Approximate Fermionic Scattering for the NISQ Era

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In the era of noisy intermediate scale quantum (NISQ) hardware, digital quantum computers are limited to shallow circuits on the order of a thousand layers due to system noise and qubit decoherence. Thus, every step of a simulation must be made efficient as possible. Using the recently proposed Givens Rotation state preparation by Chai et al and ladder operator block encoding method by Simon et al, we propose a method for large volume fermionic scattering simulations to approximate the fermionic wave packets by localizing them in space, reducing circuit depth by half. With time evolving block decimation via matrix product states, we show that the approximation holds for large near-critical weakly interacting theories, and for larger interactions in the non-critical regime for a modified transverse field Ising model. We then discuss implementation on quantum hardware. Using IonQ's Aria trapped ion and IBM's Rensselaer transom machines, we show promising results for 8, 12, 20, and 36 site systems.

Introduction - Quantum computers provide a natural pathway for large real-time scattering simulations, but in the noisy intermediate scale quantum (NISQ) era [1] system noise and qubit decoherence severely limit both simulation time and complexity. In terms of quantum circuit depth on digital hardware, this means we can only go up to around a thousand gate layers with sophisticated error correction and mitigation techniques. Nevertheless, there have already been very promising results obtained for small volume scattering simulations [2–12]. In the context of fermionic scattering, Jordan, Lee, and Preskill proposed a six step simulation process where one (1) prepares the ground state of the free theory, adiabatically turns on the (2) nearest neighbor and (3) interacting terms of the Hamiltonian to evolve into the ground state of the interacting theory, (4) excite wave packets, then (5) real-time evolve the state, and finally (6) measurement [13, 14]. Informed variational algorithms like the variational quantum eigensolver (VQE) [15] or the improved adapt-VQE [16–18], allows the state preparation steps (1-4) to be combined.

Suppose we let VQE handle the vacuum preparation (1-3), and use alternative methods to prepare fermionic wave packets. These wave packets are a sum of highly non-local fermionic creation operators in the particle basis. For standard state decomposition procedures like Möttönen[19] and quantum Shannon[20], circuit depth grows far too quickly per system size. Thus, specific state preparation techniques are needed in the near term. Using variational methods, Davoudi et. al used ancillary qubits to place the non-unitary creation operators in a larger unitary space to make wave packets for hadronic theories [21]. Another technique that has shown great promise uses Given's rotation matrices[22–24], decomposing the state into a product of approximate unitary particle conserving rotation operators when acting on a non-trivial ground state. Chai et. al [25] have used this to simulate fermion/anti-fermion scattering in the Thirring Model.

Nevertheless, in the near term more efficient and or approximate methods are needed. We introduce a modification to Chai et. al's method for the case for narrow wave packets with large initial separation that reduces circuit by half by localizing the wave packets in position space. As well, we use ancillary qubits to completely unitarize the particle creation operators. This letter is structured as follows. We first introduce a toy interacting fermionic Hamiltonian using the transverse field Ising model. We then describe the Givens state preparation method with added approximation. Then we show results with IonQ Forte 1 and IBM hardware, comparing with time evolving block decimation via matrix product states.

Theory - Consider a modified one-dimensional N-site Transverse Field Ising model whose Hamiltonian is given by

$$\hat{H} = -\sum_{j=1}^{N} \left(J\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + h\hat{\sigma}_j^z + g\hat{\sigma}_j^z \hat{\sigma}_{j+1}^z \right), \qquad (1)$$

where $J(g)$ is nearest neighbor coupling in the $X(Z)$ direction, h is the transverse field coupling, and $\hat{\sigma}_{N+1} = \hat{\sigma}_1$ for periodic boundary conditions. For $g = 0$, the model is diagonalized by three transformations: Jordan-Wigner, Fourier, and Bogoliubov [26–29]. The Jordan-Wigner fermionic operators are defined as:

$$\hat{c}_j^\dagger = \left(\prod_{i=1}^{j-1} -\hat{\sigma}_j^z \right) \hat{\sigma}_j^-, \qquad \hat{c}_j = \left(\prod_{i=1}^{j-1} -\hat{\sigma}_j^z \right) \hat{\sigma}_j^+, \qquad (2)$$

Due to the boundary term, the Hamiltonian is dependent upon the particle number of the state, so we define two sets of momentum numbers for even and odd numbers of particles:

$$k = \begin{cases} 0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \ldots, \pi & \text{(odd particle number)} \\ \pm\frac{\pi}{N}, \pm\frac{3\pi}{N}, \ldots, \pm\frac{(N-1)\pi}{N} & \text{(even particle number)} \end{cases}. \qquad (3)$$

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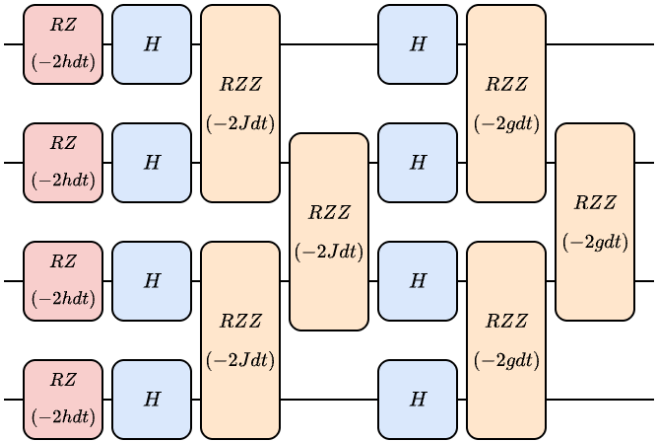

FIG. 1. The Trotterized time evolution operator for the modified Ising model. The boundary term is assumed but not shown. All Pauli-rotation gates are defined as $RP(\theta) = \exp(-i\hat{P}\,\theta/2)$. The layers $H\mathrm{RZZ}H$ correspond to RXX layers, where H is the Hadamard gate.

For all $J > 0$, the ground state is non-trivial, with a phase transition occurring at $J = h$ in the continuum.

The inspiration for the ZZ-term comes from the four fermion interaction term in discrete space given by [25]

$$\begin{aligned} 4g\sum_j \hat{c}_j^\dagger \hat{c}_j \hat{c}_{j+1}^\dagger \hat{c}_{j+1} &= g\sum_j \left(\hat{\mathbb{1}} - \hat{\sigma}_j^z\right)\left(\hat{\mathbb{1}} - \hat{\sigma}_{j+1}^z\right) \\ &= g\sum_j \left(\hat{\mathbb{1}} - 2\hat{\sigma}_j^z + \hat{\sigma}_j^z\hat{\sigma}_{j+1}^z\right) \end{aligned} \tag{4}$$

The first term is the identity and can be ignored, the second term is the transverse field coupling of the Ising model up to a negative sign, and the third term is what we added. Thus, we can think of the XX-term in the Ising model as the kinetic term. We will first treat g as a perturbation and then approach $h = 2g$. Using the Lie-Trotter formula [30, 31], the time evolution circuit (TEO) to first order in Δt is given in Figure 1. We can go to higher levels of precision, but that is not the focus of this letter.

State Preparation via Givens Rotations - In position space, a simple fermionic Gaussian wave packet with average position x_A and average momentum k_A is

$$|\psi\rangle = \mathcal{G}_A\,|\Omega\rangle = \left(\sum_{j=1}^{N} e^{-ik_A j} e^{-|j-j_A|^2/\sigma^2}\hat{c}_j^\dagger\right)|\Omega\rangle\,, \tag{5}$$

where σ is proportional to the width of the wave packet. A two-packet scattering state with position (momentum) centers $x_A(k_A)$, $x_B(k_B)$ is then $\mathcal{G}_A\mathcal{G}_B\,|\Omega\rangle$. The net operator $\mathcal{G}_A\mathcal{G}_B$ has $N(N-1)/2$ terms. Suppose we truncate the sums on the right moving and left moving wave packets to act on the left and right halves of the space respectively. Then $\mathcal{G}_A\mathcal{G}_B$ now only has $N(N/2-1)/4$ terms. The inspiration for this will be explained next.

We provide a brief overview of the Givens Rotations method of fermionic wave packet preparation on quantum computers (for a full treatment, see [25]). Let $a_j = \exp\left(-|j-j_A|^2/\sigma^2\right)$ and $\beta_j = k_A j$. The method involves diagonalizing $|\psi\rangle$ in terms of fermionic operators:

$$V\hat{c}_1^\dagger V^\dagger = \sum_j a_j e^{-i\beta_j}\hat{c}_j^\dagger \tag{6}$$

by first canceling the phase $\exp(-i\beta_j)$ and then the coefficients a_j of each term. The phases are canceled by single qubit z-rotations:

$$V^\dagger(\beta) = \prod_j \mathrm{RZ}(\beta_j) = \exp\left(-\frac{i}{2}\sum_j \beta_j\hat{\sigma}_j^z\right). \tag{7}$$

The real coefficients are canceled by iteratively diagonalizing each row of $|\psi\rangle$ with the operators

$$V^\dagger(\theta_j) = \exp\left[i\frac{\theta_j}{2}\left(\hat{\sigma}_{j-1}^x\hat{\sigma}_j^y - \hat{\sigma}_{j-1}^y\hat{\sigma}_j^x\right)\right], \tag{8}$$

acting on nearest neighbors $(N-1, N)$, $(N-2, N-1)$, $\ldots, (1,2)$ (no boundary term), for $\theta_j = \arctan(-a_j/a_{j-1})$. Beginning at $(N, N-1)$, the coefficients "up" the vector a_{j-1} are updated after each $V^\dagger(\theta_j)$ is applied. The angles are determined classically by working in the subspace spanned by the N single particle states. The operator is efficiently decomposed in terms of two CNOT gates and x and z rotations (Figure 2 (c)). The wave packet creation operator is then

$$\mathcal{G}_A = V(\beta)V(\theta)\hat{\sigma}_1^- V^\dagger(\theta)V^\dagger(\beta), \tag{9}$$

for

$$V^\dagger(\theta) = V^\dagger(\theta_1)\ldots V^\dagger(\theta_{N-2})\,V^\dagger(\theta_{N-1})\,. \tag{10}$$

The circuit for two wave packets in an eight-site model is given in Figure 2 (a). Notice that the addition of the string of σ^z's makes the fermionic operator $\hat{c}_4^\dagger$. Compared to the original formulation for fermion-fermion scattering states, the circuit depth D is reduced to $D/2+1$. For an individual site, the CNOT depth is 4, but within the M-site subspace spanned by the wave packet, all $4(M-1)$ CNOT gates are applied in series. One will see that we still have an issue because the lowering operator σ^- cannot be directly implemented on a quantum computer. Simon et al [32] introduced the Ladder Operator Block Encoding (LOBE) method where a fermionic creation operator can be placed within a larger unitary by using a single external control qubit c and an ancilla qubit a. Suppose we apply σ^- to some qubit j whose in the state $|\psi_j\rangle = a|0\rangle + b|1\rangle$. The resultant state is $\sigma^-|\psi_j\rangle = a|1\rangle$. The operator in Figure 2 (c) removes the $Ub|1\rangle$ from the system into the external control, ancilla space, so the system only has the state $a|1\rangle$. Thus, we have a non-variational method to excite wave packets that obey the

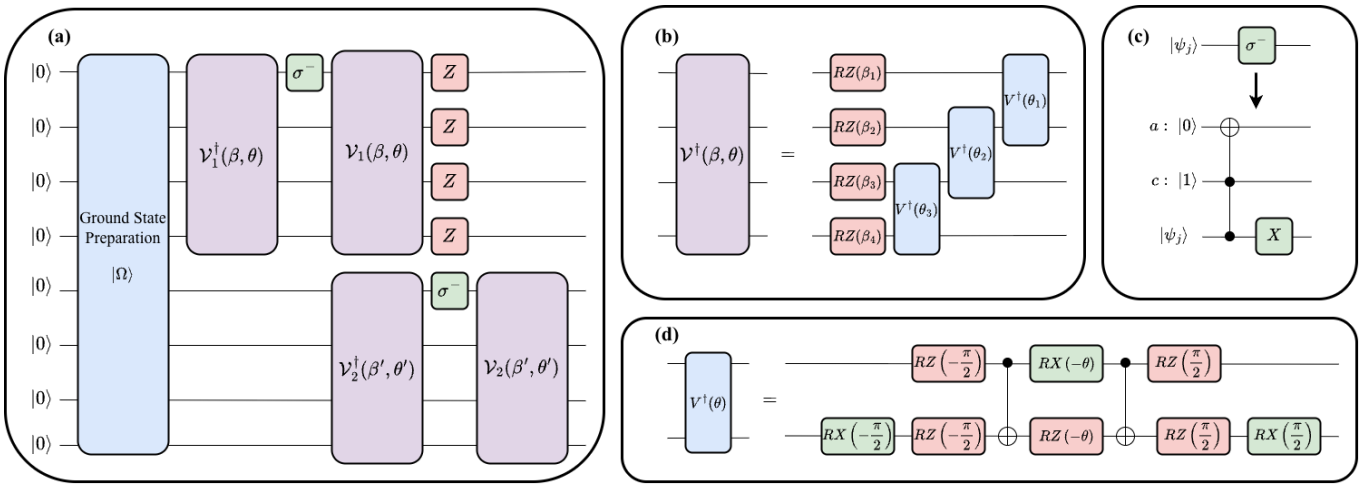

FIG. 2. (a) Truncated Givens rotation circuit to construct two Gaussian wave packets centered at sites 1 and 5 for an eight site model. (b) Decomposition of $\mathcal{V}^\dagger(\beta,\theta) = V^\dagger(\theta)V^\dagger(\beta)$ in terms one and two qubit gates. (c) Equivalent unitary operation for σ^- on qubit j using an external control qubit c and ancilla qubit a. (d) Minimal CNOT Decomposition of $V^\dagger(\theta)$.

fermionic anti-commutation relations, with the only approximation coming from VQE ground state preparation.

Results - We compare our quantum simulations with time evolved MPS states via Time Evolving Block Decimation (TEBD) [33] as well as using the density matrix renormalization group (DMRG) [34–36] method for ground state preparation. All MPS simulations are done with the ITensor library [37, 38], and the max bond dimension of the MPS will be set to 40. For $N = 8$, we use standard linear algebra techniques.

For quantum simulation, we use a VQE classical simulation with qiskit [39] to construct the ground state. Via an efficient-SU(2) ansatz and the Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer, we can generate ground states classically with a sub 10% error in energy.

N	Δt	$\langle N_j(t)\rangle$	$S(t)$
8	0.03	4.66%	3.64%
16	0.01	0.165%	0.139%
32	0.02	1.74×10^{-3}%	3.92×10^{-4}%
64	0.04	0.0224%	0.0230%

TABLE I. Average percent difference of the site occupation number and entanglement entropy between the full and truncated wave packets at criticality. For the occupation number, only occupations that were greater than 10^{-4} are considered. The period of evolution is similar to Figure **??**, just for a different Δt.

Conclusion -

- With minor adjustment to the original Givens Rotation method for fermionic scattering state preparation, we have provided useful method to generate narrow localized wave packets with respect to system size and initial separation for large volume scattering simulations.

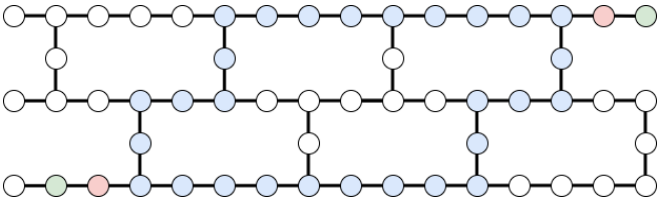

FIG. 3. Example qubit map on IBM's heavy hexagonal topology. The blue circles represent system qubits, the white non-system qubits, and the red and green as control ancilla and ancilla qubits respectively that are used to implement σ^-. In this case, the system size is 28.

- The adjustments are only having individual wave packet creation operators span only half of the space, and the inclusion of unitary particle creation operators via ancillary qubits.

- Unlike variational methods, the creation of the wave packets themselves are exact. We do still have to rely on variational methods to generate the ground state of the system.

- Readily implementable on transmon machines like IBM by reducing all operations to nearest neighbor interactions.

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Data Availability - The data that support the findings of this article are openly available [40].

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