

Gaussian Wave Packet Preparation on Quantum Computers

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1 Transverse Ising Model

Hamiltonian (PBC):

$$\hat{H} = -\lambda \sum_{j=0}^{N_s-1} \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x - \sum_{j=0}^{N_s-1} \hat{\sigma}_j^z$$

2 Gaussian Wave Packet Operator

In an N_s -qubit space, we define the Gaussian wave packet creation operator as

$$\hat{\mathcal{G}}_A = \frac{1}{\sqrt{N_s}} \sum_{j=0}^{N_s-1} e^{-ik_A x_j} e^{-r(x_j, x_A)/\sigma^2} \hat{c}_j^\dagger,$$

where k_A is the momentum center, x_A is the position center, $r(x_j, x_A)$ is the minimum distance between x_j and x_A , σ is the width in position space, and

$$\hat{c}_j^\dagger = \left(- \prod_{m=0}^{j-1} \hat{\sigma}_m^z \right) \hat{\sigma}_j^-$$

is the Jordan-Wigner fermionic creation operator. A single wave packet state is then

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

where $|\Omega\rangle$ is the vacuum. A double wave packet state is then

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

For scattering, we usually choose $k_B = -k_A$ and x_B some distance away from x_A that is greater than the width of a single packet and that the point of collision

will be occur a qubit site. For a single wave packet, the momentum numbers are given by

$$k = 0, \pm \frac{2\pi}{N_s}, \pm \frac{4\pi}{N_s}, \dots, \pm \frac{(N_s - 2)\pi}{N_s}, \pi \quad ,$$

while for two wave packets the momentum numbers are

$$k = \pm \frac{\pi}{N_s}, \pm \frac{3\pi}{N_s}, \dots, \pm \frac{(N_s - 1)\pi}{N_s}.$$

The j -th term of the sum acts on $j + 1$ qubits, so the operator is very nonlocal.

3 Approximated Operator

Suppose we want to construct a Gaussian wave packet that is M -qubits wide. That is, any qubits beyond the M -sector have near zero contribution to the overall wave packet. Then, initially, nothing happens to the system beyond the M -sector, and we can restrict our state prep to that M -sector. In that M -sector, we can generate a wave packet

$$\hat{\mathcal{G}}_A |0\rangle = \frac{1}{\sqrt{N_s}} \sum_{j=0}^{M-1} e^{-ik_A x_j} e^{-r(x_j, x_A)^2 / \sigma^2} \hat{c}_j^\dagger |0\rangle ,$$

where $|0\rangle$ is the all spin up state in the sector and j, A are in the range of the sector. For the momentum number k_A , it's possible values will be that of the larger system. Our sources of error will then come from the k_A values, and \hat{c}_j^\dagger depending upon where the wave packet is centered.

For example, suppose we want to generate a two wave packet state of momenta $\pm k$ and position centers 1 and 5. We can let $x_j = (0, 1, 2)$ and $r_j = (-1, 0, 1)$. The Jordan-Wigner operators are

$$\begin{aligned} \hat{c}_0^\dagger &= \hat{\sigma}_0^- & , \\ \hat{c}_1^\dagger &= -\hat{\sigma}_0^z \hat{\sigma}_1^- & , \\ \hat{c}_2^\dagger &= \hat{\sigma}_0^z \hat{\sigma}_1^z \hat{\sigma}_2^- & . \end{aligned}$$

The Gaussian operators are then

$$\begin{aligned} \hat{\mathcal{G}}_{\rightarrow} &= \frac{1}{\sqrt{3}} \left(e^{-1/\sigma^2} \hat{c}_0^\dagger + e^{-ik} \hat{c}_1^\dagger + e^{-2ik} e^{-1/\sigma^2} \hat{c}_1^\dagger \right) & , \\ \hat{\mathcal{G}}_{\leftarrow} &= \frac{1}{\sqrt{3}} \left(e^{-1/\sigma^2} \hat{c}_0^\dagger + e^{ik} \hat{c}_1^\dagger + e^{2ik} e^{-1/\sigma^2} \hat{c}_1^\dagger \right) & . \end{aligned}$$

For $k = +\frac{3\pi}{8}$, the equivalent quantum circuit is given in Figure 1. For $k = -\frac{3\pi}{8}$, the only thing that changes is some of the signs for the U_3 angles. We then prepend these circuits to the whole 8-site circuit on sites 0, 1, 2 and 4, 5, 6 respectively. Figure 2 shows the initial state and evolution of the system for $\lambda = 0.3$. Improved approximations could be made by making an m -site wave packet in a $M > m, M < N_s$ subspace.

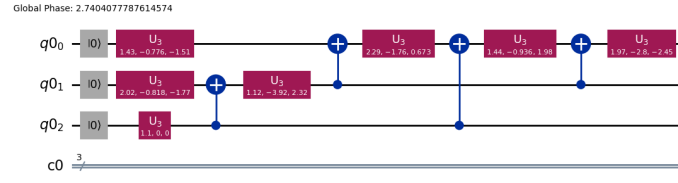


Figure 1: Equivalent circuit for to generate a 3-site Gaussian wave packet with momenta $+\frac{3\pi}{8}$. The circuit consists of 4 CNOT gates and has depth 10.

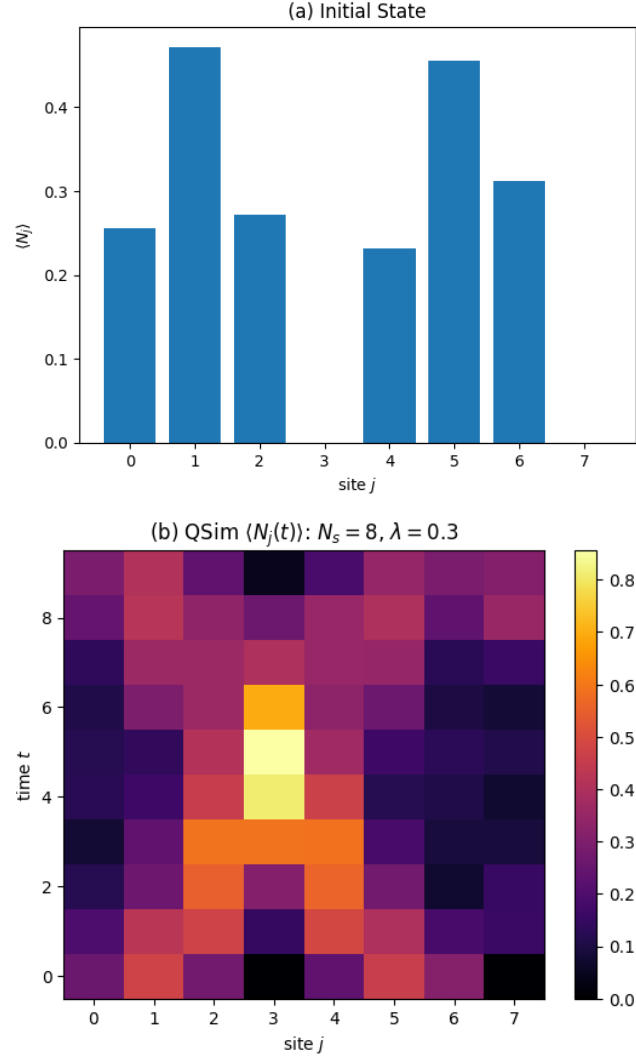


Figure 2: Scattering of two Gaussian wave packets for $\lambda = 3$. (a) shows the occupation of sites for the initial state and (b) the evolution of occupation of sites. The momenta of the wave packets are $\pm \frac{3\pi}{8}$.