Mode Entanglement in the Lieb-Liniger Model

Daniel G. Allman

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Abstract

Experiments and simulations in confined liquid helium-4 (He-4) systems have shown quasi-one-dimensional behavior consistent with quantum phases of 1D bosons [1]. In these experiments, confined He-4 becomes strongly correlated, and can be described by the linear quantum hydrodynamics known as Luttinger liquid theory, which also predicts a novel state of matter in 1D. Furthermore, 1D systems at near-zero temperature are highly entangled, and can offer insight into the use of entanglement as a resource for quantum information processing applications. In this research, I study 1D bosons with short-ranged interactions, described by the Lieb-Liniger model, by exactly diagonalizing the Hamiltonian to calculate physically important quantities, including the entanglement entropy that are inaccessible by any other means.
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1 Introduction

Entanglement is a purely quantum mechanical phenomenon in which non-classical information is shared between particles in a quantum state. The outcomes of measurements on entangled quantum states are not independent: the outcome of a measurement on one subsystem can influence the outcome of another instantaneously, in apparent violation of the laws of special relativity (no information can be transmitted faster than the speed of light). The idea of entanglement was debated heatedly by Einstein and his collaborators until John Bell, in 1964, proved that quantum mechanics is a non-local theory that allowed for entanglement [2]. Recently, Bose-Einstein condensates (BECs) have become a topic of great interest, in part because of their non-classical nature and intrinsically high levels of entanglement. Spatial entanglement (i.e. entanglement between different regions of space) has been studied in BECs, and these analyses indicate substantial entanglement, even without interactions [3]. In confined physical systems, there has been research concerning the novel state of matter known as a Luttinger liquid. Numerical methods, such as path integral Monte Carlo (PIMC), have been employed to study correlation functions that describe the long-range correlations in confined liquid He-4 systems [1]. Since 1-D systems display more quantum behavior than typical 3-D systems (due to stronger quantum and thermal fluctuations), they are good candidates for highly entangled systems. Thus, research into Luttinger liquids is another very important field of research, as they should be highly entangled, and are amenable to various mathematical methods. The Lieb-Liniger model is a useful many-body model because it has an exact solution, known as a Bethe ansatz solution [4, 5]. With it, one can calculate, but is quite limited to, the exact energies and wavefunctions. However, the Bethe ansatz is a useful benchmark for methods, since it provides a way to compare energies.

It is important for theoretical developments to be paralleled by experimental observations on such developments. Recently, experimental setups of trapped 1-D systems have attracted much interest. For instance, physicists have been seeking experimental realization of a Tonks-Giradeau (TG) gas, a special case of the low-density Lieb-Liniger gas where the repulsion becomes infinite [6, 7]. The TG gas displays many interesting properties, such as a pseudo-fermionic repulsion due to the infinite repulsive potential, similar to how fermions cannot occupy the same location in space, due to the Pauli exclusion principle. The TG regime has recently been experimentally accessed in interacting ultracold Rubidium atoms in optical lattices made using orthogonal standing waves. Implementing a shallow lattice potential, the effective masses of the atoms increase, and the interactions approach the TG limit [8]. Furthermore, theoretical criteria have been placed on experimentally creating a TG gas in cigar-shaped 1-D traps. These criteria are represented by a set of hydrostatic equations in trapped, delta-function interacting bosons [9].

Entanglement is also a necessary resource for quantum computation. In order to create a functioning quantum computer, one must generate and be able to manipulate persistent and robust entangled states. A highly entangled quantum computer
will be able to perform vast numbers of calculations simultaneously, and provide an exponential speed up over classical algorithms [10]. Thus, it is important, for the future of computing, and the transition to post-silicon technologies, to study these highly entangled systems. The Lieb-Liniger model has been studied previously using the techniques of path-integral Monte Carlo and the Bethe ansatz, but there has been little work via exact diagonalization. There are great benefits to using exact diagonalization: we can calculate quantities inaccessible to the previously mentioned techniques, including, von Neumann and Rnyi entropies under a momentum bipartition, and excited quantum states in the Lieb-Liniger model. Furthermore, exact diagonalization allows for momentum entanglement to be studied, as opposed to spatial or particle partitioned entanglement, thus offering a different perspective on this phenomenon. Unfortunately, exact diagonalization is unable to handle larger systems of particles, where huge amounts of memory are required. This is certainly a drawback, but we can still gain invaluable insight into smaller systems and calculate interesting quantities using this numerical method.

2 Background

Entanglement is one of the more shocking and unintuitive phenomena to emerge from theory of quantum mechanics, so to motivate the theory behind entanglement, I will start with a simple example: Suppose we have two ordinary coins. The outcomes of a single coin flip are simply heads or tails, with 50% probability for each. If we were to throw both coins at the same time and measure their joint outcomes, we’d find that, 25% of the time we’d measure two heads, 25% two tails, 25% heads-tails, and 25% tail-heads. In fact, we could have just predicted the joint outcomes from the individual outcomes themselves. Thus, we acquire every bit of information from the individual components: No information is gained by looking at the joint outcomes. Now, instead of classical coins, suppose we redo the experiment on two quantum spins. In particular, suppose we perform spin measurements on a pair of particles (A and B) in a Bell state, described by the ket

\[ |\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow⟩ + |\downarrow\uparrow⟩). \]  

(1)

If we measure the spin of particle A alone, we would measure up 50% of the time and down 50% of the time. The same is true for measurements on particle B alone. However, if we measure both spins simultaneously, we’d never find both spins aligned with each other. Instead, we’d find that, 50% of the time we’d measure up-down, and 50% of the time we’d measure down-up. This quantum mechanical phenomenon cannot be explained classically, and this example demonstrates the notion of “hidden information” contained in quantum states. We can only acquire part of the total information from measurements on individual particles. The other part is contained in the composite system itself. In other words, we cannot piece together the joint outcomes from the individual outcomes like we could in the case of two classical coins.

This simple example demonstrates that measurements on bipartite, entangled quantum systems are not independent. A
bipartite quantum system is one that has been divided into two subsystems, i.e. A and B. This division may be spatial (i.e. two subregions in space), particle-based, (i.e. sites on a lattice), momentum based, etc. Each subsystem also has an associated Hilbert space, i.e. \( \mathcal{H}_A \) and \( \mathcal{H}_B \) for subsystems A and B, respectively. The tensor product of the two Hilbert spaces \( \mathcal{H}_A \otimes \mathcal{H}_B \) forms the Hilbert space for the combined system, \( \mathcal{H} \). Furthermore, if A and B have bases \( \{ |i\rangle_A \} \) and \( \{ |j\rangle_B \} \) respectively, then the set \( \{ |i\rangle_A \otimes |j\rangle_B \} \) forms a basis for the combined Hilbert space. In an entangled bipartitioned quantum state, there is no way of associating a pure state to one of the subsystems. However, for a given pure quantum state \( |\Psi\rangle \), we can associate a density matrix \( \rho = |\Psi\rangle\langle\Psi| \). Then, by tracing over the complementary subsystem B, say, one obtains the reduced density matrix, \( \rho_A \), describing subsystem A.

\[
\rho_A = \text{tr}_B(\rho) = \sum_j (|j\rangle_B \rho \langle j\rangle_B )
\]

(2)

By ‘tracing out’ the complementary subsystem, the reduced density matrix refers only to subsystem A. Furthermore, the diagonal elements of the reduced density matrix are probabilities, and for an entangled state, the reduced density matrix describes a statistical ensemble of states. By direct analogy to classical information theory, the von Neumann entropy is defined as

\[
S_{VN} = -\text{tr}(\rho_A \log \rho_A)
\]

(3)

which effectively quantifies the entanglement between the two subsystems.

An entangled bipartitioned quantum state is one that cannot be written as a simple tensor product of two states in each subsystem. A product state has the form

\[
|\Psi\rangle_{\text{product}} = |\chi\rangle_A \otimes |\phi\rangle_B
\]

(4)

Here, \( |\chi\rangle_A \) and \( |\phi\rangle_B \) are any states in subsystems A and B respectively. At first glance, a state may seem entangled, i.e. not look like a product state, but an orthogonal transformation to a new basis will show that it is indeed a product state. Take for example the state

\[
|\chi\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle)
\]

(5)

where \( |\uparrow\downarrow\rangle \), say, is shorthand for \( |\uparrow\rangle_A \otimes |\downarrow\rangle_B \). While this state may seem superficially very similar to the Bell state described above, it is in fact an unentangled product state. To see this, consider reexpressing the \( |\uparrow\rangle \) and \( |\downarrow\rangle \) states in terms of the eigenstates of \( \sigma_x \). Diagonalizing \( \sigma_x \) yields \( |\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \) and \( |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle) \) as its eigenstates. Furthermore, computing \( |\rightarrow\rangle \otimes |\rightarrow\rangle \) yields the state described above in Eq. (5), and so (5) is indeed a product state.

It is nearly impossible to tell from simply looking at a state whether it is entangled or not. That information, however, is encoded in the reduced density matrix. The reduced density matrix of an unentangled state may be a mixed ensemble in
a some basis, but a pure state in another, as can be seen by diagonalization of the reduced density matrix. A pure state’s reduced density matrix is characterized in its diagonal form by a single 1 at any position along the diagonal, while the rest are 0.

3 Theory

The Lieb-Liniger model describes a 1-D system of bosons interacting via a delta function potential. In this research, we look at the particular case of N identical bosons on a ring of circumference L. The Hamiltonian for this system is given in the position basis by

$$\hat{H} = \frac{\hbar^2}{2\mu} \sum_i \frac{d^2}{dx_i^2} + g \sum_{i<j} \delta(x_i - x_j)$$  \hspace{1cm} (6)

where $\mu$ is the mass of each boson, $\hbar$ is the reduced Planck’s constant, and $g > 0$ represents the strength of the interaction.

We want to solve the Schrödinger equation

$$\hat{H}|m\rangle = E_m|m\rangle$$  \hspace{1cm} (7)

for the energies $E_m$ and eigenstates $|m\rangle$. The wavefunction $\psi_m(x) = (x|m)$ is subject to the periodic boundary condition $\psi_m(x + L) = \psi_m(x)$. This equation is impossible to solve analytically, as is often the case for N body quantum mechanical systems with a general interaction. However, it is exactly solvable if $g = 0$. In particular, for the $N = 1$ case, the eigenfunctions are simply (normalized) plane waves, i.e. $\psi_m(x) = \sqrt{\frac{1}{L}} \exp \left( \frac{2\pi imx}{L} \right)$, where $m \in \mathbb{Z}_0$ is the angular momentum quantum number. The energy is given by $E_m = \frac{2\hbar^2 \pi^2 m^2}{\mu L^2}$. The set of wavefunctions forms an orthonormal eigenbasis for the single particle Hilbert space. The eigenfunctions of the N-body non-interacting ($g = 0$) Hamiltonian are the symmeterized product of single particle eigenfunctions. For N=2 in particular, $\psi_{m_1,m_2}(x_1,x_2) = \frac{1}{\sqrt{2}} [\psi_{m_1}(x_1)\psi_{m_2}(x_2) + \psi_{m_1}(x_2)\psi_{m_2}(x_1)]$.

For large N however, it becomes cumbersome to work with the so-called first quantization notation, in which wavefunctions are represented by symmeterized products of single particle eigenstates. A quick fix to this problem is to work in second quantized notation, in which modal occupations are enumerated. For instance, a general eigenstate can be written as

$$|\vec{n}\rangle \equiv |n_0, n_1, n_{-1}, n_2, n_{-2}, ...\rangle$$  \hspace{1cm} (8)

where $n_0, n_1, ...$ represent the number of bosons in the $m = 0, m = 1, ...$ modes, respectively. This representation avoids the complication of symmeterizing the wavefunction, and is thus much easier to work with.

Remember though, the eigenstates in Eq. (8) are the eigenstates for the non-interacting Hamiltonian. So why did we bother calculating them if the problem we are interested in involves interacting particles? With Eq. (8), one can do perturbation theory calculations to find the first order shifts in the energies and eigenstates. These will give approximate
expressions for the energies and eigenstates, with better approximations as \( g \to 0 \). However, these approximations become unreliable in the large \( g \) regime. To study larger \( g \) regimes, we employ the techniques of second quantization.

Firstly, the Hamiltonian \( \hat{H} \) has a matrix representation, whose elements are given, with respect to a particular basis \( \{ |n \rangle \} \), by \( \langle m | \hat{H} | n \rangle \). One can choose as their basis the set of non-interacting eigenstates in Eq. (3), giving matrix elements

\[
H_{\vec{n}, \vec{n}'} \equiv \langle \vec{n} | \hat{H} | \vec{n}' \rangle
\]  

Once each and every matrix element has been calculated, one can construct the full Hamiltonian matrix and diagonalize it to find the eigenenergies and eigenstates. This method is general and holds true even when considering interactions between particles. Thus, the task at hand amounts to calculating matrix elements given by Eq. (4), building the full Hamiltonian, and diagonalizing it.

Since the Hamiltonian is just the sum of kinetic and potential operators, i.e. \( \hat{H} = \hat{T} + \hat{V} \), the matrix elements can be calculated as

\[
H_{\vec{n}, \vec{n}'} = \langle \vec{n} | \hat{T} | \vec{n}' \rangle + \langle \vec{n} | \hat{V} | \vec{n}' \rangle
\]  

Here, \( \vec{n} \) is just an index that labels the occupancy state \( | \vec{n} \rangle \). The kinetic part is simple, since \( \langle \vec{n} | \hat{T} | \vec{n}' \rangle = E^{(k)}(\vec{n}) \), where \( E^{(k)} = \sum_m n_mE_m \) represents the kinetic (non-interacting) energy eigenvalue. Thus,

\[
T_{\vec{n}, \vec{n}'} = E^{(k)}_{\vec{n}} \delta_{\vec{n}, \vec{n}'}
\]  

which is a diagonal matrix. The interaction term, however, is much more complicated, but can be solved using second quantization.

Most interaction potentials are pairwise, meaning they are functions of relative positions of two particular particles. In the Lieb-Liniger model for instance, the potential is a function of only \( |x_i - x_j| \). Operators of this form are called two-body operators, and such operators have a unique second quantized representation. Using the completeness relation of the non-interacting eigenstates \( | \vec{n} \rangle \), one can show that the second-quantized representation of any two-body operator \( \hat{V}_2 \) is

\[
\hat{V}_2 = \sum_{m,m',m'',m'''} \langle m,m' | \hat{V}_2 | m'',m''' \rangle a_{m'}^{\dagger}a_{m''}^{\dagger}a_{m'}a_{m''}
\]  

where \( a^{\dagger} \) and \( a \) are the creation and annihilation operators, with the properties that

\[
a_{m}^{\dagger}|n_0,n_1,\ldots,n_m,\ldots\rangle = \sqrt{n_m + 1}|n_0,n_1,\ldots,n_m + 1,\ldots\rangle
\]  

\[
a_m|n_0,n_1,\ldots,n_m,\ldots\rangle = \sqrt{n_m}|n_0,n_1,\ldots,n_m - 1,\ldots\rangle
\]  

and the “scattering” matrix element \( \langle m,m' | \hat{V}_2 | m'',m''' \rangle \) is given by

\[
\langle m,m' | \hat{V}_2 | m'',m''' \rangle = \int_0^L dx_2 \int_0^L dx_1 \psi_{m,m'}^{*}(x_1,x_2)V_2(x_1,x_2)\psi_{m'',m'''}(x_1,x_2)
\]  

where \( \psi_{m,m'}(x_1,x_2) \) is the non-interacting eigenstate.
A complete derivation can be found in [11]. For the delta function interaction in the Lieb-Liniger model, one can integrate the above equation directly to find, with $V_2 = g \delta(x_1 - x_2)$,

$$\langle m, m' | \hat{V}_2 | m'', m''' \rangle = \frac{g}{L} \delta_{m+m',m''+m'''}$$

(16)

Thus, the full second-quantized representation of the delta function interaction in the Lieb-Liniger model is

$$\hat{V}_2 = \frac{g}{L} \sum_{m,m',m''} a_m^\dagger a_{m'}^\dagger a_{m''} a_{m+m'-m''}$$

(17)

With Eq. (17), we are now in a position to calculate the matrix elements

$$\langle \vec{n} | \hat{V} | \vec{n}' \rangle = \frac{g}{L} \sum_{m,m',m''} \langle \vec{n} | a_m^\dagger a_{m'}^\dagger a_{m''} a_{m+m'-m''} | \vec{n}' \rangle$$

(18)

since we know the action of the creation and annihilation operators on the occupation states.

Once the full Hamiltonian has been constructed using equations (11) and (18), the next step is to diagonalize it to find the energies and eigenstates. Note that everything up to this point has been exact. Unfortunately, the set of non-interacting eigenstates spans an infinite dimensional space (since there are an infinite number of modes), and therefore the Hamiltonian is of infinite dimension. In order to make calculations tractable, we must introduce a mode cutoff, after which all modal occupations are zero. This approximation is reasonable as long as $g$ isn’t too large, as particles are less likely to occupy higher-momentum states in the weakly-interacting regime. With this approximation, the Hilbert space isn’t infinite dimensional, but instead has dimension

$$D = \frac{(2m_c + N)!}{(2m_c)!N!}$$

(19)

where $m_c > 0$ is the cutoff mode such that $n|m| > m_c = 0$. This factor counts the number of ways of distinctly placing $N$ indistinguishable particles in $2m_c + 1$ modes (See appendix for derivation). The reason for the $2m_c + 1$ is because we want to include modes in the range $-m_c \leq m \leq m_c$. The dimension of the Hilbert space therefore grows very rapidly as both the cutoff and system size are increased.

One can use numerical algorithms, such as the Lanczos algorithm, to calculate the eigenvalues and eigenstates of the truncated Hamiltonian. With these eigenstates, various other physically important quantities can be calculated. Of particular interest are the von Neumann entropy and condensate fraction, quantities inaccessible through other numerical methods in the Lieb-Liniger model.

In order to quantify entanglement via the von Neumann entropy, we must first define our bipartition. In this second quantized notation, which enumerates the modal occupancies, it is natural to bipartition our Hilbert space into the condensate, consisting of all particles in the $m = 0$ mode, and the depletion, consisting of all particles in the $m \neq 0$ modes. At very low temperatures, a quantum state will almost certainly exist in the ground state of the Hamiltonian. Thus, the states
we are investigating are pure states. Since the Hamiltonian was diagonalized in the \{\ket{\vec{n}}\} basis, the eigenstates are linear combinations of \ket{\vec{n}}:

\[ \ket{\Psi} = \sum_{\vec{n}} c_{\vec{n}} \ket{\vec{n}} \]  \tag{20}

Under bipartition of condensate and depletion, one can rewrite \ket{\vec{n}} as

\[ \ket{\vec{n}} = \ket{n_0} \otimes \ket{\vec{n}_d} \]  \tag{21}

where \ket{\vec{n}_d} is the depletion.

The density matrix for the ground state is

\[ \rho = \bra{\Psi} \rho \ket{\Psi} = \sum_{\vec{n}, \vec{n}'} c_{\vec{n}}^* c_{\vec{n}'} \ket{\vec{n}} \bra{\vec{n}'} \]  \tag{22}

One obtains the reduced density matrix of the condensate by tracing the density matrix over the depletion:

\[ \rho_A = \sum_{\vec{n}_d} \bra{\vec{n}_d} \rho \ket{\vec{n}_d} = \sum_{\vec{n}_d, \vec{n}, \vec{n}'} c_{\vec{n}}^* c_{\vec{n}'} \bra{\vec{n}_d} \ket{\vec{n}} \bra{\vec{n}'} \ket{\vec{n}_d} \]  \tag{23}

\[ = \sum_{\vec{n}, \vec{n}'} c_{\vec{n}}^* c_{\vec{n}'} \delta_{\vec{n}_d, \vec{n}_d} \ket{n_0} \bra{n_0'} \]  \tag{24}

We can simplify this expression further. Note that, since particle number is fixed, \( \sum_m n_m = N \). Now, if the depletions \ket{\vec{n}_d} and \ket{\vec{n}'_d} of two occupancy states \ket{\vec{n}} and \ket{\vec{n}'} respectively are equal, then they contain the same number of particles, implying, by particle number conservation, that the condensates \ket{n_0} and \ket{n_0'} are equal. In other words, since the particles that do not occupy the depletion must occupy the condensate, equal depletions requires equal condensates by the particle number constraint. Therefore, we can replace \( \delta_{\vec{n}_d, \vec{n}_d'} \) by \( \delta_{\vec{n}, \vec{n}'} \) and Eq. (24) becomes

\[ \sum_{\vec{n}, \vec{n}'} c_{\vec{n}}^* c_{\vec{n}'} \delta_{\vec{n}_d, \vec{n}_d} \ket{n_0} \bra{n_0'} \]  \tag{25}

\[ = \sum_{\vec{n}} |c_{\vec{n}}|^2 \ket{n_0} \bra{n_0} \]  \tag{26}

Implicit in these equations is the fact that \ket{n_0} = \ket{n_0}(\vec{n})}, meaning a particular \( \vec{n} \) sets the condensate occupancy. Equation (26) shows that the reduced density matrix of the condensate is a mixed ensemble, indicating an entangled state. Also note that \( \rho_A \) is diagonal in the \{\ket{\vec{n}}\} basis. The von Neumann entropy is defined as

\[ S_{VN} = - \text{tr}(\rho_A \log \rho_A) \]  \tag{27}

This equation can be manipulated into a more familiar form by using the definition of \( \rho_A \) in (26). The diagonal matrix elements of \( \rho_A \) are given by

\[ (\rho_A)_i = \sum_{\vec{n}} |c_{\vec{n}}|^2 \delta_{n_0, i} \]  \tag{28}
Since the $|c_\vec{n}|^2$ give the probability of collapse onto the $|\vec{n}\rangle$ eigenstate, the expression in (28) is the average value of some projection operator, $\hat{\delta}_{n_0,i}$, such that

$$\hat{\delta}_{n_0,i}|\vec{n}\rangle = \delta_{n_0,i}|\vec{n}\rangle$$

i.e, it is the projection operator onto a state with $i$ particles in the condensate. Therefore, one can use the identical definition of the expectation value in quantum mechanics to reexpress $(\rho_A)_i$ as

$$(\rho_A)_i = \langle \Psi|\hat{\delta}_{n_0,i}|\Psi\rangle \equiv p_i$$

Thus, the von Neumann entropy can be expressed as

$$S_{VN} = -\sum_{i=0}^{N} p_i \log p_i$$

which looks identical to the classical definition of the Shannon entropy. Computationally, the procedure described above amounts to building up the $\hat{\delta}_{n_0,i}$ for each value of $i \in \{0, 1, ..., N\}$ and then computing the $p_i$ by simple matrix multiplication, which is carried out very efficiently in Python.

A generalization of the von Neumann entropy is the Renyi entropy, given by

$$S_\alpha = \frac{1}{1-\alpha} \log(\sum_i p_i^\alpha)$$

where $\alpha \geq 0$ is the order of the Renyi entropy. Although undefined for $\alpha = 1$, one can show, using L'Hospital's rule, that the Renyi entropy becomes the von Neumann entropy in the limit as $\alpha$ approaches 1. Furthermore, the Renyi entropy is monotonically decreasing in $\alpha$. The Renyi entropies are trivial to calculate once the $p_i$'s are known, which is another distinct benefit to using exact diagonalization.

Another operator of interest is the number operator $\hat{n}_m$. This operator simply counts the number of particles occupying a mode $m$. It is diagonal in the $\{\vec{n}\}$ basis, and is very easy to construct: One simply counts the number of particles in each mode and places those numbers along the diagonal. Its expectation value, $\langle \Psi|\hat{n}_m|\Psi\rangle$ gives the average bosonic occupancy in mode $m$. The condensate fraction, the ratio of particles in the condensate ($m = 0$) to the total particle number, is a particularly interesting quantity that can be calculated in experiments through an analysis of the velocity distribution of cold atoms released from an optical trap, that is closely related to the entanglement entropy. In the non-interacting limit, the particles form a Bose-Einstein condensate, characterized by a condensate fraction of 1. In this phase, the modal entanglement entropy is zero. The condensate fraction is another quantity whose computation is facilitated by the methods second quantization and exact diagonalization.
4 Methods

The matrices we deal with can be huge (on the order of $10^5 \times 10^5$), and calculating eigenvalues and eigenstates requires an efficient means of diagonalization. The Lanczos algorithm is able to do just this. This algorithm takes a Hermitian matrix $H$ and computes an orthogonally similar tridiagonal matrix $T$ from it. Once $T$ is computed, the eigenvalues and eigenvectors can be computed via standard algorithms such as the QR and multiple relatively robust representation methods [Panju, M, Dhillon, I].

The Lanczos algorithm is implemented in Python via the scipy.sparse.linalg.eigs function, which is a wrapper to the ARPACK function. The eigs function can effectively compute the smallest (ground state) eigenvalue and corresponding eigenvector of a Hermitian matrix. It was necessary to perform a test of Python’s Lanczos algorithm to determine its reliability. As a test case, we investigated the quantum transverse-field Ising model, a well-known, well-studied model with useful benchmarking results. In particular, the magnetization and spin correlation expectations were calculated and plotted as functions of external magnetic field and spin coupling, respectively.

Once the reliability of Python’s eigs function was established, the next step was to implement the diagonalization code for the Lieb-Liniger model. To benchmark the calculations, the exact result, known as the Bethe ansatz, was used. With the Bethe ansatz, one can calculate, but is limited to, the exact energies and wavefunctions. Unfortunately, expectation values and other meaningful quantities such as the von Neumann entropy cannot be calculated with it, but the Bethe ansatz provides a means of comparing the approximate energies computed via exact diagonalization.

The algorithm for the matrix constructions in the Lieb-Liniger model is now outlined:

1: Construct Hilbert space given particle number $N$ and mode cutoff $m_c$.
2: Define creation/annihilation operator functions as well as 2nd quantized representation of $\hat{V}$.
3: for $i$ in range(number of states):
   compute $T_{\vec{n},\vec{n}}$ according to (11), compute $V_{\vec{n},\vec{n}'}$ according to (18).
   Also compute matrix elements of $\hat{n}$.
4: for $i$ in range($N+1$):
   construct $\hat{n}_{m,i}$ according to (29).
5: Save all matrices to disk for use later.
6: Diagonalize Hamiltonian using eigs function. Store ground states to disk.

With these steps, all desired matrices are constructed. It is important to save the matrices to disk to avoid having to
reconstruct them, since the construction process is very time consuming for large system sizes and/or cutoffs. For similar reasons, the eigenvectors are saved to disk. Finally, with the ground states on hand, one can compute the expectation values required for calculation of the entropies and condensate fractions using the $\hat{\delta}$ and $\hat{n}$ matrices that were also stored on disk.

To save a huge amount of memory and decrease construction time, sparse matrices were used. Both the kinetic and potential matrices contain mostly zeros, meaning a significant portion of a machine’s RAM is wasted in storing these zeros. A sparse matrix can circumvent this problem by storing only the non-zero elements along with their positions in the matrix. Furthermore, Python’s scipy module can easily work with and manipulate sparse matrices (the eigs function is designed for sparse matrices, hence the ’s’).

Construction time can be reduced further by noting that unoccupied modes will always give 0 when acted upon by the second-quantized form of the potential operator, since the right-most operator an annihilation operator, and $a|0\rangle = 0$. Thus, the number of iterations per loop can be reduced by iterating over only occupied modes, significantly reducing run time.

5 Results for Lieb-Liniger Model

Quantifying the condensate-depletion entanglement via the von Neumann entropy is only possible through the methods of exact diagonalization. Thus, the von Neumann entropy is one of the more interesting calculable quantities in this research. Since we have no way of benchmarking the entropies (as opposed to the energies, where we had the Bethe ansatz), instead, we seek convergence in the entropies as a function of the cutoff. The mode cutoff was introduced to make numerical calculations tractable, and inevitably error was introduced. However, for a fixed interaction strength, convergence can be seen with increasing cutoff, as expected. From the cutoff-convergence results, a regime of interaction strengths, in which the von Neumann entropy can be accurately calculated, can be determined. This can be accomplished by fixing the relative error

$$\epsilon(m) = \frac{|S_{VN}(m+1) - S_{VN}(m)|}{S_{VN}(m)}$$

at, say, 1% for fixed $g$, and locating the cutoff at which this convergence is reached (if possible). Since the Hilbert space dimension, and thus computation time, grows rapidly with increasing cutoff, especially for larger system sizes, the range of interaction strengths that can be studied becomes narrower. For small systems, ($N=2$ for instance), large cutoffs are accessible, and thus, a broad range of interaction strengths can be studied accurately. We do not have this luxury for larger systems sizes ($N \geq 16$) however, where only small cutoffs can be studied due to computation time and memory limitations.

Firstly, the eigenenergies calculated from exactly diagonalizing the Hamiltonian were plotted against $g$, the interaction strength, along with the Bethe ansatz energies. For $N=2$, the energies calculated using perturbation theory were also plotted.

Next, using the methods described in section (3), the von Neumann entropy was calculated and plotted as a function of $g$, the interaction strength. The Rényi entropies, the generalization of the von Neumann entropy, were also plotted for a variety
Figure 1: Plots of energy eigenvalues for various system sizes.
of orders using the maximum attainable cutoffs. Another interesting quantity, the condensate fraction, was also plotted again as a function of $g$. The condensate fraction is simply the expectation value of the condensate ($m = 0$) occupancy divided by $N$.

The scaling results were plotted to show convergence in the von Neumann entropies as a function of the cutoff, as well as finite size scaling in the system size. The first of these plots play an important role in determining the regime of studiable interaction strengths in which reliable results can be obtained. In such plots, $g$ is fixed while the relative errors are plotted against the cutoff, $m_c$. The second of these plots are intended to show convergence of the von Neumann entropy in the system size.
Figure 3: Plots of Rényi entropies of various order for various system sizes. These plots were produced using the maximum available cutoff for a given system size.
Figure 4: Plots of the condensate fractions for various system sizes.
Figure 5: Plots of scaling in the von Neumann entropies for various system sizes.
Figure 6: A plot of von Neumann entropies vs. log(N) for various interaction strengths. Uncertainties are given by the difference in entropy calculated between the maximum cutoff and the maximum cutoff minus 1.

6 Discussion

The energy plots show clear convergence to the exact energies, calculated from the Bethe ansatz, as the cutoff is increased. The energy plots, while important in their own right, indicate the validity of the Lanczos algorithm in the context of the Lieb-Liniger model.

The von Neumann entropies also show clear convergence as the cutoff is increased, as predicted. Interestingly, the plots of the von Neumann entropies show quicker convergence with increasing cutoff than the energies, at least in the regimes of interaction strengths used. The scaling plots quantify this observation, and are important because there is no way to calculate the von Neumann entropies exactly. Thus, the scaling plots are the only means of determining a regime of g values in which the entropies can be accurately calculated. For \( N = 2 \), it is easy to see that convergence to under 1% relative error is achieved even for small cutoffs for the range of g values shown. Therefore, a broad range of interactions can be studied, especially considering access to large cutoffs is possible. Similarly, for \( N = 4 \), clear convergence can be seen especially at larger cutoffs. With \( N = 8 \) particles, convergence to under 1% relative error is only seen at the maximum available cutoff (\( m = 5 \)). However, at this cutoff, a fairly large range of g values can be studied. Unfortunately, for \( N = 16 \), only the curve at g=1 comes close to satisfying the relative error criterion, even at the maximum cutoff of 3. Thus, we are limited to g values less than 1. For larger system sizes, only very small cutoffs are accessible due to memory limitations, even when the Python
The plots of the Rényi entropies show some expected results. Firstly, the $\alpha = 1$ case corresponds precisely to the von Neumann entropy, a result predicted through application of L'Hospital's rule on the Rényi entropy equation (32). Secondly, we see a hierarchy in the Rényi order, with $S_1 \geq S_2 \geq S_3,...$

The plots of condensate fractions also show some expected results. Firstly, they confirm our theory that all particles should occupy the condensate when the interaction strength is zero, since the condensate is the lowest energy state in the non-interacting limit. The ground state of the non-interacting Hamiltonian forms the Bose-Einstein condensate. As the interaction strength is increased, particles will tend to be ‘kicked out’ of the condensate, thus decreasing the condensate fraction. This quantity is closely related to the entanglement entropy: When all particles occupy the condensate, the modal entanglement entropy is zero (although there may be significant spatial entanglement [3]) since physically there is nothing for the condensate to be entangled with.

For $N = 32$ and $m_c = 3$, diagonalization could not be achieved, even when implemented on Vermont’s Advanced Computing Core using the maximum requestable memory. Since the Hamiltonian for this system is a $2.7 \times 10^6$ by $2.7 \times 10^6$ matrix, which consumes a total of around 2GB on disk (in sparse matrix form), a huge amount of memory is required to diagonalize it. Unfortunately, this is one of the main drawbacks to exact diagonalization: At certain system sizes and cutoffs, there is no way of performing numerical diagonalization, even on very powerful computers. The path integral Monte Carlo approach can effectively study large systems, but we sacrifice the ability to calculate certain quantities, most notably the von Neumann entropies and condensate fractions.

Finite size scaling plots can be used to predict the behavior of larger system sizes by studying the apparent asymptotic behavior of certain values as system size is increased. For instance, one can infer from the magnetization and spin correlation plots shown in the methods section how these quantities scale with system size. In general, the maximum von Neumann entropy for a bipartioned quantum system is $\log(D)$, where $D$ is the dimension of the subsystem’s Hilbert space [12]. In the case of condensate-depletion entanglement, the dimension of the condensate is simply $N$, and thus $\log(N)$ is a strict upper bound on the von Neumann entropy. The von Neumann entropies were thus plotted against $\log(N)$ for several interaction strengths, as shown in Figure 6. The hope was to see clear asymptotic behavior in the entropies with the system size, as we saw in the Ising model plots. However, it is not entirely clear if any finite sized scaling behavior can be observed. In order to observed clearer scaling behaviors, larger system sizes should be studied, which unfortunately is a difficult task, especially considering we are limited to only small cutoffs that introducing significant uncertainties in the entropies.
7 Conclusion

The numerical method of exact diagonalization is an effective way of studying small system sizes and allows very interesting quantities to be numerically accessed. While it has limitations, especially in its inability to study larger system sizes with accuracy, it can still be used to gain insight into the mysterious nature of entangled one-dimensional systems. In order to study larger system sizes with larger cutoffs, a transition from Python to C++ may be necessary for efficiency reasons. With results from larger system sizes, we will get a better understanding of how the entropy scales with system size, which is a necessity to study the more realistic systems consisting of large numbers of particles.

A very important benefit of using exact diagonalization however is its generality: One is not limited to studying only delta function interactions. In transforming from the first quantized to second quantized representation of the two-body interaction operator, one must compute a Fourier transform of the potential, given by the matrix element \( \langle m, m'| V(|x_1 - x_2|)|m'', m''' \rangle \). For instance, one could study a Gaussian-type interaction, and one would only require the Fourier transform (another Gaussian) to fully reexpress the two-body operator in second quantized notation. Using Python’s fast Fourier transform function, one can efficiently compute the Fourier transform to study a diversity of interaction types. The next stage of this project will involve implementing different interactions by computing the Fourier transform of the interaction and performing similar calculations as the ones done previously. Although the one-dimensional delta function interaction can be accessed experimentally in optical lattices using ultracold atoms, it would be exciting to study more natural one-dimensional bosonic systems, such as a system of He-4 atoms interacting via a pairwise Lennard-Jones potential.

8 Appendix

8.1 Ising Model Derivations

We wish to calculate the matrix elements of the Ising Hamiltonian in a transverse magnetic field. The Hamiltonian is given by

\[
\hat{H} = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x
\]  

(33)

We compute matrix elements in the spin-up spin-down \( N \)-particle basis, since we know the action of the Pauli matrices on spins in this basis.

\[
\sigma^z | \uparrow \rangle = | \uparrow \rangle
\]  

(34)

\[
\sigma^z | \downarrow \rangle = -| \downarrow \rangle
\]  

(35)

\[
\sigma^x | \uparrow \rangle = | \downarrow \rangle
\]  

(36)
Figure 7: Plots of Ising model results, showing the expectation values of the magnetization and spin correlation.

\[ \sigma^z \downarrow = \uparrow \]

Note that the spin correlation operator is diagonal in this basis, while the magnetization operator is not. Setting \( h = 0 \) simply gives the classical Ising model energies, which can be read off directly as the diagonal elements of \( \hat{H} \). In the N-spin basis, \( \{ \uparrow \uparrow \ldots, \uparrow \downarrow \ldots, \ldots, \downarrow \downarrow \ldots \} \), one can construct the matrix representation of \( \hat{H} \) and diagonalize it via the Lanczos algorithm to obtain the eigenstates and energies. Expectation values were then calculated in the groundstate. The first term in \( \hat{H} \) is the quantum mechanical operator for the spin correlation, while the second term is the total magnetization operator, i.e.

\[ \hat{C}_z \equiv \frac{1}{N} \sum_i \sigma_i^z \sigma_{i+1}^z \]

and

\[ \hat{M}_x \equiv \frac{1}{N} \sum_i \sigma_i^x \]

These operators were used to calculate expectation values, and the results were plotted vs \( J \) (for the spin correlation) and \( h \) (for the magnetization). The plots of magnetization and spin correlation show some expected results. Firstly, in the magnetization plot, one can see two fairly distinct regions: The first where \(-1 \leq h \leq 1\) and the second elsewhere. The first region is the weak-field region. There is no overwhelming tendency for spins to points in a preferred direction along the x-axis. Outside of this region, the magnetic field becomes strong, and the spins will tend to allign with the field to minimize energy. This is easily seen on the graph. The spin correlation measures the tendancy for spins to allign with eachother. Again, we see two regimes: A weakly interacting regime and a strongly interaction one. In the weakly interacting regime, the spins tends to be disordered, and show little tendancy to be alligned with eachother. However, in the strongly interacting
regime, we see preference for alignment. Furthermore, in both plots, we can see some sort of asymptotic scaling with particle number.

### 8.2 Additional Plots and Discussion

Another set of plots important to this research project are the wallclock scaling plots. In these plots, the time taken to construct the Hamiltonian (kinetic and potential matrices) is plotted versus both the system size and the cutoff, with cutoff and system size fixed, respectively. These plots can be used to predict the time required to construct Hamiltonians for larger Hilbert space dimensions. Since the matrix size grows very rapidly with both system size and cutoff (Eq (19)), the matrix construction time diverges very rapidly. Closely related to the wallclock time is the total memory consumed on disk by these matrices.

The plots of $\log_2(\text{time})$ vs. $\log_2(\text{particles})$ show linear trends, indicating an exponential increase in the construction time with the system size. As cutoff increases, we see an increase in the growth factor, the slope of the fit, as well. The memory consumption plots show how rapidly memory demand increases with cutoff in larger system sizes. For the maximum cutoffs shown, gigabytes of memory are required to store these matrices to disk, and from the trend shown, it is easy to see that higher cutoffs demand a great deal more.

### 8.3 Derivation of Hilbert Space Dimension

The dimension of the truncated Hilbert space is the number of ways of placing $N$ particles into $2m_c + 1$ modes. If we imagine each particle is represented by an ‘x’, and the $2m_c + 1$ modes are represented by $2m_c + 2$ bars, with the bars at each end fixed, then the dimension is the number of ways of permuting the order of the x’s and bars, divided by an appropriate factor that accounts for the indistinguishability of the x’s and bars. For example, take $N = 2$ and $m_c = 2$. Now, a starting configuration could be represented by $|x\ x|\ |\ |\ |$. Every possible configuration can be created by simply moving the x’s and bars around, while keeping the bars at the end fixed. For instance, the second configuration is created by moving the second bar to the left, giving $|x\ \ |\ x\ |\ |\ |$. There are $(2m_c + N)!$ possible permutations, but we must account for the indistinguishability of the x’s and bars by diving by $(2m_c)!|N|!$, giving a total number of possible configurations $D = \frac{(2m_c + N)!}{(2m_c)!|N|!}$.
Figure 8: Plots of wallclock time for fixed cutoff
Figure 9: Plots of Hamiltonian memory consumption for $N=16$ and $N=32$
9 References


