One-dimensional Bose Hubbard Ladder With An Induced Flux

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by

ANANYA MUKHERJEE

Roll Number: 22P0430004 ABC ID: 293-398-429-357 PRN: 202200044 Under the Supervision of

PROF. RAMESH V. PAI

School of Physical and Applied Sciences Master of Science in Physics (MSPH)



Goa University May 2024





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I hereby declare that the data presented in this Dissertation report entitled, "Onedimensional Bose Hubbard Ladder With An Induced Flux" is based on the results of investigations carried out by me in the discipline of Physics, at the School of Physical and Applied Sciences, Goa University under the supervision of Prof. Ramesh V.Paj and the same has not been submitted elsewhere for the award of a degree or diploma by me. Further, I understand that Goa University or its authorities will not be responsible for the correctness of observations / experimental or other findings given the dissertation. I hereby authorize the University authorities to upload this dissertation on the dissertation repository or anywhere else as the UGC regulations demand and make it available to anyone as needed.

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Signature and Name of Student Scat no: Ananya Mukherjee 2290430004

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Date: 6 5 24

Ry

Signature and Name of Supervising Teacher Prof. Rameth V. Pa

Signature of Dean of the School/HoD of Dept Date: 6|5|2-4Place: Goa University



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ABBREVIATIONS USED

| Entity | Abbreviation |
|--------------------------------------|--------------|
| Superfluid | SF |
| Chiral Superfluid | CSF |
| Mott insulator | MI |
| Chiral Mott Insulator | CMI |
| Central Mean Field Theory | CMFT |
| Density Matrix Renormalization Group | DMRG |

ABSTRACT

Condensed matter physics often relies on simplified models to understand complex systems due to the challenges of directly studying large systems. This study looks at the response of a one-dimensional bi-layered ladder system to an induced flux using the Bose-Hubbard model, extending beyond conventional density limits. The system is analyzed using two numerical techniques: Cluster Mean-Field Theory (CMFT) and Density Matrix Renormalization Group (DMRG).

By adjusting the hopping strengths (t_a, t_b, t_p) , a phase difference is induced in the lattice, effectively creating a flux within the system. Through analysis, three distinct phases are identified: the Chiral Mott Insulator, Regular Mott Insulator, and Chiral Superfluid Phase. These phases are characterized by examining the current-current correlation function $(j_i * j_k)$, superfluid order parameter (ψ) , and variation in perpendicular hopping (t_p) .

The study concludes that a non-zero current correlation function indicates the presence of chirality in the system. When the superfluid order parameter is zero, the system is in an insulator phase, while a finite order parameter signifies superfluidity. The study reveals a transition from the Chiral Mott Insulator to the Mott Insulator phase as the onsite interaction strength (u) increases. Additionally, chirality persists in the superfluid phase regardless of variations in u.

Primary reader and thesis advisor:

Dr. Ramesh V. Pai Professor School of Physical and Applied Sciences Goa University, Goa, India

Chapter 1

INTRODUCTION

1.1 Background

Ultracold atomic physics has opened up the world of physics and has led to various discoveries. It has paved the way for researchers to discover new phenomena as well as find fresh approaches to analyze known phenomena in depth. You might be curious as to how one studies ultracold atoms. To do so, we form a lattice by trapping atoms in a box. We then have to cool the atoms present in the lattice with the help of lasers. How this is done is relatively simple. Lasers are used to trap the atoms. The laser beam is expanded and sent through several holes, this creates interference patterns due to the interference of light. Atoms view this interference as an optical potential. Atoms are cooled and trapped in this optical potential. Research in ultracold physics has shown the existence of artificial gauge fields. The reason for it being called "artificial" is because although there is no magnetic field applied to the

system. In the presence of the laser, there is a field created wherein the center of mass of the neutral atoms present mimic charged particles in a magnetic field[1]. Magnetic trapping leads to the formation of a potential well where atoms are independent of the exterior conditions i.e. atoms do not touch the walls of the enclosed space and therefore they remain unaffected by the room temperature. Within the lattice, lasers are used for cooling the atoms. Previous research in the domain has been able to show the existence of three phases, namely: Chiral Mott Insulator(CMI), Mott Insulator (MI), and Chiral Superfluid(CSF) using just a single numerical technique, Density Matrix Renormalization Group(DMRG) [2]. Chirality implies the breaking of the time-reversal symmetry.

1.2 Aim and Objectives

Our main aim in this research paper is to obtain and analyze the phase transitions and properties obtained using the simple Bose-Hubbard model for a one-dimensional ladder with flux induced through hopping, without fixing the density value. We explore densities other than unity in our experiment because fixing density within the trap of an optical lattice is challenging. By investigating non-unit densities, we aim to extend our understanding beyond ideal experimental conditions.

The Hamiltonian that we worked with is described below in detail.

$$H = -t_a \sum (a_i^+ a_{i+1} + a_{i+1}^+ a_i) + t_b \sum (b_i^+ b_{i+1} + b_{i+1}^+ b_i) - t_p \sum (a_i^+ b_i + b_i^+ a_i) + u_a \sum (n_i^a (n_i^a - 1) + u_b \sum (n_i^b (n_i^b - 1) - \mu \sum (n_i^a + n_i^b))$$
(1.1)

In equation 1.1 a_i^+ creates and a_i annihilates a boson at site *i* in layer *a* respectively. Similarly, b_i^+ creates and b_i annihilates a boson at site *i* in layer *b* respectively. The number operators at site *i* in layer *a* and *b* are denoted as $n_i^a = a_i^+ a_i$ and $n_i^b = b_i^+ b_i$ respectively. t_a, t_b , and t_p are the the hopping parameters, where t_a and t_b are hopping along the chains *a* and *b* respectively, and t_p is the perpendicular hopping between the two chains. u_a and u_b are the onsite interaction terms and μ is the chemical potential. In the project we consider the onsite interaction terms to be identical and denote them as *u*.

The choice of the model comes from the fact that the Bose-Hubbard model is simple. The Bose-Hubbard model provides a framework for understanding the behaviour of interacting bosonic atoms in a lattice. In our setup, we consider two layers of bosons confined to move along a one-dimensional lattice structure. Flux is introduced through a phase difference between the hopping in different directions, adding an additional degree of freedom to the system.

In this research paper, the two numerical techniques that we make use of to simplify the Hamiltonian 1.1 are: CMFT and DMRG.

Cluster Mean Field Theory (CMFT) is a mean-field approach used to study the behaviour of strongly correlated systems. In CMFT, the lattice is divided into its central site and its neighbouring sites. The interactions between the central site and its neighbours are treated exactly, while the interactions between different clusters are treated at a mean-field level that provides a computationally efficient way to capture the essential physics of the system while incorporating some degree of correlation effects. Density Matrix Renormalization Group (DMRG): is a powerful numerical technique used to study the ground-state properties of one-dimensional quantum lattice systems. It is particularly well-suited for systems with strong correlations. DMRG iteratively constructs a low-rank approximation of the reduced density matrix to capture the most relevant states of the system. By systematically truncating the least important states, DMRG can accurately describe the ground state and low-energy excitations of the system.

The Bose-Hubbard model for a bilayer one-dimensional system with an induced flux presents a variety of quantum phenomena. Numerical techniques such as Cluster Mean Field Theory (CMFT) and Density Matrix Renormalization Group (DMRG) provide valuable tools for investigating the ground-state properties and phase transitions of such systems. By combining the theoretical model with numerical techniques, we can gain insights into the behaviour of strongly correlated bosonic systems.

1.3 Research Question

Varying some of the parameters of the system, such as the onsite interaction strength (u), chemical potential (μ), and hopping strengths (t_a, t_b, t_p), will induce phase transitions between different phases present in the system, including the transition from Chiral Superfluid to Chiral Mott Insulator and Chiral Mott insulator to regular Mott insulator. We hope to answer the questions on how these changes in the system parameters, influence the phase transitions observed in our model, and what are the critical behaviors associated with these transitions?

1.4 Literature Review

For newcomers exploring the realm of physics concerning optical lattices, Greiner and Folling, 2008 in their paper [3] simplify various aspects of condensed matter physics, particularly the how, why, and what regarding optical lattices. They emphasize the experimental convenience that lattices offer to researchers, allowing for easy manipulation of parameters and scalability of the system. The study of lattices commenced in the 1990s and continues to offer significant potential for physicists. The Hubbard Model holds particular significance due to its ability to illustrate the transition between the superfluid (SF) and Mott insulator (MI) phases. In the superfluid phase, particles move freely and exhibit delocalized behavior. In contrast, the Mott insulator phase restricts particle movement, causing them to localize at specific sites. Tokuno and Georges (2014)[1] conducted a study utilizing the same model as ours, a Bose Hubbard ladder with an artificial magnetic field. They used Density Matrix Re-normalization Group (DMRG) techniques to demonstrate transitions among three identified phases: CMI (Chiral Mott Insulator), MI (Mott Insulator), and CSF (Chiral Superfluid). Their findings revealed that transitions between CSF and CMI exhibited Berezinskii-Kosterlitz-Thouless (BKT) characteristics, while transitions between CMI and MI had characteristics of an Ising transition, and transitions between CSF and MI were of a second-order nature. Interestingly, they identified the tricritical point where these phases meet. To do this they used Luttinger parameters because this tricritical point was a feature not observable through DMRG alone. Dhar et al. (2012-2013) [2, 4] highlight crucial aspects of the aforementioned phases. They emphasize the significance of the staggered current in discerning the three distinct phases observed in the Bose-Hubbard ladder model under an artificial magnetic flux. This current is present in both the CMI and CSF phases but vanishes in the MI phase. This paper uses DMRG as well as Monte Carlo simulations for the study. It can be seen that depending on the Hubbard repulsion(U) and chemical potential μ we can differentiate the three phases.

All papers alike emphasize the importance of studying the phase diagrams of the system to achieve significant results. However, it's worth noting that existing research has primarily focused on scenarios where density remains fixed. Leveraging the insights from the literature, we intend to push the boundaries further by exploring the Bose-Hubbard system under conditions where density is not rigidly constrained.

Chapter 2

METHODS

2.1 Introduction

In this project, we used Fortran programming to analyze data and understand phase diagrams. In this chapter, we will elaborate on the methods and data being analyzed. We looked at a specific kind of model called a 1-dimensional Bose Hubbard ladder. The model in 1.1 is simplified using two numerical techniques, CMFT(Cluster Mean Field Theory) and DMRG(Density Matrix Renormalization Group) which are described below. Our goal is to explore how this model behaves when there is a flux induced and the density is not limited to 1.

2.2 Numerical Techniques

In this section, we have described the numerical techniques that we have employed for our research.

Cluster Mean Field Theory which we will often refer to as CMFT in the paper, is a numerical technique used commonly in condensed matter physics to simplify the interactions between particles in many-body systems. It approximates the interactions by treating each particle as if it were independent of the others. We assume that it interacts only with a mean field. The advantage of this method is that it reduces the computational complexity while still capturing important features of the system.

Density Matrix Renormalization Group we will further often refer to as **DMRG** throughout the paper. It is a numerical technique used to effectively study onedimensional quantum systems. It's particularly helpful for systems with strong correlations, like the Bose Hubbard ladder model. It is an iterative method used to optimize a reduced density matrix to keep the most relevant states of the system while discarding less important ones.DMRG is a method helpful in describing the ground state and low-lying excited states of the system.

In this paper, we use the combination of the two numerical techniques mentioned above: CMFT and DMRG.

CMFT provides an initial approximation of the system's ground state by simplifying the interactions between particles. This approximation acts as a starting point for further DMRG calculations. DMRG takes this initial approximation and refines it, iteratively optimizing the reduced density matrix to capture more accurately the relevant states of the system. DMRG can handle strong quantum correlations that CMFT might overlook, thus providing a more accurate description of the system.

2.3 Mean Field Calculations

Our starting point is the Hamiltonian mentioned in equation 1.1, The mean field approximation is applied as follows:

$$a_i^+ = \psi_i^* + \delta a_i^+$$

$$a_i = \psi_i + \delta a_i$$

Where, $\psi_i = \langle a_i \rangle$ is the superfluid order parameter and $\langle \rangle$ denotes average over the ground state. The mean field is felt only by the sites at the extremities of the cluster. We apply the above approximation to the Hamiltonian mentioned in 1.1

$$H = -t_a \sum (a_i^+ a_{i+1} + a_{i+1}^+ a_i) + t_b \sum (b_i^+ b_{i+1} + b_{i+1}^+ b_i)$$
$$-t_p \sum (a_i^+ b_i + b_i^+ a_i) + u_a \sum (n_i^a (n_i^a - 1))$$
$$+u_b \sum (n_i^b (n_i^b - 1)) - \mu \sum (n_i^a + n_i^b)$$

and ignore terms outside the cluster and those consisting solely of the fluctuations. When we do this we achieve a system decoupled and simplified my mean field approximation. Dividing the Hamiltonian into parts and applying the mean-field approximation we get the following:

Part I:

$$-t_a \sum (a_i^+ a_{i+1} + a_{i+1}^+ a_i) = -t_a \psi_a(a_i + a_i^+) + t_a \psi_{a_i}^2 - t_a(a_i^+ a_{i+1} + a_{i+1}^+ a_i)$$

Part II:

$$t_b \sum (b_i^+ b_{i+1} + b_{i+1}^+ b_i) = t_b (\psi_b (b_i + b_i^+) - t_b \psi_{b_i}^2 + t_b (b_i^+ b_{i+1} + b_{i+1}^+ b_i))$$

The rest remains the same, unaffected by the Mean Field. Part III:

$$u_a(n_i^a(n_i^a - 1)) + u_b(n_i^b(n_i^b - 1)) - \mu(n_i^a + n_i^b)$$

The mean field approximation aims to simplify the study of complex systems by approximating interactions between individual components as if they were only influenced by an average or mean effect of the rest of the system.

The Hamiltonian after Mean field approximation is applied becomes,

$$H = \sum_{i} -t_a \psi_a(a_i + a_i^+) + t_a \psi_{a_i}^2 - t_a(a_i^+ a_{i+1} + a_{i+1}^+ a_i) + t_b(\psi_b(b_i + b_i^+))$$
$$-t_b \psi_{b_i}^2 + t_b(b_i^+ b_{i+1} + b_{i+1}^+ b_i) - t_p(a_i^+ b_i + b_i^+ a_i)$$
$$+u_a(n_i^a(n_i^a - 1)) + u_b(n_i^b(n_i^b - 1)) - \mu(n_i^a + n_i^b)$$

CMFT is used to simplify the Hamiltonian by decoupling the terms. DMRG is then used to truncate/reduce the number of states to an order we can handle in our code.

Before delving into the code's functionality, let's discuss its underlying concept and approach to addressing our current problem. We have a 1-dimensional Bose Hubbard ladder that we have now simplified using the Mean field approximation. The subsequent step involves diagonalizing the Hamiltonian to determine the ground state energy (eigenvalue) and wave function (eigenvector). We then employ a self-consistent method to minimize the superfluid order parameter, ψ . We divide our system into two identical blocks (Left and Right) and utilize the concept of density matrix to construct a reduced density matrix of the left block, ρ_L , achieved by integrating out the right block. We then diagonalize the reduced density matrix of the left block ρ_L to find the eigenvalues and vectors. From the numerous states N >> n, we select "n" states with the highest energy values to truncate our density matrix system size from N to n. We assume symmetry between the Left and Right blocks. In this process, we perform calculations for the left block and then replicate the same block on the right side when forming our lattice to reduce computational complexity. We then add one (two) site(s) in the center for odd (even) lattice lengths to create a superblock which we calculate the Hamiltonian and diagonalize until our desired length is achieved.

For a lattice with an odd number of sites, if we initiate with 3 sites, considering 2 for the left block and symmetry for the right block, we then append one site to the cluster. Consequently increasing the lattice by 2 at each step. Below is an outline of how the building of a superblock takes place for an even number of sites.



Figure 2.1: Building a superblock

(a) The above picture has been taken from "Density matrix renormalization group (DMRG) for cyclic and centrosymmetric linear chain", a paper by Kumar et al. (2016)[5]

In 2.1a, they start with a 4-site cluster and divide it equally into two parts. Then, one site is added to each part, resulting in an increase in length by 2 sites. This process is repeated until the ideal length of the superblock is achieved.

2.4 Unveiling the Inner Workings

In this section, we outline the setup of the codes, describing their organization and structure. A comprehensive outline is provided, detailing the functions of both the main code and the subroutines used for various tasks.



Figure 2.2: Mind map for the flow of codes

Let's thoroughly examine the code breakdown.

Section I:

We start with SRC, which serves as the repository for our source code, organized

within a single folder. The five primary programs are outlined as follows:

| Program name | Function | |
|--------------|--|--|
| Hcy0 | Constructs the one site Hamiltonian and then stores the whole Hamiltonian in sparse form | |
| Omatlt | Constructs the reduced density matrices | |
| Hmatlt | Used to change basis using the reduced density matrix | |
| Hcy1 | Used to increase the length of the ladder by adding sites in the middle of the cluster block in steps and generating the new Hamiltonian on each addition of a cluster | |
| Makefile.lx | Used to compile all the codes with a single command and gives the path to the executable files | |

Table 2.1: Source Codes

Below are the various subroutines that constitute integral parts of the aforementioned main programs:

| Subroutine name | Function |
|--------------------|---|
| Inputdata | Reads input data such as maximum matrix size, multiplicity, etc. and stores it in a common block for global access |
| Onesite | Generates the operators for a single site |
| Hcy3 | Hamiltonian of the whole lattice is calculated |
| SparseEigenSolve | Diagonalizes the Hamiltonian using the Davidson code and returns the eigenvalues and eigenvectors |
| Averages | Calculates averages of operators(creation, annihilation, and number operators) |
| Matexpand | Takes a matrix represented in sparse form, where only nonzero ele- ments are stored and expanded to a full matrix with zero elements in their respective positions. |
| Matmulnorm | Renormalizes the operators written in the new basis |
| Matmultb | Changes the operators into the new basis |
| Matnonzero | Turns a matrix into a sparse representation |

 Table 2.2:
 Subroutines used in the Source Code

Section 2:

Under DSQ(Data, Setup, and Quality) we have 3 subfolders with the following functionalities:

| Folder name | Function |
|-------------|---|
| Data | Stores all the necessary data after the codes have been complied and executed |
| DSQ | Stores run files that contain initial and final parameter values and execution instructions |
| OBJ | Objective files generated during the compilation of the main OBJ file are transferred to this folder to facilitate their utilization during code execution. |

| Table | 2.3: | DSQ | files |
|-------|------|-----|-------|
|-------|------|-----|-------|

As mentioned the main OBJ folder contains the objective files created when the codes are compiled.

2.5 Phases

Returning to the core objective of our project, our focus revolves around examining phase diagrams derived from the 1-Dimensional Bose Hubbard Model, with the incorporation of an induced flux. To discern the different phases, our investigation centers on analyzing the following plots:

- ψ and ρ vs μ, to identify if there is a change of phase (From Superfluid(SF) to Mott Insulator(MI))
- current-current correlation function vs length to see if there exists a finite current in the lattice and if it has a staggered nature.

The different phases we look at are :

Superfluid Phase: In this phase, particles exhibit coherent motion without any resistance. It's characterized by a non-zero order parameter (ψ) and the absence of long-range order. Particles exhibit fluid-like behavior, moving freely throughout the system

Chiral Superfluid Phase: This phase is distinguished by the breaking of time-reversal symmetry, resulting in a preferred direction of circulation within the superfluid. It's characterized by a non-zero current, indicating the presence of a net circulation of particles as well as a non-zero superfluid order parameter (ψ).

Mott Insulator Phase: In this phase, the interaction between particles dominates over their kinetic energy, leading to a localization of particles at each lattice site. As a result, each site becomes occupied by a fixed number of particles. Particles are strongly confined to their respective sites and cannot move freely between neighboring sites. The Mott insulator phase typically arises in systems with strong on-site repulsion between particles.

Chiral Mott Insulator Phase: This phase combines the properties of the Mott insulator with chiral behavior. While the particles are localized at each lattice site as in the Mott insulator, there's also a preferred direction in the flow of currents within the system. This can arise due to an external factor like the induced flux in our case.

In the following table, we have tabulated the distinct features of the various phases we were hoping to identify with our model:

| Phase | Features | |
|----------------------------|---|--|
| Superfluid(SF) | Superfluid order parameter (ψ) is non-zero and no stag- gered current (j) in the lattice | |
| Chiral Superfluid(CSF) | Similar to superfluid but the order parameter of the two layers have magnitudes equal but opposite direc- tions and there is a finite staggered current (j) in the lattice | |
| Mott insulator(MI) | Superfluid order parameter (ψ) is zero and no staggered current (j) in the lattice | |
| Chiral Mott Insulator(CMI) | Superfluid order parameter (ψ) is zero and there is a finite staggered current (j) in the lattice | |

Table 2.4: Various phases and their properties

2.6 Current

Current is an important observable for us to find in this project to show chirality in the system. In [2] current is calculated using the following method wherein the methods of DMRG and Monte Carlo simulations were employed.

$$j_{i,i+1}^{a} = -it_{a}(a_{i}^{+}a_{i+1} - a_{i+1}^{+}a_{i})$$

$$j_{i,i+1}^{b} = -it_{b}(b_{i}^{+}b_{i+1} - b_{i+1}^{+}b_{i})$$

$$j_{i}^{ab} = -it_{p}(a_{i}^{+}b_{i} - b_{i}^{+}a_{i})$$
(2.1)

[(i) denotes the site, (j) denotes current, and (a,b) denotes the leg of the ladder]

The equations presented above provide the current generated at each bond, Inter-layer j^{ab} between layers a and b, and intra-layer j^a , j^b between two sites of the same layer. By summing over one loop as seen in 2.3, encompassing two sites of the lattice, both interlayer and intralayer currents contribute to determining the current direction. For the presence of staggered currents to be evident, it's imperative that adjacent loops exhibit currents flowing in opposing directions.



Figure 2.3: Direction of the current flow

In the depicted diagram, site 1 occupies the far left position within the lattice, whereas site 5 resides at the far right end, i.e. where the mean field is felt. Sites 2, 3, and 4 are positioned centrally, equidistant from both ends of the lattice. Symmetry is maintained across the lattice concerning site 3, under the assumption of identical left and right blocks. A particle has the potential to transition between sites a and b, with varying probabilities for each direction, thus establishing a directional bias conducive to current flow. Our analysis primarily centers on the behavior of particles within the three central sites. Letting the loop formed by sites 2 and 3 be called the left loop and the loop formed by sites 3 and 4 be the right loop. Current within these loops are calculated as follows, using the equations in 2.1.

$$Left - loop: b_2^+ a_2 + b_3^+ b_2 + a_3^+ b_3 + a_2^+ a_3$$
(2.2)

$$Right - loop: a_3^+b_3 + a_4^+a_3 + b_4^+a_4 + b_3^+b_4$$
(2.3)

The equations mentioned above are formed under the assumption of a staggered nature in the flow of current.

Above is the background of current calculations so far. As current is a real quantity, we can deduce from 2.1 that the term within the bracket is a complex. Consequently, in our project, computing the precise value of current in the system poses a challenge. As an alternative, we utilize the current-current correlation function -the product of the current at two sites- to ascertain the presence of staggered current within the system. Additionally, we check whether this correlation vanishes for high values of U when $\psi = 0$, indicating a transition from the Chiral Mott Insulator phase to the Mott Insulator phase.

The current-current correlation function is given as:

$$j_{i}j_{k} = -it_{p}(a_{i}^{+}b_{i} - b_{i}^{+}a_{i}) * -it_{p}(a_{k}^{+}b_{k} - b_{k}^{+}a_{k})$$
$$j_{i}j_{k} = -t_{p}^{2}[(a_{i}^{+}b_{i} - b_{i}^{+}a_{i}) * (a_{k}^{+}b_{k} - b_{k}^{+}a_{k})]$$
(2.4)

[i and k denote two sites over which the current-current correlation function is calculated] To conclude this chapter, From the above methods and equations we must examine the obtained results to ascertain the phases identifiable within the 1-Dimensional Bose Hubbard Model featuring induced flux through hopping terms using two numerical techniques mentioned above in detail(CMFT and DMRG). We analyze the superfluid order parameter ψ , density ρ , and current correlation relative to variations in chemical potential μ and on-site interaction u, aiming to identify the various phases present in our system.

Chapter 3

RESULTS AND ANALYSIS

3.1 Introduction

In the previous chapters, we explored the project's conceptual framework and outlined our approach to addressing the research problem. In this chapter, we will delve into the outcomes and conclusions derived from extensive data collection. To reiterate, our focus is on the 1-dimensional Bose Hubbard model, where we introduced a flux through the hopping terms and allowed for varying density. We utilized the methods of Central Mean Field Theory and Density Matrix Renormalization Group (CMFT and DMRG) to analyze the system.

3.2 Even Lattice Lengths and Site Clusters

In this section, we examine the outputs obtained using programs for even-length lattices, starting with a 4-site cluster. At each iteration, the length of the lattices increases by 2. We use 35 density matrix states, onsite interaction(u)=5, and the length of the lattice goes from 4 sites up to 300 sites in our results.



(b) Mott Insulator phase(U=5, μ =1.4)

Figure 3.1: Convergence of ψ and ρ at the lattice edge 1 and center $\frac{L}{2}$

From 3.1, it is clear that various parameters tend to converge as the length of the lattice over which they are calculated increases. In 3.1a when $\mu = 0.6$, a disparity exists in the Superfluid(SF) phase regarding the density ρ between the center of the lattice $(\frac{L}{2})$ and its edges (1), with ρ exhibiting an increase from the edges towards the center. The SF order parameter ψ at the edges is higher than at the center due to the effect of the Mean Field, which overestimates its value at the edges. In 3.1b, we observe that the SF order parameter ψ goes to zero at the center where the Mean Field is not felt, and the SF phase density ρ converges to one, both at the center and at the edges. These features indicate that the system enters the Mott Insulator phase at $\mu = 1.4$.

The above plots were generated using the following parameters: $t_a = 1, t_b = -1, t_p = 0$. This choice of parameters ensures that both intralayer hopping terms are in the same direction. This is because we have considered a Hamiltonian where these terms are opposing in nature 1.1.

In the later stages of the study, we found it necessary to transition to odd-cluster systems. This adjustment became imperative when we encountered difficulties discerning the system's nature, particularly when t_a and t_b pointed in opposite directions. The even-cluster configuration proved inadequate in capturing the staggered characteristics of the order parameters ψ_a, ψ_b . Conversely, the odd-size cluster configuration effectively captured the essence of this staggered nature as depicted in the diagram below.



Figure 3.2: Even cluster drawback

Since we consider the left block identical to the right block, in the case of the even cluster at the center, there exists a disparity between what is observed and what the expected outcome should have been. This occurs because two identical sites are inserted in the middle. In contrast, for an odd number of sites, only one site is added to the center of the lattice, preserving the staggered nature.

3.3 Odd Lattice Lengths and Site Clusters



 $\rho_{a}(3) vs \mu: 0-2$ for u:4.5, 5, 5.5, 6, tp=1.0, length=1001 u=45 - u=50 - u=55 - u=50 0.55 - u=0 0.55 - u=0 0.50 - u=0 0.55 - u=0 0.50 - u=00

(b) ρ vs μ for U=4.5,5,5.5,6

Ψa(3) vs µ:0-2 for u:4.5,5,5.5,6 ,tp=1.0,length=1001

- u4.5 - u5.0 - u5.5 - u6.0

1.0

(d) ψ_b vs μ for U=4.5,5,5.5,6

1.5

2.0

(a) ρ vs μ for various values of one site repulsion(U)



(c) ψ_a vs μ for various values of one site repulsion(U)





(e) ψ_b vs μ for various values of one site repulsion(U)

(f) ψ_b vs μ for U=4.5,5,5.5,6

Figure 3.3: ρ and ψ as a function of μ for varying U

0.5

0.4

0.3

0.1

0.0

-0.1 _____ 0.0

0.5

(E) 0.2

The figures in, 3.3 illustrate the behavior of ψ and ρ for varying values of μ at different u conditions. On the left-hand side, graphs are plotted for u values ranging from 4 to 6, while on the right-hand side, we focus solely on graphs corresponding to a select few u values. This selective approach enables a more nuanced understanding of the system's behavior.

We can identify two phases: The Mott insulator phase, characterized by $\psi = 0$ and $\rho = 1$, and the Chiral-Superfluid phase where ψ assumes finite values and ρ increases with μ . Chirality arises from the equal but opposite nature of ψ_a and ψ_b , but to confirm the chiral order, we need to verify if the current is finite within the phase. Similarly, we have to verify whether the Mott insulator exhibits chiral behaviour.

It becomes evident that as u increases, the system goes into the Mott insulator phase at higher μ values and remains within this phase over a longer range of chemical potential μ . Furthermore, calculating the current is necessary to confirm the chirality of the system.

3.4 Varying perpendicular hopping



Figure 3.4: Varying t_p in the Superfluid (SF) phase to observe the behavior of ψ as a function of length



Figure 3.5: Varying t_p in the Superfluid (SF) phase to observe the behavior of ψ as a function of length

| t_p | $ \psi_3^a - \psi_2^a $ | $ \psi_3^b - \psi_2^b $ |
|-------|---------------------------|---------------------------|
| 0.0 | 0.00 | 0.00 |
| 0.5 | 0.06 | 0.06 |
| 1.0 | 0.12 | 0.12 |
| 1.5 | 0.16 | 0.16 |

Table 3.1: Variation of order parameter ψ with t_p

We see that increasing the perpendicular hopping t_p within the superfluid phase enhances tunneling between different chains of the ladder structure. This enhanced tunneling is reflected by a larger amplitude of the order parameter ψ , indicating that the bosons become more delocalized and exhibit greater coherence across the ladder. As a result, the system demonstrates stronger superfluid behavior, with bosons able to flow more freely between chains, contributing to a more robust superfluid phase. The figures demonstrating its nature are given in 3.4 and 3.5.

3.5 Current-current correlation function



Figure 3.6: Value of Current-current correlation function and ψ as a function of u



Figure 3.7: Current-current Correlation Function vs μ for various u

In 3.6 and 3.7 we present plots for increasing values of u. On the left, we've graphed the order parameter ψ against μ to clarify the system's phases. It is evident that when $\psi = 0$, the system behaves as an insulator, whereas in other regions, it demonstrates a superfluid phase. On the right, we've analyzed the current-current correlation function to discern the system's chiral characteristics. Observing the figures, we note that at U = 5, finite current-current correlations persist consistently implying that the phases that are present are the Chiral Superfluid phase(CSF) and Chiral Mott Insulator phase(CMI). However, as U increases, these correlations tend towards zero and there is a phase transition from the Chiral Mott Insulator(CMI) to the regular Mott Insulator phase(MI).

From the graphs above, we can conclude that our system exclusively exhibits the chiral superfluid phase, as opposed to the regular superfluid phase when ψ is finite. This conclusion is supported by the fact that the system consistently maintains a finite

staggered order parameter ψ along with finite current-current correlation function values throughout our observations. Conversely, in the insulator region where $\psi = 0$, we observe a transition from the Chiral Mott insulator (CMI), characterized by finite current correlation, to the regular Mott Insulator (MI) phase, where the current correlation tends towards zero as u increases.

We examined the current correlation function between two sites, i and k, in equation 2.4 to identify the staggered pattern of current within the lattice.

| Current-current correlation | | |
|-----------------------------|-------------|--|
| $j_2 * j_3$ | $j_2 * j_4$ | |
| 0.409595 | -0.246191 | |
| 0.399491 | -0.230475 | |
| 0.405419 | -0.245394 | |
| 0.409213 | -0.249794 | |

Table 3.2: The current-current correlation function between first and second neighbors

The subscript numbers correspond to the site numbers of the lattice, with 2, 3, and 4 positioned at the center of the lattice length.

As can be seen in 3.2, we observe a change in sign as we transition from the current correlation of one site to the next in the lattice. This variation indicates the staggered nature and the continuous shift in directional preference of the current within the lattice.

Chapter 4

CONCLUSIONS

4.1 Introduction

In this Chapter, we will conclude our research paper by summarizing the findings derived from our results and discussing potential future endeavors in this field that may have broader implications for the field of physics.

4.2 Conclusions

In summary, our study of the one-dimensional Bose-Hubbard ladder model with an induced flux has provided insights into the behavior of quantum systems under the influence of perturbations. Through the combined use of Cluster Mean Field Theory (CMFT) and Density Matrix Renormalization Group (DMRG) techniques, we have been able to understand the interplay between particle interactions and flux-induced effects.

Our results shed light on key phenomena, including the emergence of special phases such as the Chiral Mott insulator (CMI), regular Mott Insulator(MI), and Chiral Superfluid(CSF) phases when flux is induced through hopping. By systematically varying parameters such as the onsite interaction strength (u), chemical potential (μ) , and inter-layer and intra-layer hopping strengths t_a, t_b, t_p , we have identified the critical behaviour of our system. Our study has uncovered features unique to the one-dimensional Bose-Hubbard ladder model where the induced flux introduces an additional degree of freedom.

We conclude that using the techniques of combined Central Mean Field Theory(CMFT) and Density Matrix Renormalization Group(DMRG) we have been able to show the existence of unique phases. At small interactions(U) we see that Chiral Superfluid(CSF) transitions into Chiral Mott insulator(CMI) as μ increases. At higher interaction values(u) in the insulator region, we see a transition from Chiral Mott Insulator(CMI) to regular Mott Insulator(MI). Chirality which is a time reversal symmetry is identified in our system from finite values of the current-current correlation function.

4.3 Future work

Looking ahead, our findings lay the groundwork for future research directions in this domain. There is scope in calculating the current-current correlation function across the entire lattice length as the distance between the two sites i and k in 2.4, over which we calculate current correlations tends to infinity to understand its features and identify points where it vanishes in the Mott Insulator phase and remains finite in the Chiral Mott and Chiral Superfluid phases. Plotting the phase diagrams of the system will provide significant insight into the significance of each phase as functions of μ and u. We can anticipate two sections within a Mott lobe: a Chiral Mott part where current exists and a regular Mott section where current vanishes.

Exploring the connections between the one-dimensional Bose-Hubbard ladder model and other quantum systems, such as spin model systems, could result in interesting insights into aspects of quantum phase transitions.

In summary, our research contributes to the ongoing task of understanding the complexities of quantum matter and provides a platform for future explorations. By addressing fundamental questions in quantum physics, we aim to contribute to the advancement of scientific knowledge.

4.4 Drawbacks

- A higher number of density matrix states was causing the code to slow down, and at around 45 states, it encountered a segmentation error due to insufficient space for allocation.
- There have been few studies on ultracold atoms utilizing the combined techniques of CMFT with DMRG, resulting in limited available literature on the subject.
- Current is a complex quantity, so in a system where we have assumed real quantities, we are unable to calculate the true value of the current present.

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