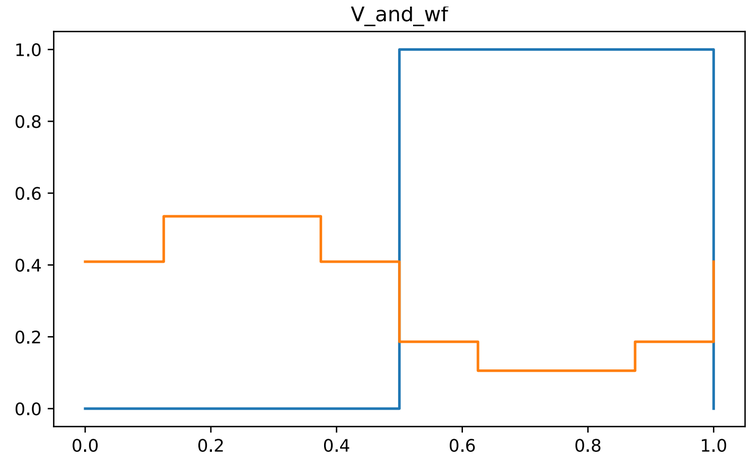
$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} -10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \end{pmatrix}$$

This is a 3-qubit example (2^3 lattice sites in 1D)
Periodic boundary conditions
Real potentials can be encoded entirely on the diagonal

Qubit mapping

Solution in general is a superposition in the computational basis

$$\begin{pmatrix} -10 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & -10 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -10 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -10 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 10 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 10 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 10 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 10 \end{pmatrix}$$



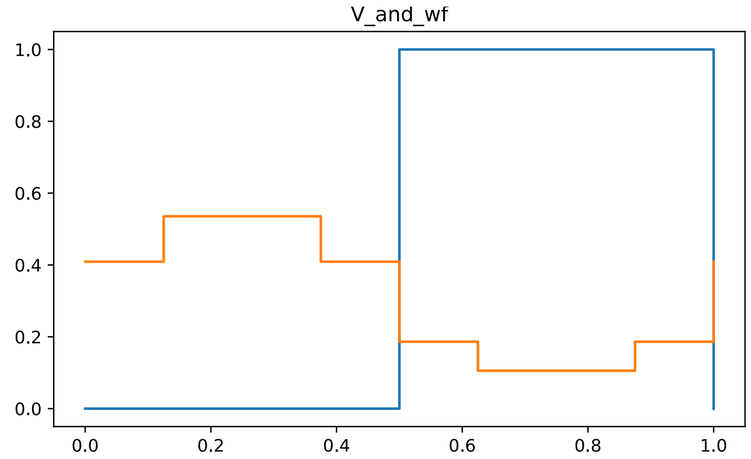
$$\Psi(1) = \begin{aligned} &- 0.6\,|\downarrow\downarrow\downarrow\rangle - 0.4\,|\downarrow\downarrow\uparrow\rangle \\ &- 0.4\,|\downarrow\uparrow\downarrow\rangle - 0.6\,|\downarrow\uparrow\uparrow\rangle \\ &+ 0.0\,|\uparrow\downarrow\downarrow\rangle + 0.0\,|\uparrow\downarrow\uparrow\rangle \\ &+ 0.0\,|\uparrow\uparrow\downarrow\rangle + 0.0\,|\uparrow\uparrow\uparrow\rangle \end{aligned}$$

Qubit mapping

Solution in general is a superposition in the computational basis

Qubits in the computational basis map to position in binary

$$\begin{pmatrix} -10 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & -10 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -10 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -10 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 10 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 10 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 10 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 10 \end{pmatrix}$$



$$\begin{aligned} \downarrow\downarrow\downarrow &= 000 = 0 \\ \downarrow\downarrow\uparrow &= 001 = 1 \\ \downarrow\uparrow\downarrow &= 010 = 2 \\ &\dots \end{aligned}$$

$$\begin{aligned} \Psi(1) = &-0.6\,|\downarrow\downarrow\downarrow\rangle - 0.4\,|\downarrow\downarrow\uparrow\rangle \\ &-0.4\,|\downarrow\uparrow\downarrow\rangle - 0.6\,|\downarrow\uparrow\uparrow\rangle \\ &+0.0\,|\uparrow\downarrow\downarrow\rangle + 0.0\,|\uparrow\downarrow\uparrow\rangle \\ &+0.0\,|\uparrow\uparrow\downarrow\rangle + 0.0\,|\uparrow\uparrow\uparrow\rangle \end{aligned}$$

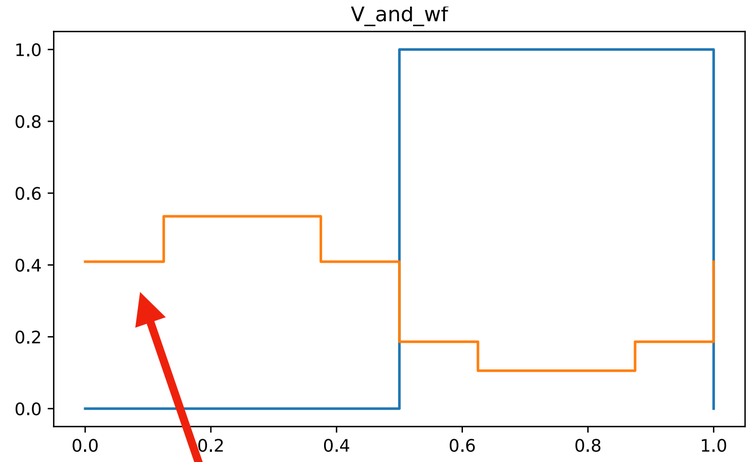
Qubit mapping

Solution in general is a superposition in the computational basis

Qubits in the computational basis map to position in binary

Amplitude maps to value of the wave function at the given position

$$\begin{pmatrix} -10 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & -10 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -10 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -10 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 10 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 10 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 10 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 10 \end{pmatrix}$$



$$\begin{aligned} \Psi(1) = & -0.6\,|\downarrow\downarrow\downarrow\rangle - 0.4\,|\downarrow\downarrow\uparrow\rangle \\ & - 0.4\,|\downarrow\uparrow\downarrow\rangle - 0.6\,|\downarrow\uparrow\uparrow\rangle \\ & + 0.0\,|\uparrow\downarrow\downarrow\rangle + 0.0\,|\uparrow\downarrow\uparrow\rangle \\ & + 0.0\,|\uparrow\uparrow\downarrow\rangle + 0.0\,|\uparrow\uparrow\uparrow\rangle \end{aligned}$$

Qubit mapping

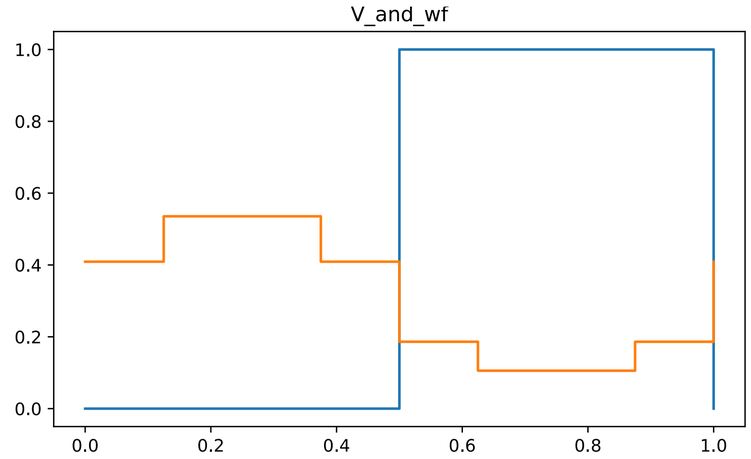
Solution in general is a superposition in the computational basis

Qubits in the computational basis map to position in binary

Amplitude maps to value of the wave function at the given position

Eigenvalue is the energy of the state

$$\begin{pmatrix} -10 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & -10 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -10 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -10 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 10 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 10 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 10 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 10 \end{pmatrix}$$



$$\begin{aligned} \Psi(1) = &- 0.6\,|\downarrow\downarrow\downarrow\rangle - 0.4\,|\downarrow\downarrow\uparrow\rangle \\ &- 0.4\,|\downarrow\uparrow\downarrow\rangle - 0.6\,|\downarrow\uparrow\uparrow\rangle \\ &+ 0.0\,|\uparrow\downarrow\downarrow\rangle + 0.0\,|\uparrow\downarrow\uparrow\rangle \\ &+ 0.0\,|\uparrow\uparrow\downarrow\rangle + 0.0\,|\uparrow\uparrow\uparrow\rangle \end{aligned}$$

Mapping the Laplacian to spin models

We want an efficient mapping to qubits

Space complexity improvements

- Exponential number of lattice sites
- Polynomial number of terms in the Hamiltonian
- Fixed Pauli weight
- Small Pauli support

} Achieved by efficient mapping to spin models

Time complexity improvements

- Polynomial time to recover ground-state wavefunction

} Achieved by knowing the “general enough” spectral gap of H(s)

Binary encoding of the Laplacian

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

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

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

Binary encoding of the Laplacian

0	1	2	3	4	5	6	7

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

For this 3 qubit example

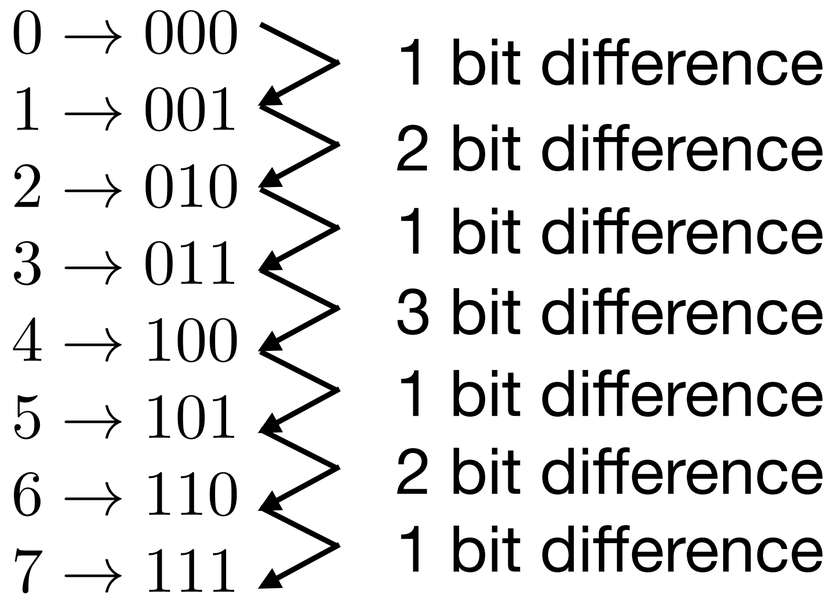
$$\begin{aligned} 0 &\to 000 \\ 1 &\to 001 \\ 2 &\to 010 \\ 3 &\to 011 \\ 4 &\to 100 \\ 5 &\to 101 \\ 6 &\to 110 \\ 7 &\to 111 \end{aligned}$$

Binary encoding of the Laplacian

0	1	2	3	4	5	6	7

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

For this 3 qubit example



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)

Binary encoding of the Laplacian

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

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

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

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

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

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

Realistically this is not going to be realized any time soon (50 years? Never?)

Laplacian in binary reflected Gray code

Binary reflected Gray code definition

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

BRGC is an alternative mapping of a **bit-string** to an integer

The binary bit-string is also the base-2 integer

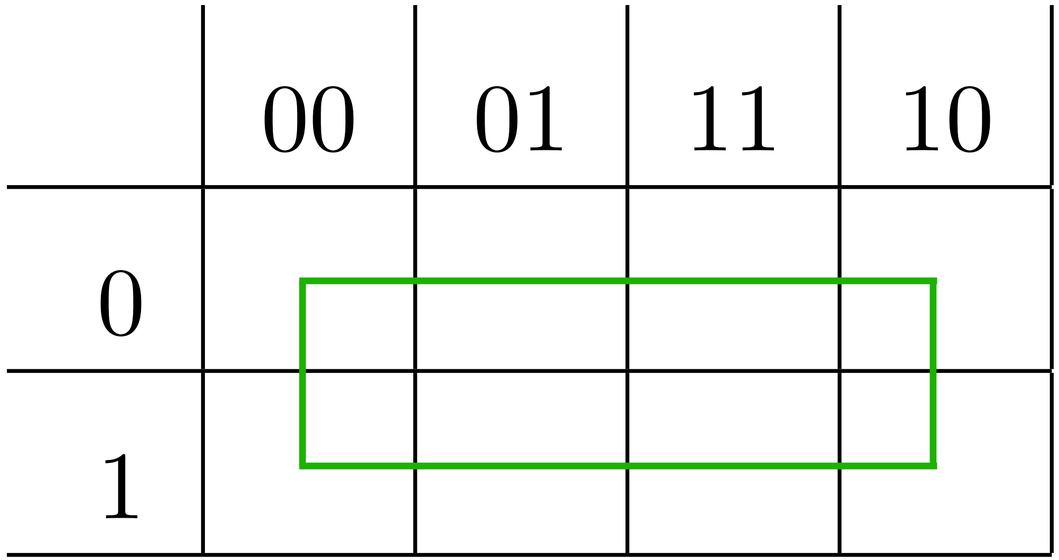
But any 1:1 mapping is a valid representation

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



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

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

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

Laplacian in binary reflected Gray code

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

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

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

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

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

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

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

This can possible be realized much sooner

Hamming distance 2 Gray code

How do we further reduce the complexity of the spin model?

Instead of X, XZ and ZZ, we want just X, Z and ZZ

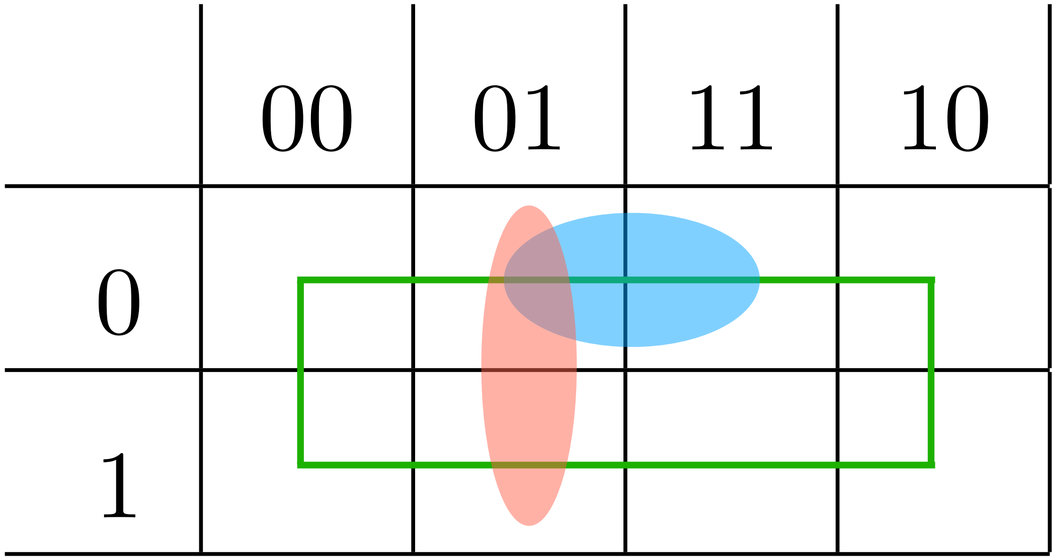
In other words…

Can we map the Schrodinger equation to

Transverse Ising model in polynomial number of qubits?

Hamming distance 2 Gray code

Why does BRGC need an XZ coupling?



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

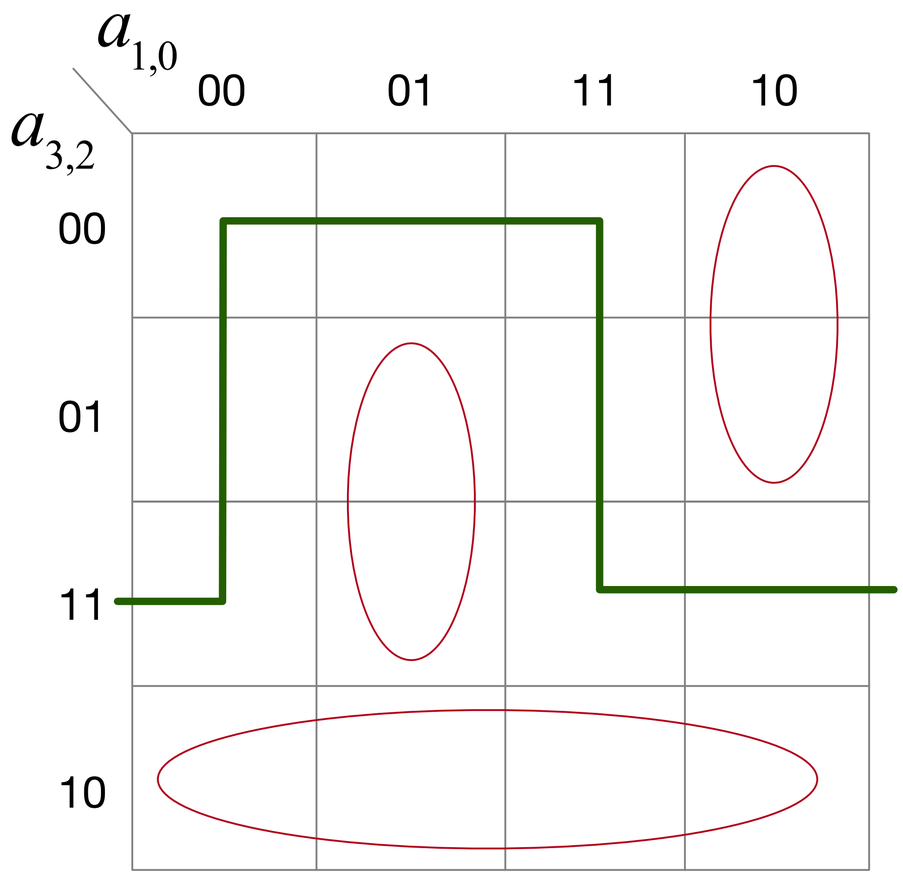
There are non-adjacent lattice sites that are also 1 bit different

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

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

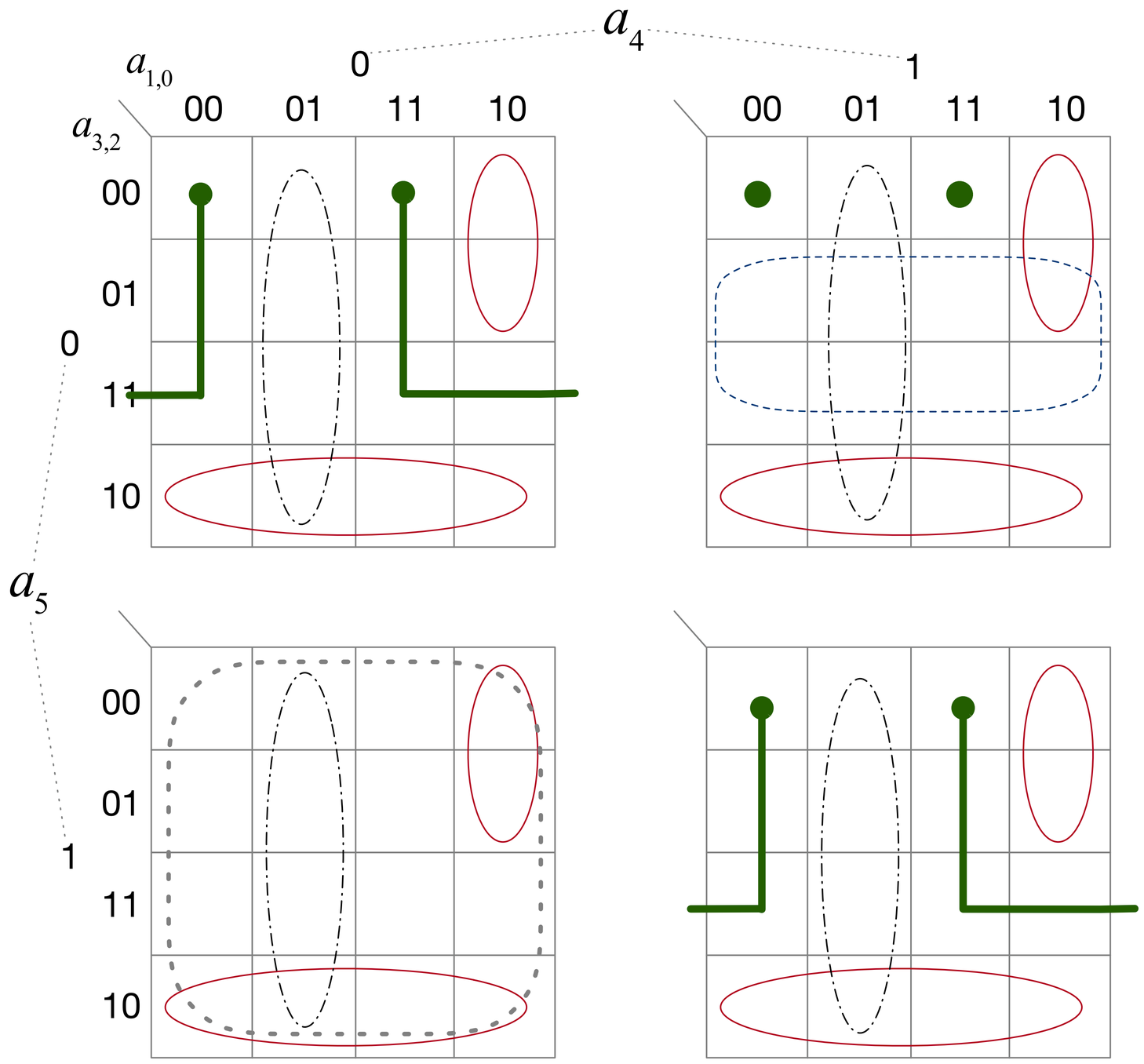
H2GC

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



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!

D-dimension and *A*-body extension

D-dimensions is straightforward
A-particles is the same for Boltzmann statistics (molecule simulations for now)

Reflected Gray code
1D A=1

00
01
11
10

Reflected Gray code
2D A=1 or 1D A=2

0000
0001
0011
0010

1100
1101
1111
1110

0100
0101
0111
0110

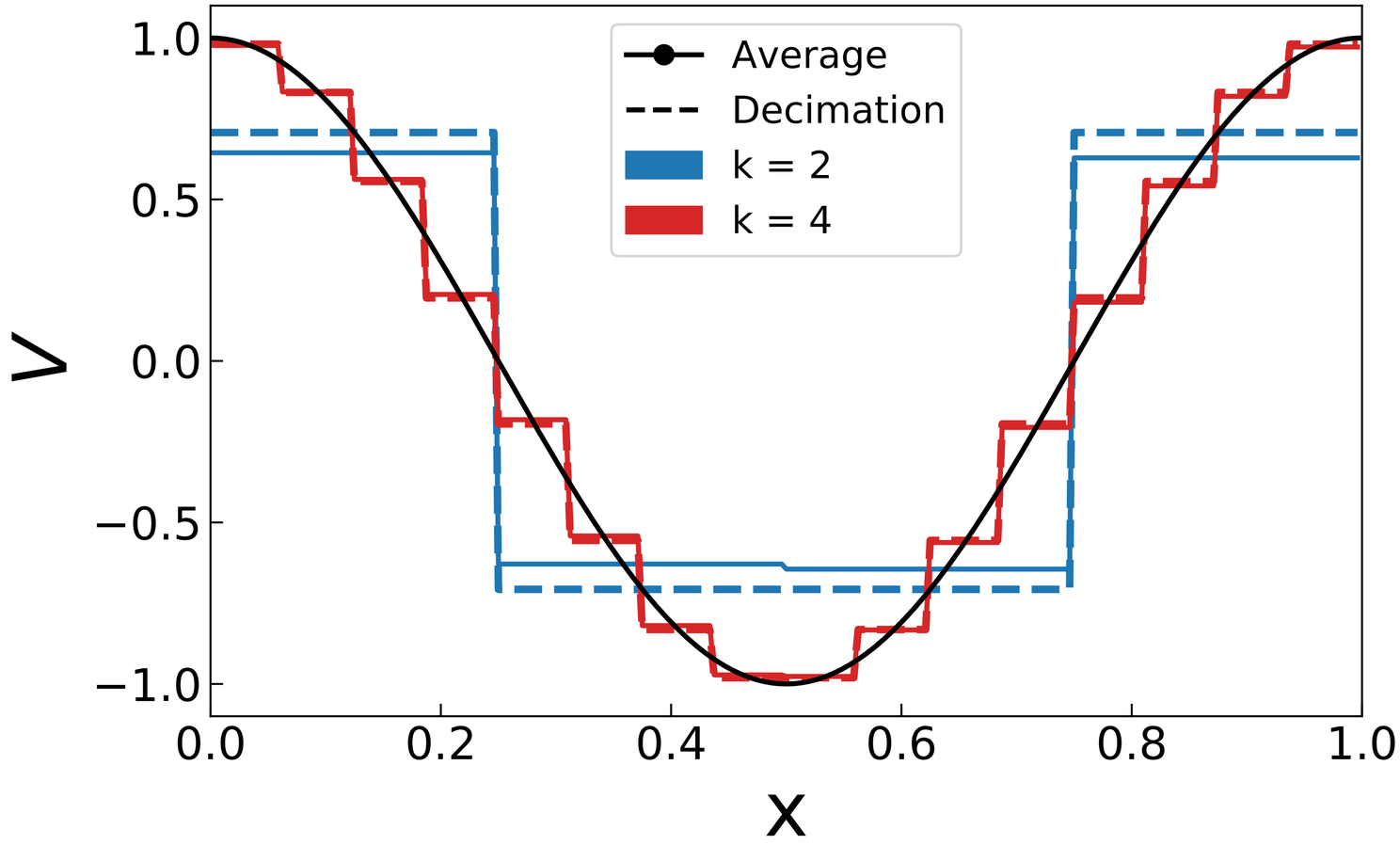
1000
1001
1011
1010

Nested Gray code

Qubit scaling is
$DA \log(\text{sites/dim})$

Mapping real potentials to Ising Model

Next I will focus on mapping arbitrary real potentials to *k*-local Ising Model

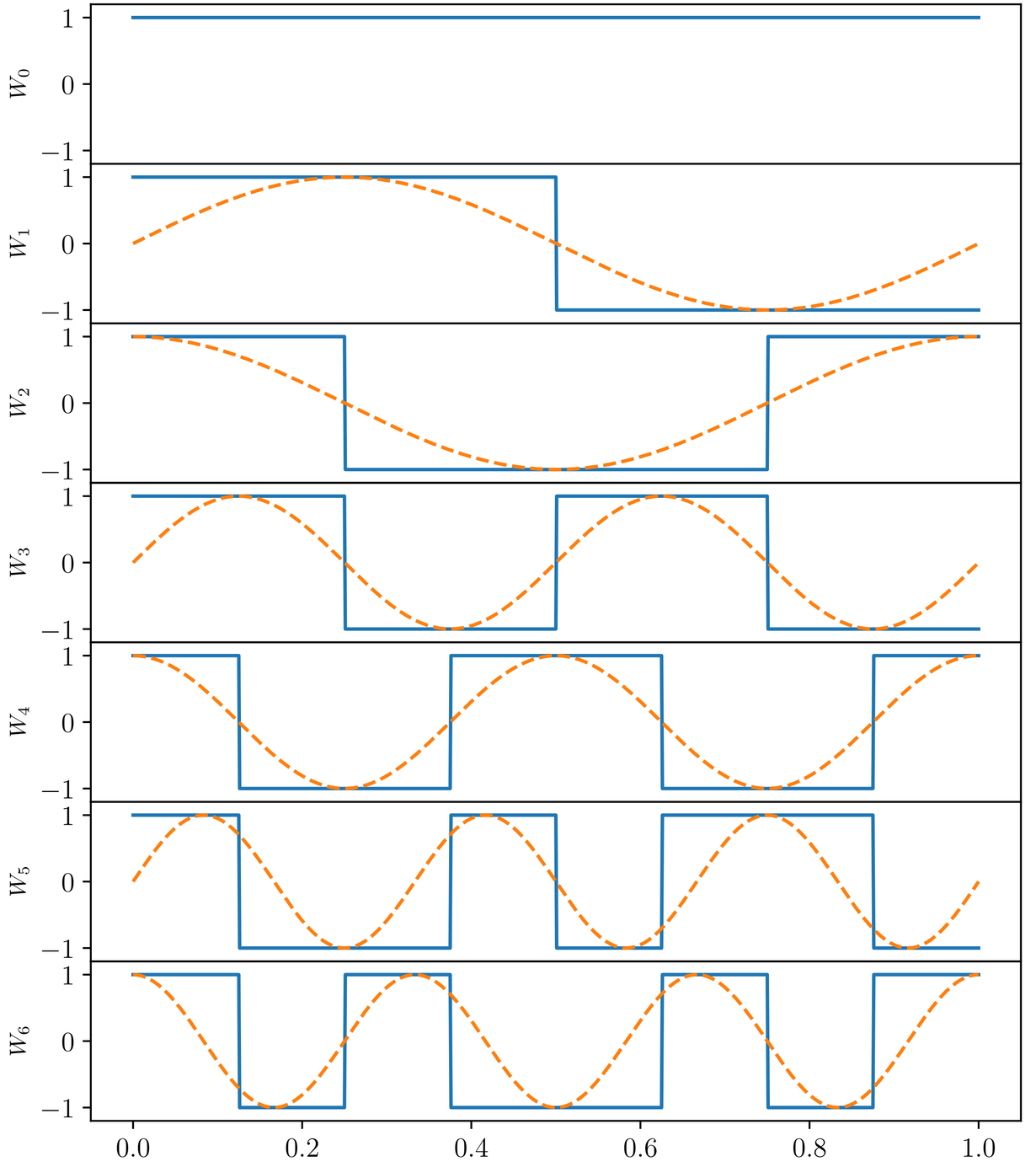


Walsh series

The Walsh functions can be organized with respect to sequency.

Has even/odd modes.

Free of Gibbs phenomena.



Adiabatic evolution

Start from free field and adiabatically turn on potential.
(basically textbook adiabatic theorem of quantum mechanics)

$$H(t) = H_L + B(t)H_V$$

The ground state of the Laplacian is identical to transverse field Hamiltonian.
(this is the zero-frequency state)

$$\Psi(0) = (|\uparrow\rangle + |\downarrow\rangle)^{\otimes A}$$

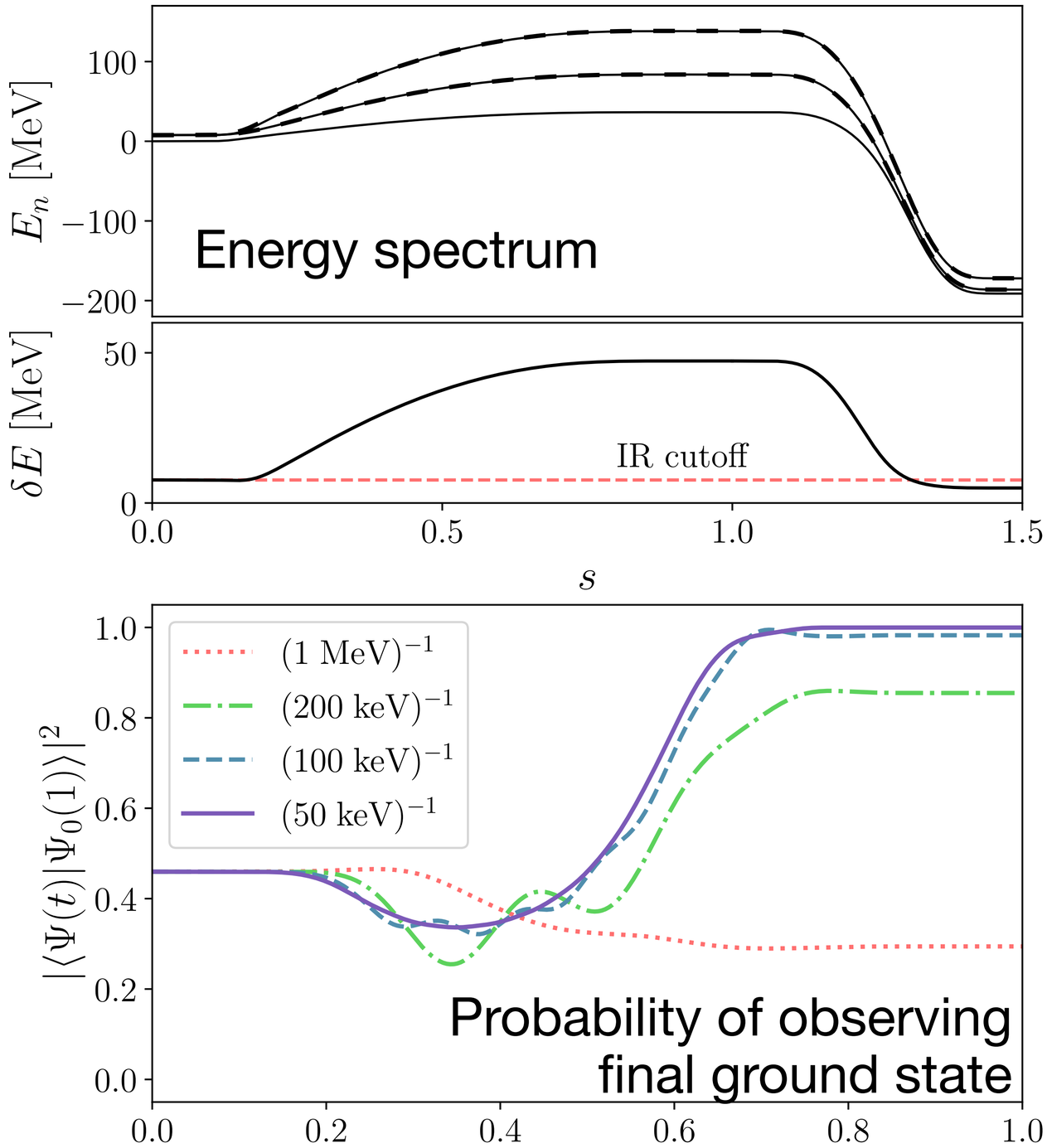
Adiabatic evolution

Integrate the time-dependent schrodinger equation to simulate the schrodinger equation… at least until there is a suitable AQC.

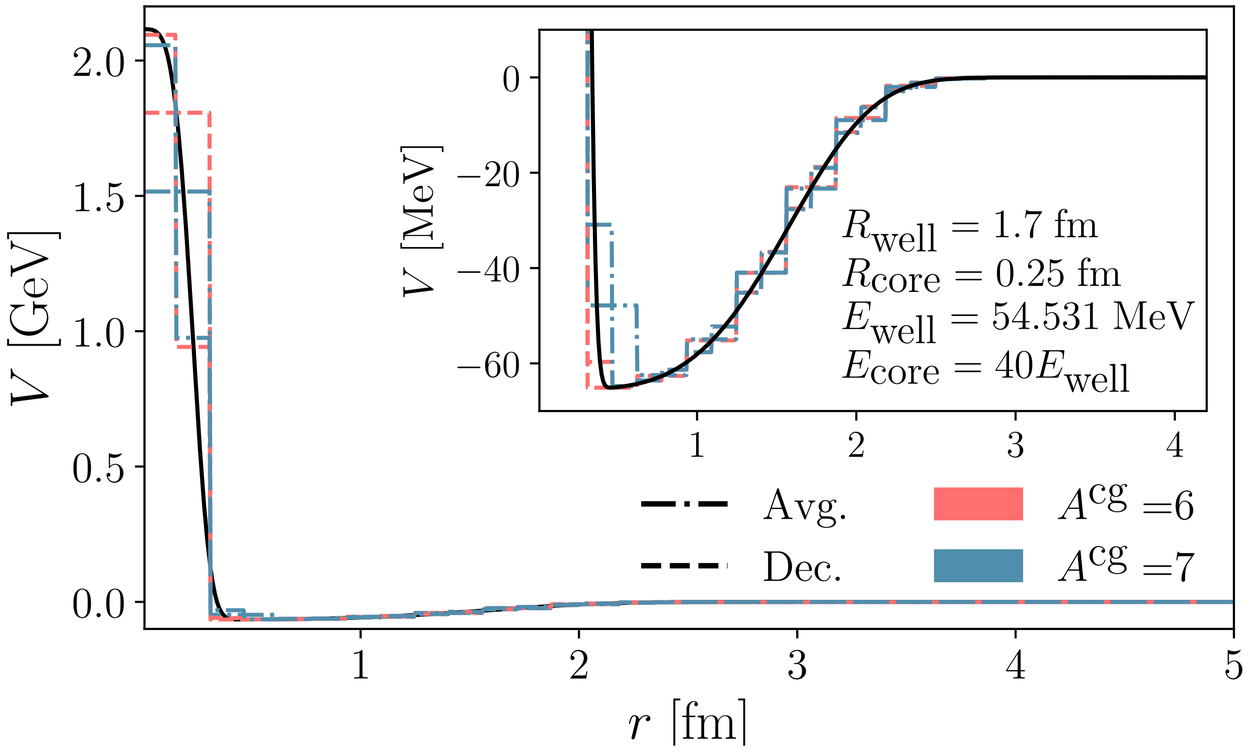
We have parallelized GPU code to simulate up to 20+ qubits.

Gap of the spectrum for initial state preparation will typically be simple.

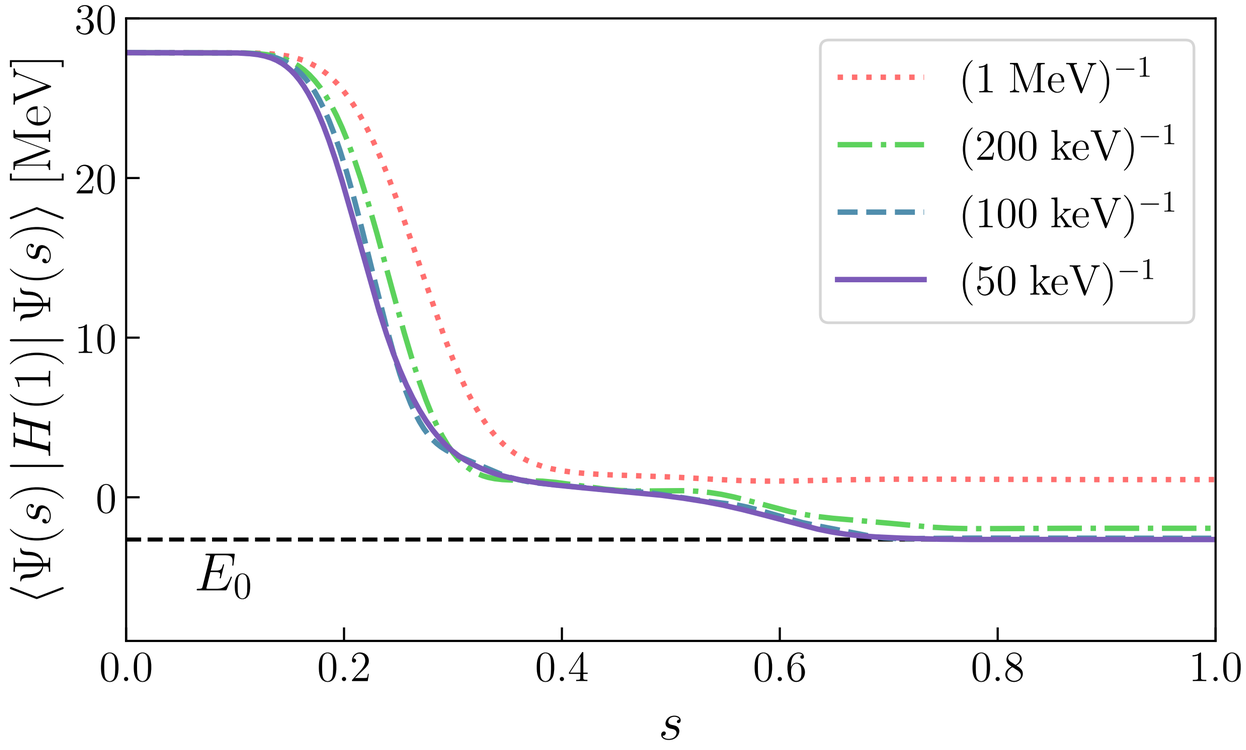
Probability converges to 1 as expected.



Deuteron binding energy



Discretize potential



Obtain binding energy with adiabatic evolution

Some final thoughts

We have mapped the Schrodinger equation to spin models

Given that

1) The potential can (at some point) be coarse grained

2) There isn’t any fine-tuning in the potential such that the first excited-state is abnormally gapped from the ground-state

Then the Schrodinger equation is polynomially mapping in both space and time complexity to the XZ and Transverse Ising model

Collaborators

Kenneth S. McElvain
Ermal Rrapaj
Yantao Wu
University of California Berkeley
RIKEN iTHEMS

This work is supported by the DOE office of NP Quantum Horizons grant

Rademacher functions

There is a class of orthogonal functions which are analogous to sin and cos

The Rademacher functions are the basic building blocks

$$R_n = \operatorname{sign} \sin\left(2^{n+1}\pi t\right)$$

Discrete Rademacher is exactly the diagonal elements of the 1-local Ising Model

$$R_n = \sigma_n^Z$$

$$\sigma^z \otimes 1 \otimes 1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

Rademacher functions

There is a class of orthogonal functions which are analogous to sin and cos

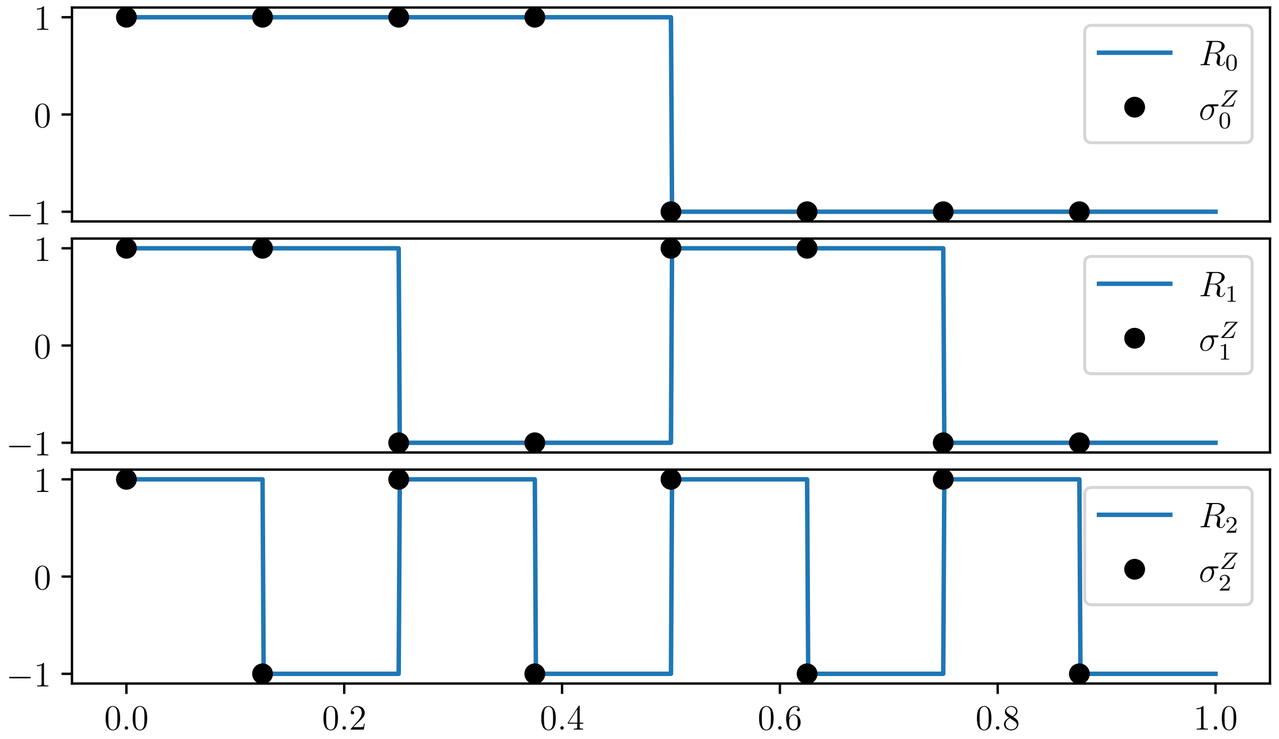
The Rademacher functions are the basic building blocks

$$R_n = \text{sign} \sin\left(2^{n+1}\pi t\right)$$

Discrete Rademacher is exactly the diagonal elements of the 1-local Ising Model

$$R_n = \sigma_n^Z$$

A qubit system has *A* Rademachers



Walsh functions

A qubits has 2^A dimensional Hilbert-space. Need more basis states.

The complete orthonormal functions are the 2^A Walsh functions.

Walsh functions are related to Rademacher functions by binary representation

$$
\begin{aligned}
1 \to 001 \quad & \therefore W_1 = R_1 = \sigma_0^Z \\
2 \to 010 \quad & \therefore W_2 = R_2 = \sigma_1^Z \\
3 \to 011 \quad & \therefore W_3 = R_2 R_1 = \sigma_1^Z \sigma_0^Z
\end{aligned}
$$

And is a bijective map to the complete set of *k*-local Ising-like Hamiltonians

Decimation coarse-graining

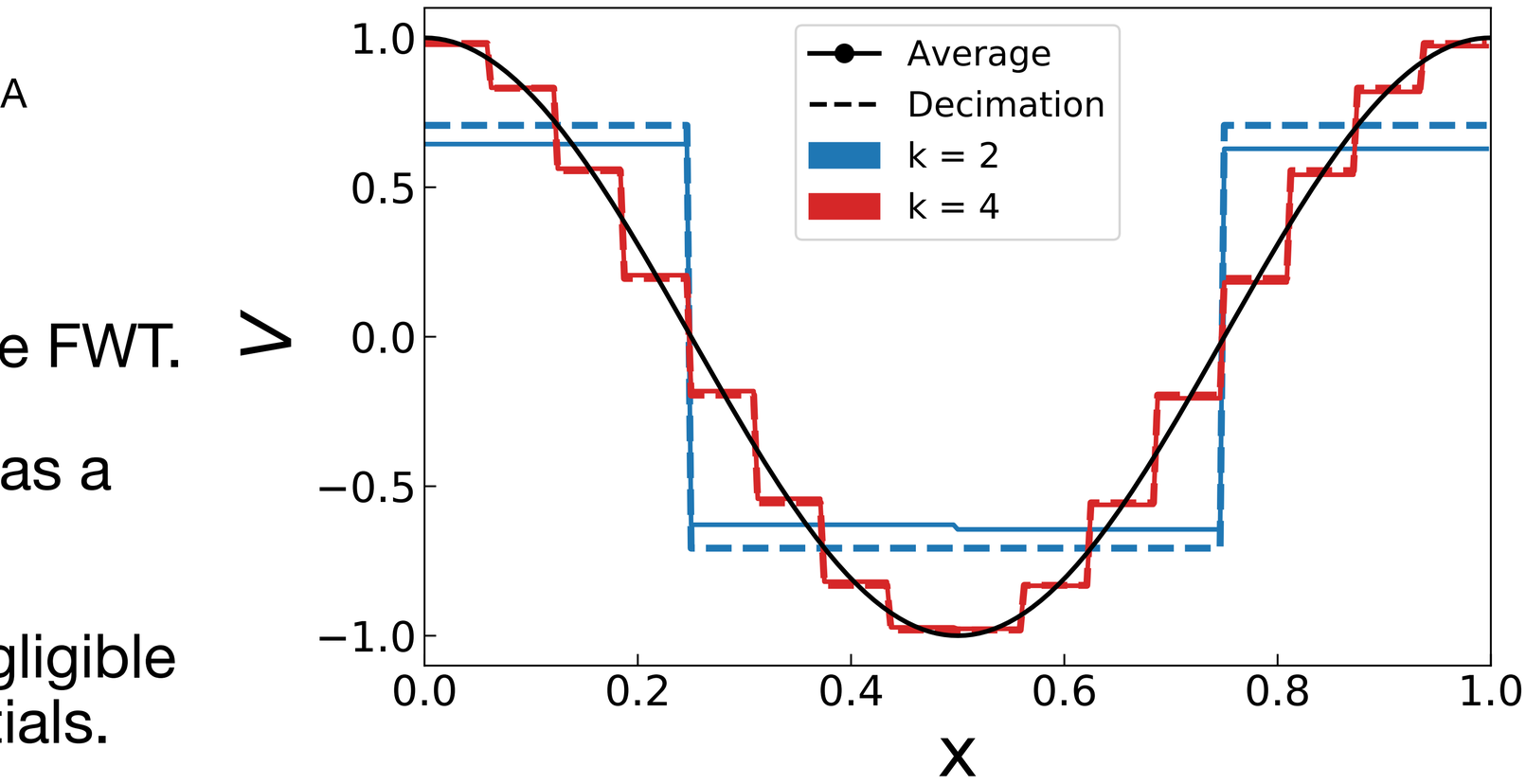
Fast Walsh Transform to get coeff.
with N log(N) complexity

However, for *A* qubits, $N = 2^A$

Coarse-grain potential before FWT.

Decimation coarse-graining as a cheap alternative.

Setup complexity is now negligible given “well-behaved” potentials.



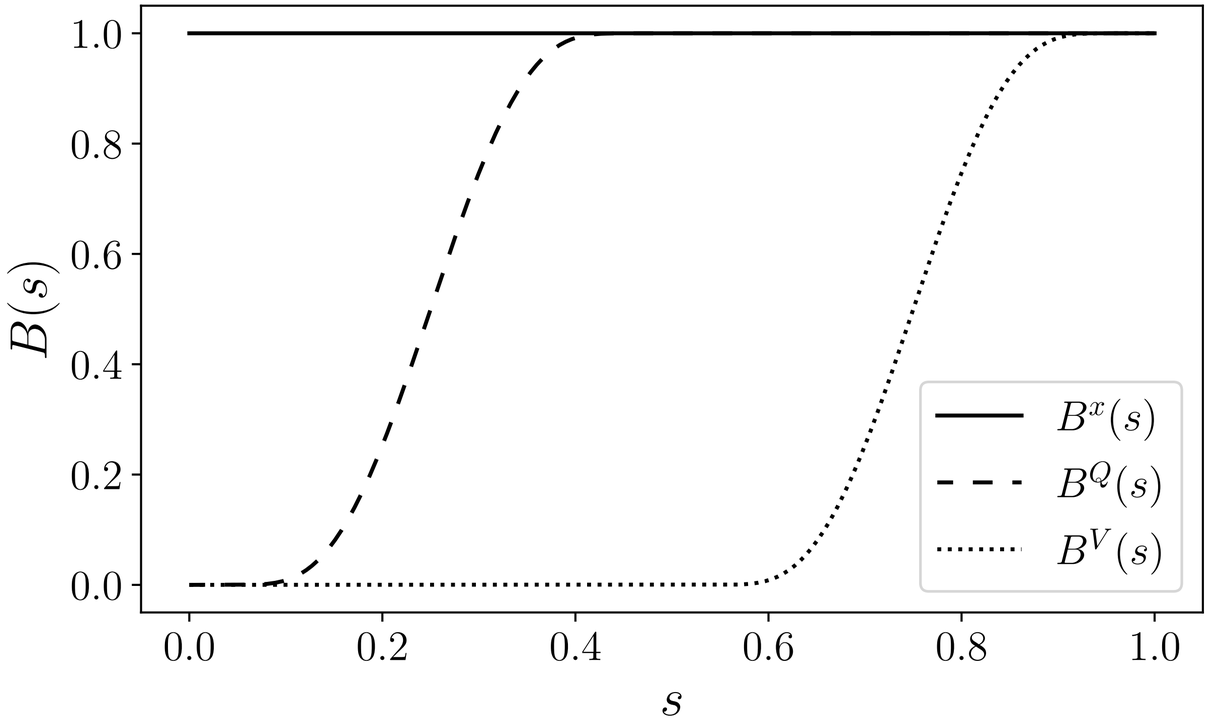
Potential construction summary

If we can coarse grain the potential

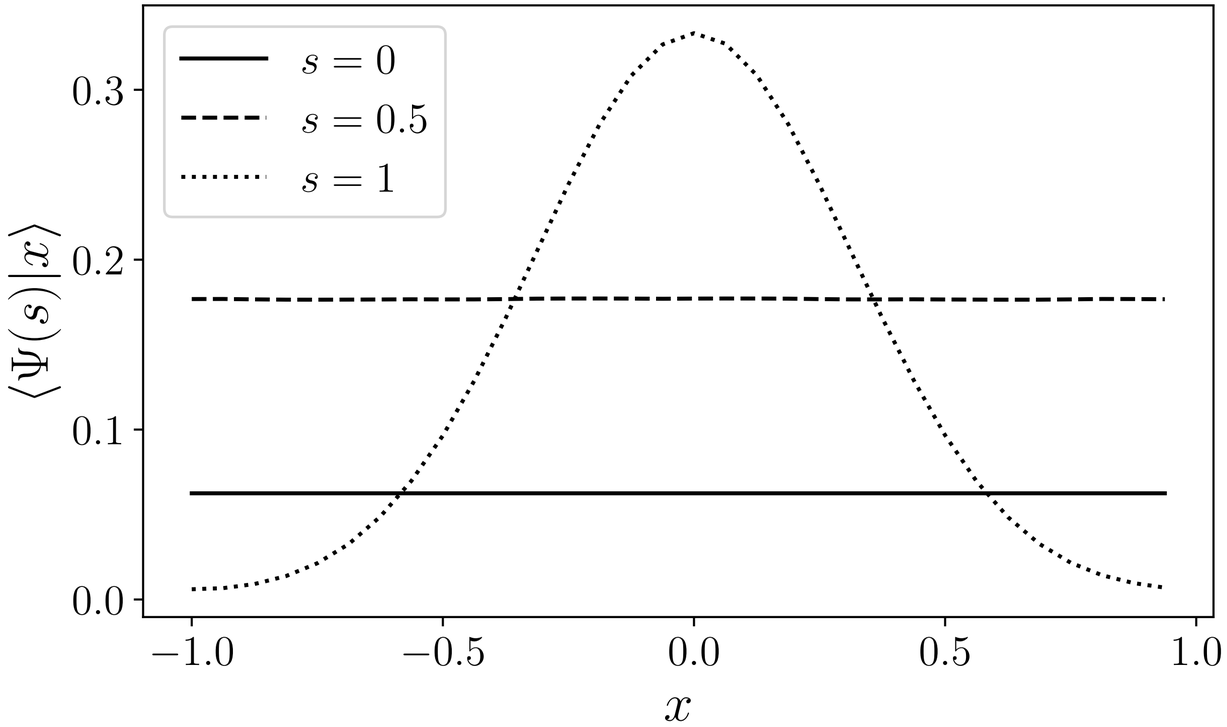
Then the (classical) time complexity of setting up the problem can be exponentially reduced

This is of course application dependent

Harmonic Oscillator with H2GC

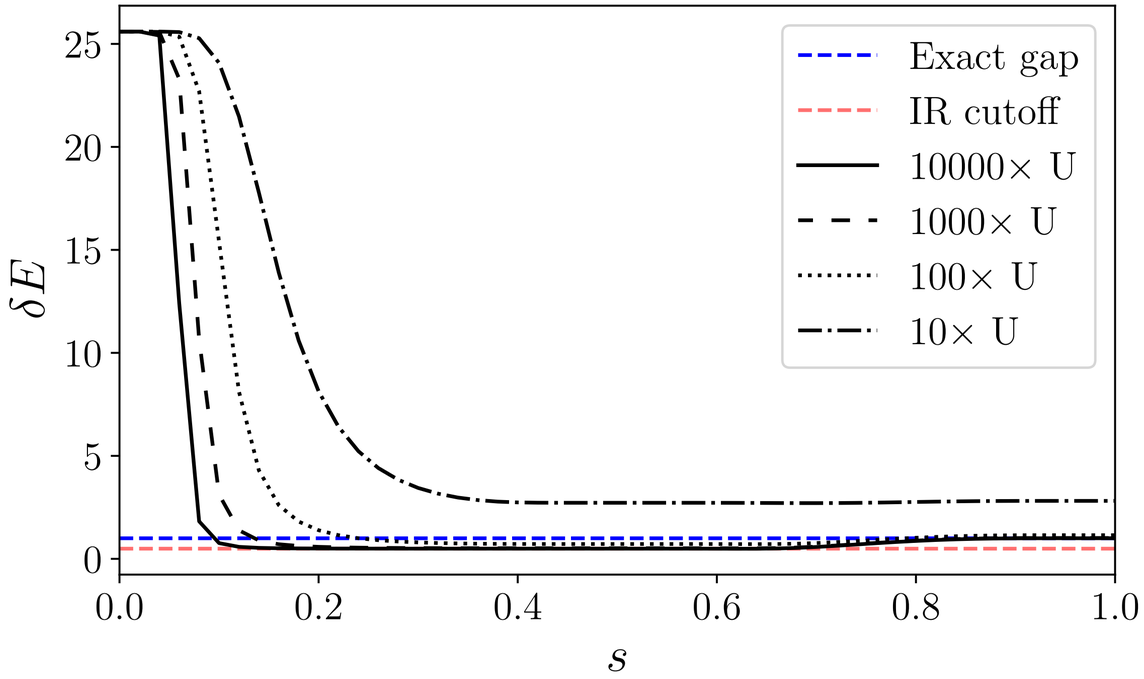


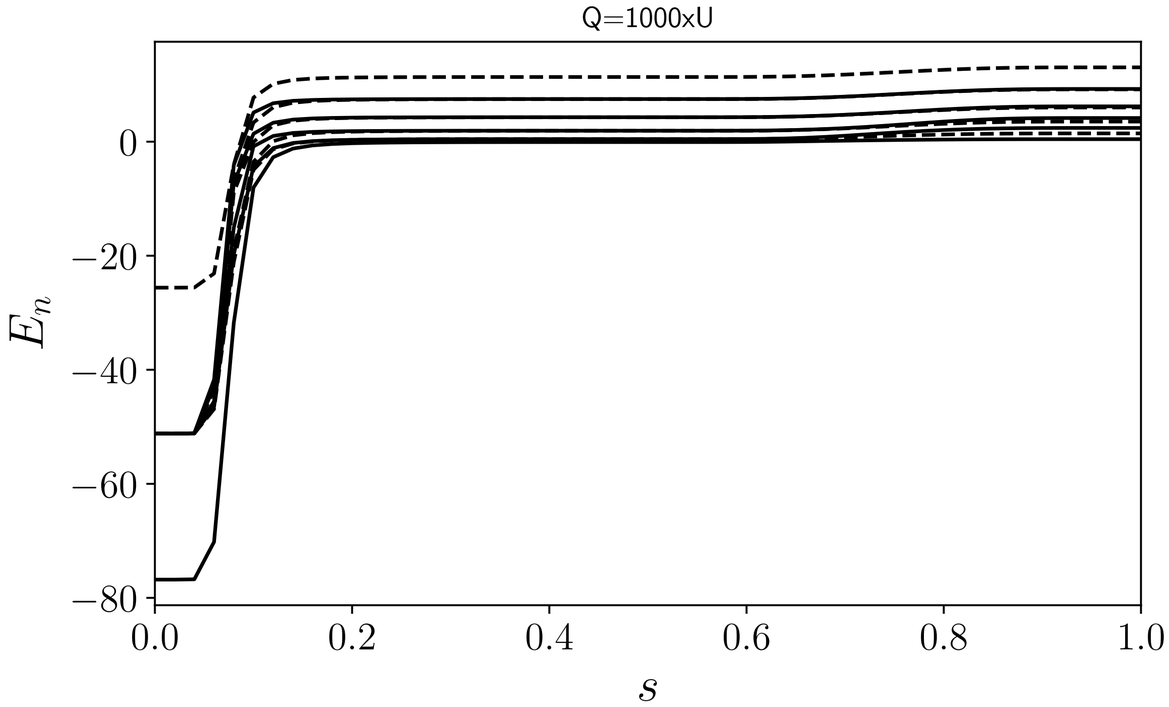
Time dependence of coefficients



Wavefunction at different points in time

H2GC penalty term challenges





Gap is typically protected by the IR cutoff

The slope of the spectrum requires us to slow down