Fermionic State Preparation using Givens Rotations

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1 Wave Packet Definition

Consider the simplfied fermionic wave packet definition

$$|\psi\rangle = \hat{\mathcal{G}}|\psi\rangle = \sum_{j=0}^{N-1} a_j e^{-i\beta_j} \hat{c}_j^\dagger |\Omega\rangle$$

where

$$a_j = e^{-(j-j')^2/\sigma^2} \in \mathbb{R} > 0$$

and

$$\beta_j = kj = \frac{n_k \pi}{N} j$$

for

$$n_k = \begin{cases} -N+2, -N+4, \ldots, N-2, N & \text{odd \# of fermions} \\ -N+1, -N+3, \ldots, N-3, N-1 & \text{even \# of fermions} \end{cases}.$$

The mean position of the wave packet is j' and width in position space is proportional to σ. The ground state of the Hamiltonian is denoted $|\Omega\rangle$.

2 Givens Rotations

Our wave packet can be completely defined in the subspace with basis vectors

$$\left\{ \hat{c}_j^\dagger |\Omega\rangle : j \in \ \mathbb{Z}_N \right\}.$$

In this basis, our wave packet has the form

$$|\psi\rangle = \begin{pmatrix} a_0 e^{-i\beta_0} \\ a_1 e^{-i\beta_1} \\ a_2 e^{-i\beta_2} \\ \vdots \\ a_{N-1} e^{-i\beta_{N-1}} \end{pmatrix}.$$

We seek to diagonalize $|\psi\rangle$ in this subspace:

$$\hat{u}|\psi\rangle = \hat{c}_0^\dagger |\Omega\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

This is equivalent to diagonalizing an $N \times N$ matrix ψ whose first column is $|\Omega\rangle$. We will do this in two broad steps: (1) Cancel out the phases and (2) iteratively diagonalize the rows.

To cancel out the phases, all we have to do is multiply by a diagonal matrix whose elements are the complex conjugate of the phases:

$$\hat{p} = \begin{pmatrix} e^{i\beta_0} & & & & \\ & e^{i\beta_1} & & & \\ & & e^{i\beta_2} & & \\ & & & \ddots & \\ & & & & e^{i\beta_{N-1}} \end{pmatrix},$$

so

$$\hat{p}|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{N-1} \end{pmatrix}.$$

Now for the magnitudes. A Givens rotation matrix is defined as

$$\hat{g}_n(\theta) = \begin{pmatrix} 1 & 0 & \cdots & & & \cdots & 0 \\ 0 & 1 & & & & & \vdots \\ \vdots & & \ddots & & & & \\ & & & \cos\theta & -\sin\theta & & \\ & & & \sin\theta & \cos\theta & & \\ \vdots & & & & & \ddots & \vdots \\ 0 & \cdots & & & & \cdots & 1 \end{pmatrix},$$

where the $(n-1)$-th and n-th row is non-diagonal. Applied to the $N-1$ and N row of $|\psi\rangle$, we have

$$\hat{g}_N(\theta_N)\, p|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{N-1}\cos\theta_N - a_N \sin\theta_N \\ a_{N-1}\sin\theta_N + a_N\cos\theta_N \end{pmatrix}.$$

If we let

$$\theta_N = \arctan\left(-\frac{a_N}{a_{N-1}}\right),$$

then

$$\hat{g}_N(\theta_N)\, \hat{p}|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ \tilde{a}_{N-1} \\ 0 \end{pmatrix}$$

where $\tilde{a}_{N-1} = a_{N-1}\cos\theta_N - a_N\sin\theta_N$. For the next row, let

$$\theta_{N-1} = \arctan\left(-\frac{\tilde{a}_{N-1}}{a_{N-2}}\right),$$

so

$$\hat{g}_{N-1}\left(\theta_{N-1}\right)\hat{g}_{N}\left(\theta_{N}\right)\hat{p}|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ \tilde{a}_{N-2} \\ 0 \\ 0 \end{pmatrix}$$

and $\tilde{a}_{N-2} = a_{N-2}\cos\theta_{N-1} - \tilde{a}_{N-1}\sin\theta_{N-1}$. Repeating this procedure $N-1$ times, we recover $\hat{c}_0^\dagger|\Omega\rangle$. The net operator has the form

$$\hat{u} = \hat{g}\hat{p} = \left[\prod_{j=1}^{N-1}\hat{g}_j\left(\theta_j\right)\right]\hat{p}.$$

3 Implementation on a Quantum Computer

We seek to write the fermionic wave packet creation operator as a unitary transformation of the creation operators

$$\hat{\mathcal{G}} = \sum_{j=0}^{N_s-1}\mathcal{G}_j\hat{c}_j^\dagger = \hat{V}(u)\hat{c}_0^\dagger\hat{V}^\dagger(u)$$

for

$$\hat{V}(\hat{u}) = \exp\left[\sum_{nl}\hat{c}_j^\dagger\left(\log u\right)_{nl}\hat{c}_j\right].$$

This mapping is a homomorphism under multiplication, so we can decompose the operator into a product of $\hat{V}\left(p_j\right)$ and $\hat{V}\left(\hat{g}_j\right)$:

$$\hat{V}\left(\hat{u}\right) = \hat{V}^\dagger\left(\hat{p}\right)\hat{V}^\dagger\left(\hat{g}_{N-1}\right)\cdots\hat{V}^\dagger\left(\hat{g}_1\right)$$

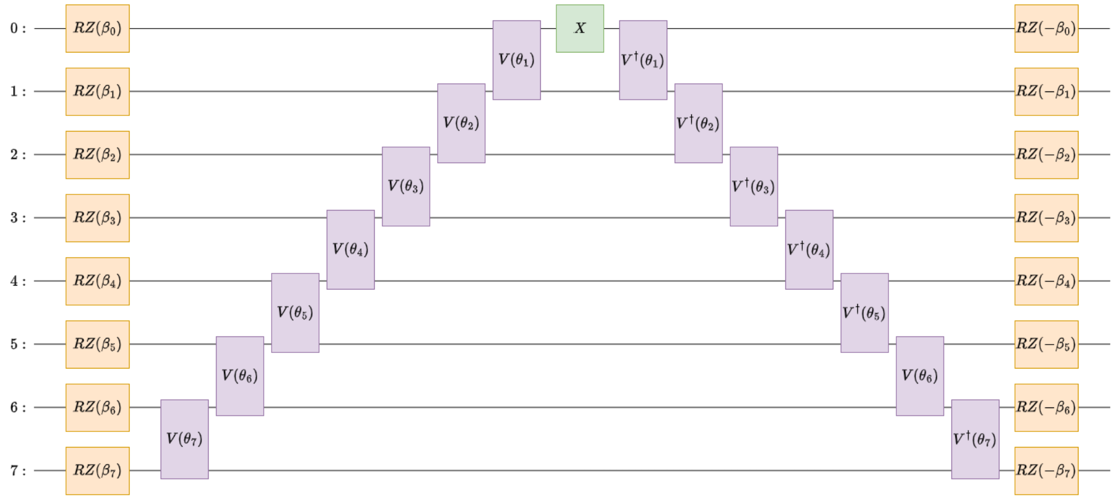
where

$$\begin{aligned}\hat{V}^\dagger\left(\hat{p}\right) &= \exp\left[-\sum_{jl}\hat{c}_j^\dagger\left(\log p\right)_{jl}\hat{c}_l\right]\\ &= \exp\left[-i\sum_j\beta_j\hat{c}_j^\dagger\hat{c}_j\right]\\ &= \exp\left[-i\sum_j\frac{\beta_j}{2}\hat{\sigma}_j^z\right]\end{aligned}$$

up to an overall phase, and

$$\begin{aligned}\hat{V}^\dagger\left(g_j\right) &= \exp\left[-\sum_{jl}\hat{c}_j^\dagger\left(\log g\right)_{jl}\hat{c}_l\right]\\ &= \exp\left[\theta_j\left(\hat{c}_{j-1}^\dagger\hat{c}_j - \hat{c}_j^\dagger\hat{c}_{j-1}\right)\right]\\ &= \exp\left[i\frac{\theta_j}{2}\left(\hat{\sigma}_{j-1}^x\hat{\sigma}_j^y - \hat{\sigma}_{j-1}^y\hat{\sigma}_j^x\right)\right],\end{aligned}$$

which has an efficient decomposition with only two CNOT gates. Below shows a full circuit to generate a single wave packet.



To generate two wave packets

$$|\psi\rangle = \hat{\mathcal{G}}_A \hat{\mathcal{G}}_B |\Omega\rangle,$$

we need only apply the above circuit twice, where $\theta_j^{A(B)}, \beta^{A(B)}$ reflect the different mean position and momentum centers of the two wave packets. CNOT depth is shallow, but the staggered application will increase preparation time.