Exploring the Hard-Core Bose-Hubbard Model through Exact Simulations

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Abstract

In this paper we present Qiskit simulations for a XY spin model, which through the Jordan-Wigner transform can be mapped to a 1D Hard-Core Bose-Hubbard model [VGR06] and many other toy models of physical systems depending on the tuning of interaction strengths. This is done through an analytic method that disentangles the XY model's Hamiltonian [FV09, CL18]. We discuss the results of this simulation [VGR06] and provide explicit circuits that were used in qiskit simulations. While a similar simulation was done previously [CL18], the circuit was smaller (4 qubits as opposed to 8) and did not explore different tuning parameters. Through these results, we better illustrate a general method first proposed by [FV09] for the exact simulation of integrable Hamiltonians that can be mapped through the Jordan-Wigner transformation. Finally, we discuss possible extensions to richer models.
Code @ github.com/nsong03/XYmodelQiskitSimulation

1 Introduction

The Bose-Hubbard model describes a system of interacting bosons on a lattice strucure. Within a simple Hamiltonian (below), it has been shown to contain the physics of a superfluid to Mott-insulator transition.

$$\hat{H}/\hbar = -t\sum_{\langle i,j\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i \tag{1}$$

Where $\langle i,j\rangle$ sums over nearest neighbors, $\hat{b}_i^\dagger, \hat{b}_i$ are the bosonic creation and annihilation operators, and $\hat{n}_i = \hat{b}_i^\dagger\hat{b}_i$ is the familiar number operator. Going term by term, the first refers to hopping amplitudes between neighboring sites with weight t, the second refers to the on-site energy penalty that is paid for multiple particles with weight U, and the third is the chemical potential μ which is usually ignored. The Hilbert space of this model scales as $(N_b + L - 1)!/N_b!(L-1)!$ where N_b is the number of bosonic particles and L is the number of lattice sites used in the model. It is well known that there is no analytic solution for the general Bose-Hubbard model - Like the TFI or Fermi-Hubbard model, we must make approximations such as mean field theory to solve their dynamics.

For this work, we will explore the Hard-Core regime [IH10]. That is, we will assume that a maximum of a single particle is allowed on a site. Formally, this means that $\hat{b}_i^\dagger\hat{b}_i^\dagger = \hat{b}_i\hat{b}_i = 0$, and $\{\hat{b}_i, \hat{b}_i^\dagger\} = 0$. Also, when acting on different sites $i \neq j$ the bosonic operators of course commute $[\hat{b}_i, \hat{b}_j] = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = [\hat{b}_i, \hat{b}_j^\dagger] = 0$. To give some variety to our Hamiltonian, we will also include an uniform external potential. So we write

$$\hat{H}/\hbar = -\sum_{i=1}^{L} t(\hat{c}_i^\dagger\hat{c}_{i+1} + \hat{c}_{i+1}^\dagger\hat{c}_i) + \lambda\hat{c}_i^\dagger\hat{c}_i \tag{2}$$

Where, considering the hard-core limit, we have written our bosonic operators instead as fermionic operators. In this regime we find that this Hard-Core model is actually contained within the XY model's Hamiltonian, which has already been explicitly solved. We will explore that model first.

2 The XY Model

The Hamiltonian used for the XY model in [FV09] was:

$$H_{XY} = \sum_{i=1}^{n}(\frac{1+\gamma}{2}\sigma_i^x\sigma_{i+1}^x + \frac{1-\gamma}{2}\sigma_i^y\sigma_{i+1}^y) + \lambda\sum_{i=1}^{n}\sigma_i^z + [\text{boundary terms}] \tag{3}$$

Where the boundary terms are included to correctly map periodic boundary conditions. Taking the Jordan-Wigner transform of this ($\hat{c}_i = (\prod_{m<i}\sigma_m^z)(\sigma_i^x - i\sigma_i^y)/2$) then gives us:

$$H_{XY}[JW] = \frac{1}{2}\sum_{i=1}^{n}((\hat{c}_{i+1}^\dagger\hat{c}_i + \hat{c}_i^\dagger\hat{c}_{i+1}) + \gamma(\hat{c}_i^\dagger\hat{c}_{i+1}^\dagger + \hat{c}_i\hat{c}_{i+1})) + \lambda\sum_{i=1}^{n}\hat{c}_i^\dagger\hat{c}_i \tag{4}$$

with periodic boundary conditions imposing $\hat{c}_{n+1} = \hat{c}_1$, and $\hat{c}_i$ being the fermionic annihilation operator. Conveniently, it turns out that this Jordan-Wigner transform directly maps the computational basis states to eigenstates of the XY Hamiltonian! This can be seen as:

$$|\psi\rangle = \sum_{i_1,i_2,...i_n=0,1}\psi_{i_1,i_2,...i_n}|i_1,i_2,...,i_n\rangle \rightarrow \sum_{i_1,i_2,...i_n=0,1}\psi_{i_1,i_2,...i_n}(\hat{c}_1^\dagger)^{i_1}(\hat{c}_2^\dagger)^{i_2}...(\hat{c}_n^\dagger)^{i_n}|\Omega_c\rangle \tag{5}$$

Where $|\Omega_c\rangle$ is the vacuum state, or simply all inputs of our circuit being $|0\rangle$. And so that transform is done for free - we just need to adjust the Hamiltonian intended to be written on the circuit to a fermionized one. We can also see that the XY model is exactly the 1D HCBH model when $\gamma = 0$.

2.1 Diagonalization

We now take a step back to sketch the method developed in [CL18, FV09] that explicitly encodes an XY Ising Hamiltonian into a circuit for exact simulation. Our goal, in general, is to find some unitary gate U_{dis} that will *disentangle* our Hamiltonian of interest so that:

$$H = U_{dis}\tilde{H}U_{dis}^\dagger, \qquad \text{where} \quad \tilde{H} = \sum_i \omega_i\sigma_i^z \tag{6}$$

$\tilde{H}$ does not necessarily have to be in terms of σ_i^z (Pauli-Z operator), but we can write it like this without loss of generality. We wish to find a circuit that implements U_{dis} efficiently, which would allow us to explore the time evolution of our system starting from **any** thermal state for long times. To see why this is the case, observe the time evolution operator.

$$e^{-itH} = e^{-itU_{dis}\tilde{H}U_{dis}^\dagger} = U_{dis}e^{-it\tilde{H}}U_{dis}^\dagger \tag{7}$$

We see that regardless of the time-evolution of the system, only a fixed number of single qubit gates would be needed as $\tilde{H}$ is diagonal. Thermal states ($e^{-\beta H}$) of any kind could also be prepared using the same scheme. So, how can this be done?

For analytically solvable spin systems, we can use some well-known transformations [EL61]. Namely, the Fourier Transform and Bogoliubov transformations.

$$\text{Defining} \quad U_{dis} = U_{FT}U_{Bog}, \quad H = U_{FT}U_{Bog}\tilde{H}U_{Bog}^\dagger U_{FT}^\dagger \tag{8}$$

To convince ourselves that this truly diagonalizes the Hamiltonian, we can work through it. Details are in the Appendix. Applying the Fourier transform to $H_{XY}[JW]$, we find:

$$H_{XY}[FT] = \sum_k[2(\lambda - \cos k)\hat{c}_k^\dagger\hat{c}_k + i\gamma\sin k(\hat{c}_{-k}\hat{c}_k + \hat{c}_{-k}^\dagger\hat{c}_k^\dagger) - \lambda] \tag{9}$$

Where $k = -\frac{n}{2}+1, ..., \frac{n}{2}$. We can then apply the Bogoliubov transform with $\hat{a}_k = \cos(\frac{\theta_k}{2})\hat{c}_k - i\sin(\frac{\theta_k}{2})\hat{c}_{-k}^\dagger$ and choose $\cos(\theta_k) = \frac{\lambda-\cos k}{\sqrt{(\lambda-\cos k)^2+\gamma^2\sin^2 k}}$. Making use of the commutation relations for fermionic operators, we then obtain:

$$H_{XY}[Bog] = \sum_k \omega_k\hat{a}_k^\dagger\hat{a}_k \tag{10}$$

where $\omega_k = \sqrt{(\lambda - \cos(\frac{2\pi k}{n}))^2 + \gamma^2 \sin^2(\frac{2\pi k}{n})}$. And so, with application of U_{FT}, U_{Bog}, we are able to obtain a single-qubit Hamiltonian that can be used for arbitrary thermal state preparation or time evolution simulation. We will show exactly how that can be done in the next subsection.

2.2 Circuitization

We first translate these U_{FT}, U_{Bog} operations into circuit form. Further justification for the exact choice of matrices and circuitization is found in [FV09]. Define the following two-qubit gates:

$$U_{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad F_k = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{\alpha(k)}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{\alpha(k)}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -\alpha(k) \end{bmatrix} \tag{11}$$

$$B_k = \begin{bmatrix} \cos\theta_k & 0 & 0 & i\sin\theta_k \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i\sin\theta_k & 0 & 0 & \cos\theta_k \end{bmatrix}, \quad \text{with} \quad \alpha(k) = e^{\frac{i2\pi k}{n}}. \tag{12}$$

The full circuit for U_{dis}, then, is:

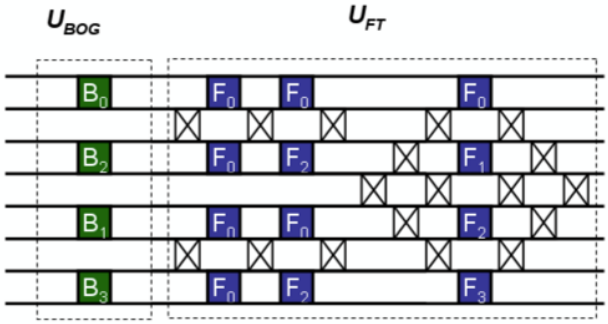


Figure 1: Circuit for the XY Hamiltonian with exact diagonalization on 8 sites, taken from [FV09]. The crosses are fermionic SWAP gates to account for anticommuting wavefunctions, while the Fourier transform (F) gates carry out a fast fourier transform on two subsets of qubits. The Bogoliubov transform is implemented in the (B) gates. Note that the full information of our XY model is stored solely in the θ_k of the Bogoliubov gates.

(A demonstration of how this circuit might be decomposed into rotation and CX gates is shown in the appendix.) And now we're done! This is exactly the circuit we need to run; There's no more to it. We input computational basis state qubits from the left side, and perform measurements on the right side. To see why this is so, consider our disentangling procedure once more. We know that

$$\tilde{H}|\psi_i\rangle = \epsilon_i|\psi_i\rangle \tag{13}$$

From the diagonalization. Which means that, from $H = U_{dis}\tilde{H}U_{dis}^\dagger$, we get $HU_{dis} = U_{dis}\tilde{H}$. So,

$$HU_{dis}|\psi_i\rangle = U_{dis}\tilde{H}|\psi_i\rangle = \epsilon_i U_{dis}|\psi_i\rangle \tag{14}$$

And so the application of U_{dis}, which is shown above, creates eigenvectors $|\phi_i\rangle = U_{dis}|\psi_i\rangle$ of our XY Hamiltonian with energies ϵ_i. What's more, we can input *any* state into this circuit, provided we give the right computational basis state of $\tilde{H}$ as an input. So we can plot the dynamics of a system that starts in an excited state, which is very difficult to do with non-exact circuit approaches.

3 Simulation Results

In the following simulations I'll focus only on the magnetization of our model, that is, $\langle \sigma_z \rangle$. We will obtain this from our simulation by running our circuit $N = 1024$ times, calculating the magnetization value of each shot, and averaging over the number of runs. We will also take advantage of the nature of our exact simulation by testing the impact of different starting energies. With 8 spins on our circuit, we can input anywhere from 0 excitations $\rightarrow \otimes^n|0\rangle$ to 8 excitations $\rightarrow \otimes^n|1\rangle$.

As a reference, for the Ising model where $\gamma = 1$, the analytic solution can be found as:

$$\langle \sigma_z \rangle = \frac{1 + 2\lambda^2 + \cos(4t\sqrt{1+\lambda^2})}{2 + 2\lambda^2} \tag{15}$$

3.1 Hard-Core Bose-Hubbard model: $\gamma = 0$

The simulation results for the Hard-Core model are as expected. To observe how the 1D Hard-Core Bose-Hubbard model works under a spin model, we can look at it's Hamiltonian:

$$H_{HCBH} = \sum_{i=1}^{n} \left(\frac{1}{2}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \lambda \sum_{i=1}^{n} \sigma_i^z + [\text{boundary terms}]\right) \tag{16}$$

And so it is indeed expected that there would be no change in the magnetization until we hit the critical value of $\lambda = 1$. At $\lambda = 1$ we observe an effective insulative spike in energy, which is expected for the Bose-Hubbard model!

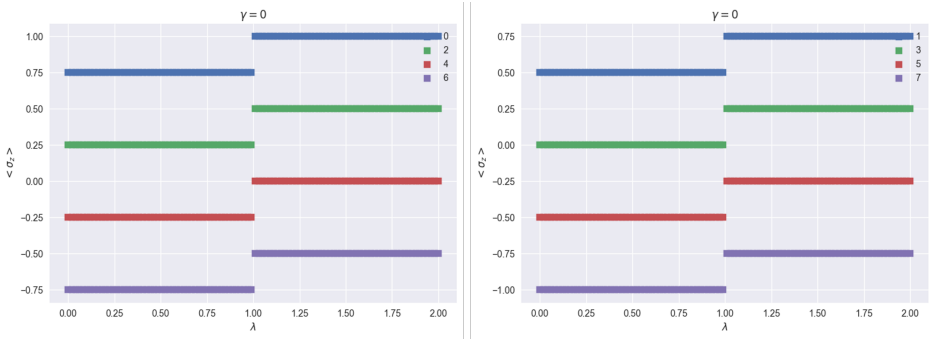


Figure 2: Expectation value of magnetization for the Hard-Core Bose-Hubbard model for different starting state excitations. Insulator behavior observed across all starting states, with different initial magnetization (energies).

3.2 Ising model: $\gamma = 1$

For the Ising model, we can now consider our Hamiltonian as:

$$H_{Ising} = \sum_{i=1}^{n} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^{n} \sigma_i^z + [\text{boundary terms}] \tag{17}$$

For this model, the jumps primarily come from the discretization of our circuit. The Ising model is known to have a smooth transition as we reach the critical point of $\lambda = 1$, but due to our circuit only having 8 qubits, the transition is discontinuous. Otherwise though, this behavior is also in-line with the analytic solution for the Ising model (Eq. 15).

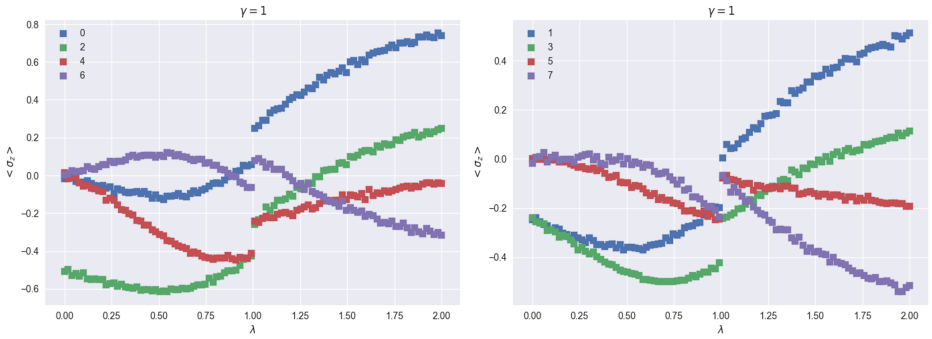
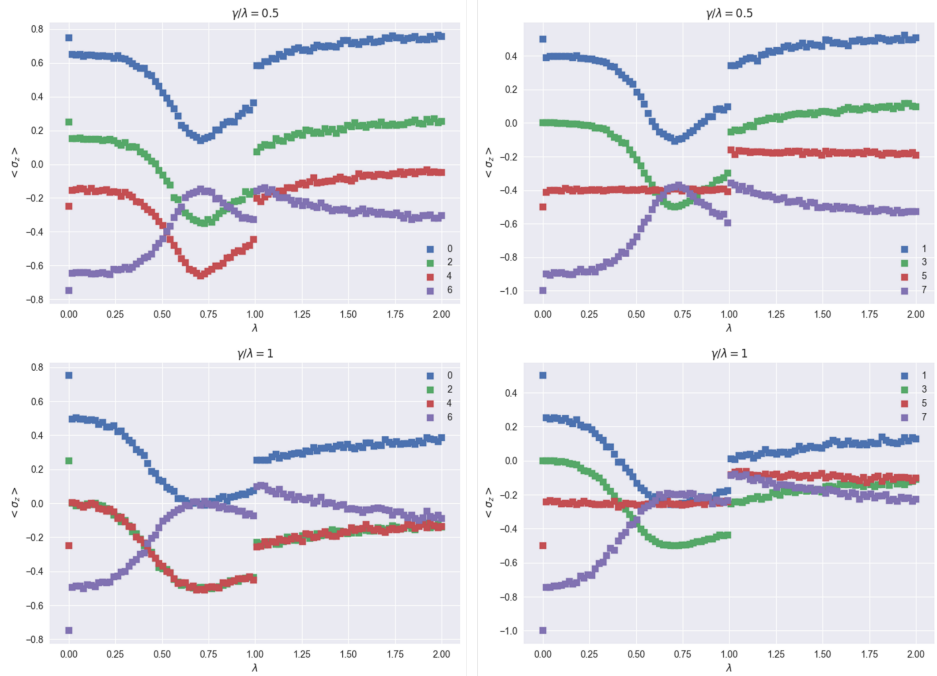


Figure 3: Expectation value of magnetization for Ising model regime for different starting state excitations.

3.3 Further Testing: $\gamma/\lambda = C$

The following models are not necessarily well-known physical models, except for the special case $\gamma/\lambda = 1$.



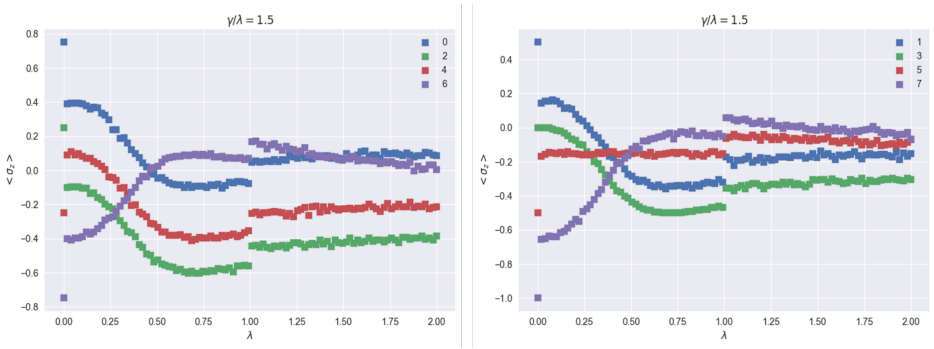


Figure 4: Expectation value of magnetization for different tunings of the Ising model, and different starting state excitations.

Some things we can observe with the relative tuning strengths: A larger ratio of γ/λ binds the spectrum of excitations more tightly together. This makes physical sense! The smaller the strength of our external field, the less effect individual spin excitations have on our energy spectrum. This is akin to Zeeman splitting observed in the presence of an external field in atomic physics - The gap between energy levels increases with the strength of an external magnetic field.

4 Conclusions

Neutral atoms have made great progress in quantum simulation of the Bose-Hubbard Hamiltonian [MG02, CSC18, LB20], mostly from Markus Greiner's work. With single atoms in optical tweezers, implementing bosonic statistics and arbitrary external / hopping potentials is relatively easy. The hopping potential can be set by atom-atom spacing and the external potential is set by a literal external field. While scaling beyond 1D and 2D is a challenge, synthetic dimensions [LB20] found in the energy level of atoms can help circumvent this obstacle. And yet, all of these demonstrations are direct physical simulations. There has yet to be a useful, digital circuit implementation of the Bose-Hubbard Hamiltonian. This is a problem from a quantum computing standpoint because such physical simulations cannot be error-corrected! There is no circuit process, simply a 'plug and play' approach that is unsuitable for extreme tuning regimes, excited dynamics, or long-time experiments. Developing near term algorithms to explore these dynamics is of key interest. While the method of exact simulation described in this paper is limited in scope to toy models that already have analytic solutions, the circuits produced allow for immediate testing on existing computation platforms. Exact simulations such as the ones highlighted in this paper can serve as useful benchmarks of NISQ devices, and provide justification for more exotic results.

5 Future Directions

Addressing the full Bose-Hubbard model, even in 1D or 2D, is very difficult. We cannot simply apply the above procedure to the full Bose-Hubbard model due to the bosonic nature of the system. When multiple particles are allowed on a single site the Jordan-Wigner transform fails, and it is no longer trivial to map the computational basis states to site occupation. Also, while exact diagonalizations of the Bose-Hubbard model can be computed [JZ10], circuitization of such a procedure is not clear. Apart from the standard techniques of Trotterization or an adiabatic approximation for Hamiltonian simulation, we suggest an alternative, imperfect scheme to further simulate the dynamics of the Bose-Hubbard model.

5.1 Soft-core Simulation

Instead of directly jumping to the generalized Bose-Hubbard model, we propose an extension of the scheme for the Hard-Core model by allowing a finite number of particles to exist on the same site. For convenience,

set the maximum allowable number of such particles as 2^p. The occupation number of each site could then be stored on p qubits. A similar sort of approach was suggested in [FV09] in the context of a 2D Kitaev Hamiltonian on a honeycomb lattice. Such a simulation would allow exploration of the full dynamics of the Bose-Hubbard model at non-negligible temperatures. Although the full extent of our tunings would be limited ($U >> J$ would need to be imposed to prevent large single site particle densities from accumulating), given the direct applicability for long-time simulations this might still be worthwhile.

Of course, there is no need to limit ourselves to the XY Hamiltonian or the Bose-Hubbard model for this venture. Other models that we attempted to explore but failed to coherently explore in time include the Dicke-Ising model [ECL17] and Fermi-Hubbard model [Ess10]. A particular approach used to obtain the polariton spectrum of the Dicke-Ising model might provide guidance for this 'soft-core' simulation. Given the Dicke-Ising Hamiltonian, the authros applied the Holstein-Primakoff transformation to map spins onto bosonic operators, which could then be reformulated into an exact diagonalisation.

5.2 Varying External Field Simulation

We could also add richness to this toy model by including a position-dependent external field. This is a typical case for neutral atom experiments, in which optical lattices are created using laser light. In this case, our Hard-Core Bose Hubbard model might look like the following.

$$\hat{H}/\hbar = -\sum_{i=1}^{L} t(\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i) + A\cos(\frac{2\pi i}{T})\hat{c}_i^\dagger \hat{c}_i \tag{18}$$

Where, considering the hard-core limit, we have written our bosonic operators instead as fermionic operators. Note that the periodic potential does not restrict our site placement such that atoms are on the nodes or antinodes of the lattice. Were that the case, our function would be $(-1)^i$ instead of $\cos(\frac{2\pi i}{T})$ [IH10]. Applying our standard technique of the Fourier Transform, we find that the Hamiltonian becomes (See Appendix):

$$H[FT]/\hbar = -2t\sum_k \cos k \hat{c}_k^\dagger \hat{c}_k - \frac{A}{2}\sum_k \hat{c}_{k+\frac{2\pi}{T}}^\dagger \hat{c}_k + \hat{c}_{k-\frac{2\pi}{T}}^\dagger \hat{c}_k \tag{19}$$

It is non-trivial to convert the second term into a diagonalizable form, but some transformation similar to Bogoliubov might suffice. Other improvements might include the presence of second-order hopping terms, or position-dependent hopping amplitudes [YZ23] that could better simulate systems with multiple species of atoms.

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6 Appendix

6.1 Derivation of Fourier Transform Terms

In applying the Fourier transform to prepare a Hamiltonian for diagnolization, it was difficult to find explicit derivations in [FV09, CL18]. As such, we provide one here. It seems that this is a standardized approach for finding analytic solutions to toy models which fails when including multiple particles on a single site (Bosonic particles). Let's calculate the transform for each term in the XY model, and the models proposed in the conclusion. This should cover most of the interesting interactions (nearest neighbor, on-site, etc.).

We will use the following equations:

$$\hat{c}_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj} \hat{c}_k, \quad e^{ikN} = 1, \quad k = \frac{2\pi n}{N}, \qquad \text{and} \quad \frac{1}{N} \sum_{j=1}^{N} e^{ij(k \mp k')} = \delta_{k,\pm k'} \tag{20}$$

Let's first start with the number operator (counting particles on a site) for a constant penalty λ.

$$\hat{H}_{11}/\hbar = \lambda \sum_j \hat{c}_j^\dagger \hat{c}_j \tag{21}$$

$$= \lambda \sum_j \frac{1}{N} (\sum_k e^{-ikj} \hat{c}_k^\dagger)(\sum_k e^{ikj} \hat{c}_k) = \frac{\lambda}{N} \sum_j \sum_{k,k'} e^{ij(k-k')} \hat{c}_{k'}^\dagger \hat{c}_k = \frac{\lambda}{N} \sum_{k,k'} N \delta_{k,k'} \hat{c}_{k'}^\dagger \hat{c}_k = \lambda \sum_k \hat{c}_k^\dagger \hat{c}_k \tag{22}$$

We can do the same for an external potential from, say, an optical lattice.

$$\hat{H}_{12}/\hbar = A \sum_j \cos(\frac{2\pi j}{T}) \hat{c}_j^\dagger \hat{c}_j \tag{23}$$

$$= \frac{A}{2} \sum_j (e^{i\frac{2\pi j}{T}} + e^{-i\frac{2\pi j}{T}}) \frac{1}{N} (\sum_k e^{-ikj} \hat{c}_k^\dagger)(\sum_k e^{ikj} \hat{c}_k) = \frac{A}{2} \sum_j \frac{1}{N} (e^{i\frac{2\pi j}{T}} + e^{-i\frac{2\pi j}{T}}) \sum_{k,k'} e^{ij(k-k')} \hat{c}_{k'}^\dagger \hat{c}_k \tag{24}$$

$$= \frac{A}{2} \frac{1}{N} \sum_j \sum_{k,k'} (e^{ij(k-k'+\frac{2\pi}{T})} + e^{ij(k-k'-\frac{2\pi}{T})}) \hat{c}_{k'}^\dagger \hat{c}_k = \frac{A}{2} \sum_{k,k'} (\delta_{k,k'-\frac{2\pi}{T}} + \delta_{k,k'+\frac{2\pi}{T}}) \hat{c}_{k'}^\dagger \hat{c}_k \tag{25}$$

$$= \frac{A}{2} \sum_k \hat{c}_{k+\frac{2\pi}{T}}^\dagger \hat{c}_k + \hat{c}_{k-\frac{2\pi}{T}}^\dagger \hat{c}_k \tag{26}$$

We can also do this for the hopping terms, weighted by t,

$$\hat{H}_2/\hbar = t \sum_j \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \tag{27}$$

$$= t\sum_j \frac{1}{N}[(\sum_k e^{-ikj}\hat{c}_k^\dagger)(\sum_k e^{ik(j+1)}\hat{c}_k) + (\sum_k e^{-ik(j+1)}\hat{c}_k^\dagger)(\sum_k e^{ikj}\hat{c}_k)] \tag{28}$$

$$= t\sum_j \frac{1}{N}(\sum_{k,k'} e^{-ik'j}e^{ik(j+1)}\hat{c}_{k'}^\dagger\hat{c}_k + \sum_{k,k'} e^{-ik'(j+1)}e^{ik}\hat{c}_{k'}^\dagger\hat{c}_k = t\sum_j \frac{1}{N}\sum_{k,k'}(e^{ij(k-k')+ik} + e^{ij(k-k')-ik'})\hat{c}_{k'}^\dagger\hat{c}_k \tag{29}$$

$$= t\sum_k \frac{1}{N}N2\cos k\hat{c}_k^\dagger\hat{c}_k = 2t\sum_k \cos k\hat{c}_k^\dagger\hat{c}_k \tag{30}$$

And the creation and annihilation of particles on neighboring sites weighted by γ.

$$\hat{H}_3/\hbar = \gamma\sum_j \hat{c}_{j+1}\hat{c}_j + \hat{c}_j^\dagger\hat{c}_{j+1}^\dagger \tag{31}$$

$$= \gamma\sum_j \frac{1}{N}[(\sum_k e^{ik(j+1)}\hat{c}_k)(\sum_k e^{ikj}\hat{c}_k) + (\sum_k e^{-ikj}\hat{c}_k^\dagger)(\sum_k e^{-ik(j+1)}\hat{c}_k^\dagger)] \tag{32}$$

$$= \gamma\sum_j \frac{1}{N}(\sum_{k,k'} e^{ij(k+k')+ik'}\hat{c}_{k'}\hat{c}_k + e^{ij(-k-k')-ik}\hat{c}_{k'}^\dagger\hat{c}_k^\dagger) = \gamma\sum_k \frac{1}{N}Ni\sin k(\hat{c}_{-k}\hat{c}_k + \hat{c}_{-k}^\dagger\hat{c}_k^\dagger) \tag{33}$$

$$= i\gamma\sum_k \sin k(\hat{c}_{-k}\hat{c}_k + \hat{c}_{-k}^\dagger\hat{c}_k^\dagger). \tag{34}$$

6.2 Limits of Exact Circuitization

Upon review, it has become clear that nearly all models that can be written under the Jordan-Wigner transform are similar in implementation. From [FV09], we see that the 1D XY spin chain's Hamiltonian can be written as:

$$\hat{H}/\hbar = -\sum_j [(\hat{c}_{j+1}^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_{j+1}) + \gamma(\hat{c}_{j+1}\hat{c}_j + \hat{c}_j^\dagger\hat{c}_{j+1}^\dagger) - 2\lambda\hat{c}_j^\dagger\hat{c}_j + \lambda] \tag{35}$$

To which we apply U_{FT} and U_{Bog} to obtain our desired circuit. We can add or subtract terms to this model, but we run into the core problem: The JW transform is only valid as a mapping from spin operators to spinless fermions to hard core bosons. And so while it provides a valuable resource for the circuitization of most spin models, bosonic statistics are prohibited almost completely. The Bogoliubov transform is quite limited - It does not directly allow for the incorporation of, say, non-uniform external potentials. It only allows for special fermionic terms, such as $\hat{c}_{j+1}^\dagger\hat{c}_j$ and h.c., $\hat{c}_{j+1}\hat{c}_j$ and h.c., $\hat{c}_j^\dagger\hat{c}_{j+1}^\dagger$ and h.c. to be diagonalized.

6.3 Sample circuit for XY model simulation with 8 qubits

Figure 5: Sample circuit decomposition for a set θ_k of the 8-qubit XY model using controlled-X gates and single qubit rotations.