The Bose-Hubbard Model and Machine Learning

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I. INTRODUCTION

II. METHODS

A. Bose-Hubbard Calculations

1. 2^{nd} *Quantization Von Nuemann Entanglement Entropy Calculation*

To get a better initial feeling for this calculation, begin with the simpler case: 2^{nd} quantization or spatial entanglement. The basis for 2^{nd} quantization is as follows:

$$|20\rangle, |11\rangle, |02\rangle. \tag{1}$$

The full Hamiltonian for the Bose-Hubbard system is

$$\hat{H} = -J\sum_i b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i + \frac{U}{2}\sum_i n_i(n_i-1) - \mu\sum_i n_i, \tag{2}$$

where J is the hopping term, U is the potential energy, and μ is the chemical potential. $b^\dagger$ and b are the creation and annhilation operators, respectively. They act as follows:

$$b^\dagger|n\rangle = \sqrt{n+1}\ \ |n+1\rangle \tag{3}$$

$$b|n\rangle = \sqrt{n}\ \ |n-1\rangle. \tag{4}$$

The full Hamiltonian can be calculated by calculating the kinetic and potential pieces separately, then simply adding them together. Start by calculating the kinetic energy piece of the full matrix Hamiltonian. The kinetic energy part of the full hamiltonian above for the 2 particle, 2 site system is

$$\hat{H}_{KE} = -J(b_1^\dagger b_2 + b_2^\dagger b_1). \tag{5}$$

The matrix elements of the kinetic energy part of the Hamiltonian are calculated as follows:

$$\begin{aligned}
\langle 20|H_{KE}|20\rangle &= 0\\
\langle 11|H_{KE}|20\rangle &= -\sqrt{2}J\\
\langle 02|H_{KE}|20\rangle &= 0\\
\langle 20|H_{KE}|11\rangle &= -\sqrt{2}J\\
\langle 11|H_{KE}|11\rangle &= 0\\
\langle 02|H_{KE}|11\rangle &= -\sqrt{2}J\\
\langle 20|H_{KE}|02\rangle &= 0\\
\langle 11|H_{KE}|02\rangle &= -\sqrt{2}J\\
\langle 02|H_{KE}|02\rangle &= 0.
\end{aligned}$$

From these matrix elements, the full kinetic energy piece of the Hamiltonian is written as:

$$\hat{H}_{KE} = \begin{pmatrix} 0 & -\sqrt{2} & 0\\ -\sqrt{2} & 0 & -\sqrt{2}\\ 0 & -\sqrt{2} & 0 \end{pmatrix}. \tag{6}$$

Next, the potential part of the hamiltonian can be calculated as follows:

$$\hat{H}_P = \frac{U}{2}\sum_i n_i(n_i - 1) = \frac{U}{2}[n_1(n_1 - 1) + n_2(n_2 - 1)], \tag{7}$$

where $n_i = b_i^\dagger b_i$. The elements of the potential part of the Hamiltonian matrix are:

$$\begin{aligned}
\langle 20|H_P|20\rangle &= U \\
\langle 11|H_P|20\rangle &= 0 \\
\langle 02|H_P|20\rangle &= 0 \\
\langle 20|H_P|11\rangle &= 0 \\
\langle 11|H_P|11\rangle &= 0 \\
\langle 02|H_P|11\rangle &= 0 \\
\langle 20|H_P|02\rangle &= 0 \\
\langle 11|H_P|02\rangle &= 0 \\
\langle 02|H_P|02\rangle &= U.
\end{aligned}$$

From these matrix elements, the full potential energy part of the Hamiltonian is written as:

$$\hat{H}_P = \begin{pmatrix} U & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & U \end{pmatrix}. \tag{8}$$

The separate kinetic and potential energy pieces of the matrix Hamiltonian can be combined together to make the full matrix as follows:

$$\hat{H} = \begin{pmatrix} U & -\sqrt{2} & 0 \\ -\sqrt{2} & 0 & -\sqrt{2} \\ 0 & -\sqrt{2} & U \end{pmatrix}. \tag{9}$$

Now that we have the full matrix Hamiltonian, we can find the energy states of the system by solving the Schrodinger equation. The general form of the Schrodinger equation is

$$\hat{H}|\psi\rangle = E|\psi\rangle. \tag{10}$$

This equation can then be manipulated to look like the following equation:

$$\left(\hat{H} - E\hat{I}\right)|\psi\rangle = 0. \tag{11}$$

Since we're not interested in the solution where $|\psi\rangle = 0$, then $\hat{H} - E\hat{I}$ must be zero. This yields the following characteristic equation:

$$\hat{H} - E\hat{I} = 0. \tag{12}$$

This characteristic equation can be solved via expanding the matrix minors and solving the resulting polynomial, where

$$-E^2 + 2UE^2 + 4J^2E - U^2E - 4J^2U = 0. \tag{13}$$

Solving this equation yields

$$\begin{aligned}
E_1 &= U \\
E_2 &= \frac{1}{2}\left(U - \sqrt{16J^2 + U^2}\right) \\
E_3 &= \frac{1}{2}\left(U + \sqrt{16J^2 + U^2}\right).
\end{aligned}$$

These are the eigenvalues for the Hamiltonian calculated earlier. Looking at the three energies listed above, it is obvious that E_2 is the ground state energy since it is the lowest of the three. Before the entanglement entropy can

be calculated, the density matrix and reduced density matrix must be found. The full density matrix is defined as $\rho = |\psi\rangle\langle\psi|$. The calculation is as follows:

$$\hat{\rho} = (\alpha|20\rangle + \beta|11\rangle + \gamma|02\rangle)\,(\alpha^*\langle 20| + \beta^*\langle 11| + \gamma^*\langle 02|)\,. \tag{14}$$

Putting our result in matrix notation yields the following:

$$\hat{\rho} = \begin{bmatrix} \alpha\alpha^* & \alpha\beta^* & \alpha\gamma^* \\ \beta\alpha^* & \beta\beta^* & \beta\gamma^* \\ \gamma\alpha^* & \gamma\beta^* & \gamma\gamma^* \end{bmatrix}. \tag{15}$$

The reduced density matrix is calculated as follows:

$$\hat{\rho}_A = \sum_{n=0}^{2} {}_B\langle n|\psi\rangle\langle\psi|n\rangle_B = {}_B\langle 0|\psi\rangle\langle\psi|0\rangle_B + {}_B\langle 1|\psi\rangle\langle\psi|1\rangle_B + {}_B\langle 2|\psi\rangle\langle\psi|2\rangle_B \tag{16}$$

$$\hat{\rho}_A = |\alpha|^2{}_A|2\rangle\langle 2|_A + |\beta|^2{}_A|1\rangle\langle 1|_A + |\gamma|^2{}_A|0\rangle\langle 0|_A. \tag{17}$$

These elements written in matrix notation are as follows:

$$\hat{\rho}_A = \begin{bmatrix} |\alpha|^2 & 0 & 0 \\ 0 & |\beta|^2 & 0 \\ 0 & 0 & |\gamma|^2 \end{bmatrix} \tag{18}$$

Now, we want to calculate the ground state eigenvector. This can be done by plugging our ground state eigenvalue into equation [10] and solving the resulting augmented matrix. This matrix is as follows:

$$\begin{bmatrix} U - \frac{1}{2}\left(U - \sqrt{16J^2 + U^2}\right) & -\sqrt{2}J & 0 \\ -\sqrt{2}J & -\frac{1}{2}\left(U - \sqrt{16J^2 + U^2}\right) & -\sqrt{2}J \\ 0 & -\sqrt{2}J & U - \frac{1}{2}\left(U - \sqrt{16J^2 + U^2}\right) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = 0. \tag{19}$$

Solving the above equation provides the solutions for α, β, & γ, which are as follows:

$$\alpha = \frac{2}{\sqrt{U'^2 + U'\sqrt{U' + 16} + 16}} = \gamma$$

$$\beta = \frac{U' + \sqrt{U' + 16}}{\sqrt{2}\sqrt{U'^2 + U'\sqrt{U' + 16} + 16}},$$

where U' is defined as $U' = \frac{U}{J}$ for simplicity. Finally, the spatial entanglement entropy is calculated as follows:

$$S_1 = -Tr\left(\rho_A \ln \rho_A\right) = -Tr \begin{bmatrix} |\alpha|^2 \ln|\alpha|^2 & 0 & 0 \\ 0 & |\beta|^2 \ln|\beta|^2 & 0 \\ 0 & 0 & |\gamma|^2 \ln|\gamma|^2 \end{bmatrix} \tag{20}$$

$$S_1 = -\left[|\alpha|^2 \ln|\alpha|^2 + |\beta|^2 \ln|\beta|^2 + |\gamma|^2 \ln|\gamma|^2\right] \tag{21}$$

2. 1^{st} *Quantization Von Nuemann Entanglement Entropy Calculation*

Now, we want to run through the same process with 1^{st} quantization to obtain the particle entanglement. The basis for 1^{st} quantization is as follows:

$$|1_1 2_1\rangle, |1_1 2_2\rangle, |1_2 2_1\rangle, |1_2 2_2\rangle. \tag{22}$$

We begin by calculating the full Hamiltonian, which behaves the same way for 1^{st} quantization as it did for 2^{nd} quantization:

$$\hat{H} = \begin{bmatrix} \langle 1_1 2_1|\hat{H}|1_1 2_1\rangle & \langle 1_1 2_1|\hat{H}|1_1 2_2\rangle & \langle 1_1 2_1|\hat{H}|1_2 2_1\rangle & \langle 1_1 2_1|\hat{H}|1_2 2_2\rangle \\ \langle 1_1 2_2|\hat{H}|1_1 2_1\rangle & \langle 1_1 2_2|\hat{H}|1_1 2_2\rangle & \langle 1_1 2_2|\hat{H}|1_2 2_1\rangle & \langle 1_1 2_2|\hat{H}|1_2 2_2\rangle \\ \langle 1_2 2_1|\hat{H}|1_1 2_1\rangle & \langle 1_2 2_1|\hat{H}|1_1 2_2\rangle & \langle 1_2 2_1|\hat{H}|1_2 2_1\rangle & \langle 1_2 2_1|\hat{H}|1_2 2_2\rangle \\ \langle 1_2 2_2|\hat{H}|1_1 2_1\rangle & \langle 1_2 2_2|\hat{H}|1_1 2_2\rangle & \langle 1_2 2_2|\hat{H}|1_2 2_1\rangle & \langle 1_2 2_2|\hat{H}|1_2 2_2\rangle \end{bmatrix} \tag{23}$$

$$\hat{H} = \begin{bmatrix} U & -\sqrt{2} & -\sqrt{2} & 0 \\ -\sqrt{2} & 0 & 0 & -\sqrt{2} \\ -\sqrt{2} & 0 & 0 & -\sqrt{2} \\ 0 & -\sqrt{2} & -\sqrt{2} & U \end{bmatrix}. \tag{24}$$

The full density matrix is then given by $|\psi\rangle\langle\psi|$, where ψ, the ground state, is given by:

$$\psi = \alpha|1_1 2_1\rangle + \frac{\beta}{\sqrt{2}}\left(|1_1 2_2\rangle + |1_2 2_1\rangle\right) + \gamma|1_2 2_2\rangle.$$

$$\hat{\rho} = \begin{bmatrix} |\alpha|^2 & \frac{\alpha\beta^*}{\sqrt{2}} & \frac{\alpha\beta^*}{\sqrt{2}} & \alpha\gamma^* \\ \frac{\beta\alpha^*}{\sqrt{2}} & \frac{|\beta|^2}{2} & \frac{|\beta|^2}{2} & \frac{\beta\gamma^*}{\sqrt{2}} \\ \frac{\beta\alpha^*}{\sqrt{2}} & \frac{|\beta|^2}{2} & \frac{|\beta|^2}{2} & \frac{\beta\gamma^*}{\sqrt{2}} \\ \gamma\alpha^* & \frac{\gamma\beta^*}{\sqrt{2}} & \frac{\gamma\beta^*}{\sqrt{2}} & |\gamma|^2 \end{bmatrix}. \tag{25}$$

We then needed to calculate the reduced density matrix, which is given by tracing out the degrees of freedom of the second particle. The reduced density matrix is as follows:

$$\hat{\rho}_A = \sum_{n=1}^{2} {}_B\langle n|\psi\rangle\langle\psi|n\rangle_B = {}_B\langle 2_1|\psi\rangle\langle\psi|2_1\rangle_B + {}_B\langle 2_2|\psi\rangle\langle\psi|2_2\rangle_B \tag{26}$$

$$\begin{aligned}\hat{\rho}_A = &\left(|\alpha|^2 + \frac{|\beta|^2}{2}\right) {}_A|1_1\rangle\langle 1_1|_A + \left(\frac{\alpha\beta^* + \beta\gamma^*}{\sqrt{2}}\right) {}_A|1_1\rangle\langle 1_2|_A \\ &+ \left(\frac{\beta\alpha^* + \gamma\beta^*}{\sqrt{2}}\right) {}_A|1_2\rangle\langle 1_1| + \left(\frac{|\beta|^2}{2} + |\gamma|^2\right) {}_A|1_2\rangle\langle 1_2|_A.\end{aligned}$$

$$\hat{\rho}_A = \begin{bmatrix} {}_A\langle 1_1|\hat{\rho_A}|1_1\rangle & {}_A\langle 1_1|\hat{\rho_A}|1_2\rangle \\ {}_A\langle 1_2|\hat{\rho_A}|1_1\rangle & {}_A\langle 1_2|\hat{\rho_A}|1_2\rangle \end{bmatrix} = \begin{bmatrix} |\alpha|^2 + \frac{|\beta|^2}{2} & \frac{\alpha\beta^* + \beta\gamma^*}{\sqrt{2}} \\ \frac{\beta\alpha^* + \gamma\beta^*}{\sqrt{2}} & \frac{|\beta|^2}{2} + |\gamma|^2 \end{bmatrix} \hat{\rho}_A = \begin{bmatrix} \frac{1}{2} & \sqrt{2}\alpha\beta \\ \sqrt{2}\alpha\beta & \frac{1}{2} \end{bmatrix}. \tag{27}$$

To get the Von Nuemann entanglement entropy, the eigenvalues of the above matrix are needed. To obtain these eigenvalues, the following equation must be solved:

$$\hat{\rho}_A - \lambda\hat{I} = 0. \tag{28}$$

In matrix form, this becomes:

$$\begin{bmatrix} \frac{1}{2} - \lambda & \sqrt{2}\alpha\beta \\ \sqrt{2}\alpha\beta & \frac{1}{2} - \lambda \end{bmatrix} = 0. \tag{29}$$

Taking the determinant of this equation yields the characteristic equation:

$$\frac{1}{4} - \lambda + \lambda^2 - 2\alpha^2\beta^2 = 0 \tag{30}$$

$$\lambda^2 - \lambda - 2\alpha^2\left(1 - 2\alpha^2\right) + \frac{1}{4} = 0 \tag{31}$$

$$\lambda^2 - \lambda - 2\alpha^2 + 4\alpha^4 + \frac{1}{4} = 0. \tag{32}$$

The eigenvalues can then be solved for using the quadractic equation:

$$\lambda_\pm = \frac{1 \pm \sqrt{1^2 - 4\left(1\right)\left(-2\alpha^2 + 4\alpha^4 + \frac{1}{4}\right)}}{2} = \frac{1 \pm 2\alpha\sqrt{2 - 4\alpha^2}}{2}. \tag{33}$$

The Von Nuemann entanglement entropy is then calculated as follows:

$$S_1 = -Tr\left(\rho_A \ln \rho_A\right) = -Tr\begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix}\begin{bmatrix} \ln\lambda_+ & 0 \\ 0 & \ln\lambda_- \end{bmatrix} \tag{34}$$

$$S_1 = -\lambda_+ \ln\lambda_+ - \lambda_- \ln\lambda_-. \tag{35}$$

III. DISCUSSION

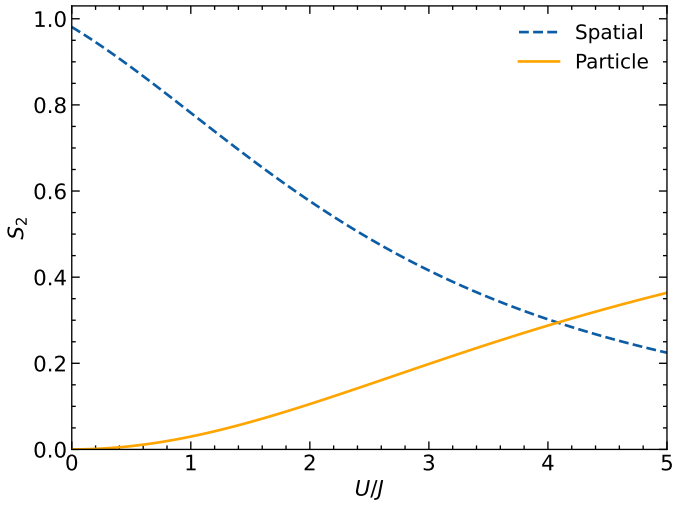

FIG. 1. The figure above is a graph of the Renyi entanglement entropy for both spatial and particle bipartitions versus the ratio of the interaction term to the hopping term.

A. PIGSFLI Algorithm

A Monte Carlo simulation is a stochastic (random) method of integration, which allows for accurate estimations of desired values. Monte Carlo is necessary for situations where exact calculations are too computationally expensive, such as in the exact diagonalization of the reduced density matrix for high particle/site number Bose Hubbard systems. The size of the Hilbert space is calculated by Eq. (36) and shown by Fig. 2:

$$D = \frac{(N+L-1)!}{(N)!\,(L-1)!} \tag{36}$$

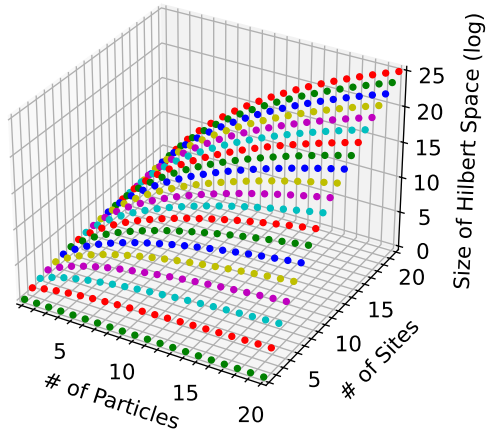

FIG. 2. The figure above shows the size of the Hilbert space as a function of number of sites and particles. This 3-dimensional plot for the number of combinations in the Hilbert space goes up to 20 sites and 20 particles.

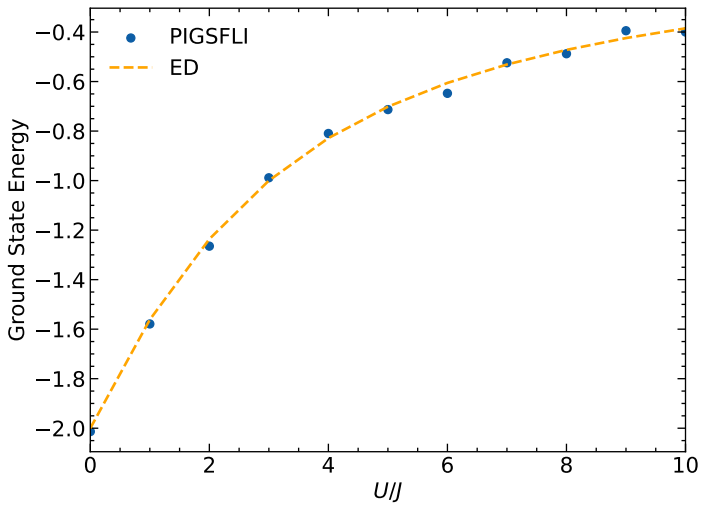

FIG. 3. A plot of the ground state energy versus the ratio between U, the potential term, and J, the hopping term for both exact diagonalization and PIGSFLI algorithm. From this plot, the PIGSFLI reults match very well to our ED calculation.

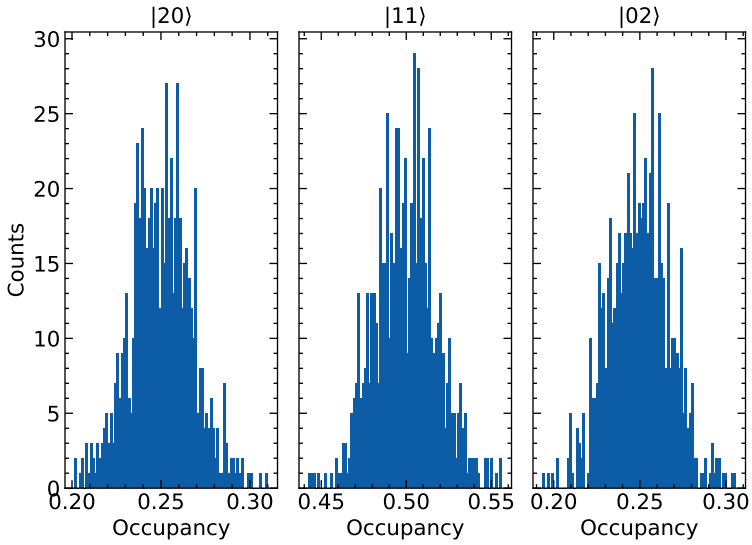

FIG. 4. The figure above shows the histogram of the occupation number for the particle bipartition as a function of the ratio of the interaction term to the hopping term. This graph specifically shows the case where the interaction term is 10 times the hopping term.

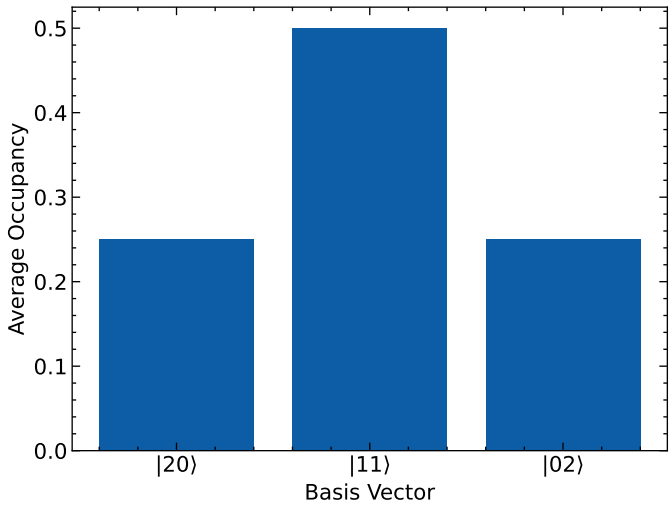

FIG. 5. The figure above shows the average occupation number for the spatial bipartition as a function of the ratio of the interaction term to the hopping term. This graph specifically shows the case where the interaction term is 10 times the hopping term.

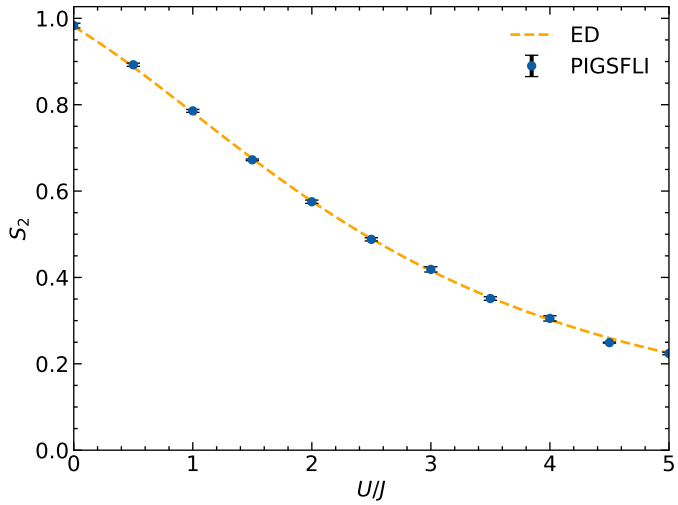

FIG. 6. The second Rényi spatial entanglement entropy as a function of U/J for both exact diagonalization (ED) and PIGSFLI. This plot shows excellent agreement between the PIGSFLI estimation and that of our ED calculation, showing that PIGSFLI is a viable option for computation on much larger system sizes.