2022 Summer Project Report

Numerical simulation of low temperature phases of a bosonic gas in an optical lattice

Name:
Akshay Shankar

Supervisor:
Dr. Sanjeev Kumar

1 Introduction

Ultra-cold atoms trapped in optical lattices have been one of the top candidates for the construction of analog quantum simulators since the idea was conceived in Feynman's seminal paper [1]. With the recent development of various cooling and trapping mechanisms for atoms, realizing such an experimental setup has become an achievable goal today. This opens up the scope to understand many strongly correlated systems in condensed matter physics that are otherwise hard to study analytically or through numerical simulations [2]. This summer project focuses on studying the physics of the Bose-Hubbard model which can then be mapped to an experimental optical lattice setup that serves as a quantum simulator.

2 Bose-Hubbard model

Neutral bosonic atoms can be trapped using lasers [3], as the electric field induces a temporary dipole moment which then couples to same the field to generate an effective periodic potential modulating over space. This creates an optical lattice for the bosons. Further, at low temperatures, we can assume only lowest energy-band physics will dominate, and the bosons only weakly interact with each other.

Given these assumptions, we can re-write the general second-quantized hamiltonian in terms of the Wannier basis to get the Bose-Hubbard model:

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_1 n_i(n_i - 1)$$

Where, $a_i(a_i^\dagger)$ is the annihilation (creation) operator of the Wannier states at the i^{th} lattice site, and n_i is the corresponding number operator. t is the "hopping" parameter, and U is the on-site interaction energy; both of which set the energy scales of competing mechanisms in the system. It is interesting to note that when t and U are mapped to the experimental parameters (laser intensity, atomic polarizability, etc), they are not independent parameters. However, using the phenomenon of Feshbach resonance [4] and varying laser intensities, it is possible to tune U independently to explore a wider range of the parameter space.

2.1 Quantum phases of the system

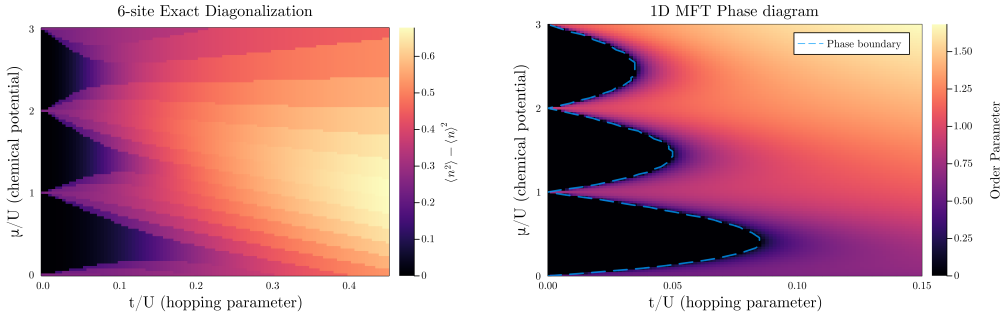
At low temperatures, thermal fluctuations are dominated by quantum fluctuations which drive the phase transitions in this regime. As there are two competing terms in the hamiltonian, two phases can be realized in the system, characterized by the breaking of the U(1) symmetry (global phase invariance) of the hamiltonian.

- **Mott insulator:** When $U/t >> 1$, the bosons are restricted to occupy a single lattice site with minimal hopping. This results in an integer filling of all the sites, and this incompressible phase characterizes the mott insulator.

- **Superfluid:** When $U/t << 1$, the bosons can easily hop across lattice sites and condense to form a BEC. In the presence of weak interactions, the condensate also exhibits superfluid properties. As opposed to the mott insulator, this phase has non-integer filling of the lattice sites as the bosons are delocalized over the entire lattice.

3 Numerical approaches

A complete analytical solution is not possible for the BHM beyond the 1-D case. As a result, we turn to numerical simulations to study the phase diagram of complicated geometries in higher dimensions. Following are a few basic approaches that were implemented, along with the corresponding phase diagrams generated using them.



(a) Exact Diagonalization (b) Mean Field

Figure 1: 1D Bose Hubbard Model; Phase Diagram

The purple regions indicate Mott Insulator lobes, and the rest indicate a Superfluid phase. The order parameter utilized varies based on the specific numerical method, but we still see some resemblance of the phase boundary in the diagrams generated. The 1-D case is pathological as it exhibits a BKT transition at the tip of the Mott Insulator lobes, but qualitatively, we see that the Mean-Field diagram is not too bad (and it gets better as the dimensionality is increased).

3.1 Exact Diagonalization

If we consider N bosons in M lattice sites, we can enumerate the number basis for the system to create an N-particle hilbert space (or a $1...N$-particle fock space, depending on the ensemble used) of dimensionality $(N+M-1)!/N!(M-1)!$. The hamiltonian matrix can then be constructed and diagonalized to obtain the ground state of the system [5]. The superfluid order parameter in this case would be the variance of the number operator on a particular lattice site. This algorithm however does not scale well with the lattice size (exponential growth of the matrix dimension), and smaller lattices are polluted with finite-size effects (for e.g. the lack of a sharp phase transition). This motivates us to look for better methods.

3.2 Mean Field theory

In this approach, we decompose the hopping term (using the approximation $\hat{a}_i = \psi + \delta\hat{a}_i$ where ψ is a c-number) which decouples neighbouring lattice sites to reduce the hamiltonian as a sum of single site hamiltonians. In doing so, we ignore all higher order quantum fluctuations $\mathcal{O}(\delta\hat{a}^2)$ and represent the global state as a product wave-function over the lattice sites. By nature of this construction, the MFT cannot predict non-local phases which becomes important in case of the extended BHM. For the BHM, however, we see that the phase diagrams are qualitatively quite insightful. The superfluid order parameter in this case is $\psi = \langle \Psi_{gs} | a_i | \Psi_{gs} \rangle$ which can be obtained by solving the mean-field hamiltonian in a self-consistent manner.

3.3 Cluster Mean Field theory

While the mean field approach gives a qualitative picture, the exact phase boundaries are not captured with good accuracy. To improve upon this, we can combine the ideas of exact diagonalization with the mean field theory in the following way; we can divide the lattice into clusters, and treat the sites inside the cluster exactly, while treating the inter-cluster couplings at the edges in the mean-field level [6]. In general, there can be several order parameters based on the geometry of the clusters and these can be obtained in a self-consistent manner similar to the naive mean field approach. As we would expect, the phase boundary seems to converge to its exact values as the number of sites in the cluster is increased.

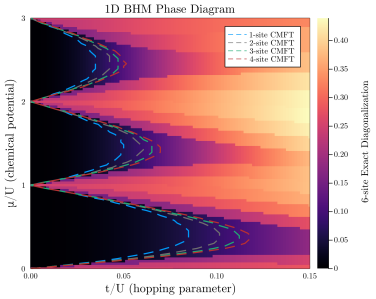


Figure 2: CMFT phase diagram of the BHM

Regardless, the cluster mean field theory clearly has better results over naive mean field theory. There are more accurate methods that one can use, such as Density Matrix Renormalization Group (DMRG) or Quantum Monte Carlo (QMC), however these were not implemented in this project.

4 Extended Bose-Hubbard model

Another closely related model that is of interest is the eBHM which builds upon the BHM with an extra term encompassing the inter-site interaction (in addition to the on-site interaction):

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_1 n_i(n_i - 1) + \boxed{V \sum_{\langle i,j \rangle} n_i n_j}$$

This hamiltonian can be mapped to any bosonic lattice system with atoms that have long-range interactions (such as dipole moments). In this manner, one can engineer different kinds of hamiltonians (including new terms) by using bosonic atoms interacting in different ways. The introduction of the new term in the eBHM gives rise to two new density modulated phases [6, 7], Density Waves (analogue to Mott Insulator) and Supersolid (analogue to Superfluid). Both of these phases have rich physics involved, and have been a widely discussed topic in the cold atom community over the past few decades.

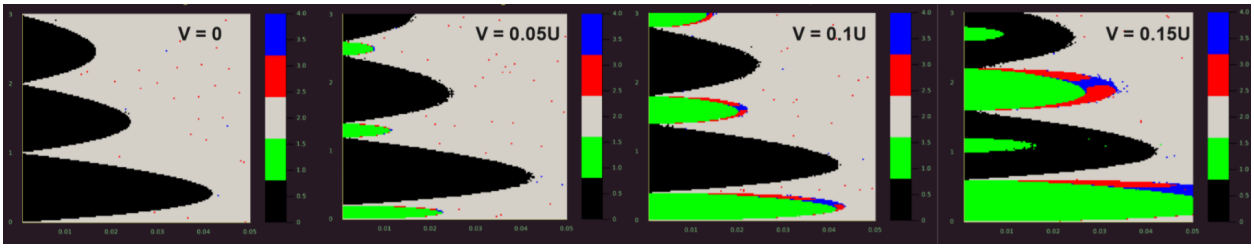


Figure 3: MFT phase diagram of the eBHM

Above is a mean-field plot of the eBHM phase diagram as the interaction term is increased, and we see that other than the BHM phases (Black - Mott Insulator, Grey - Superfluid), two new phases start to emerge (Green - Density wave, Red - Supersolid), giving rise to a richer phase diagram. The implementation of MFT for the eBHM faced several convergence issues due to which the phase diagram has some noise and non-physical phases (Blue).

5 Conclusion

This work served as a preliminary exploration of the BHM and the eBHM, as a means to characterize and understand the various phases that can be detected in the system. Further work is planned to implement Quantum Monte Carlo algorithms to obtain more accurate details of the phases in the eBHM. This is being done in collaboration with an experimental group in Stuttgart that is setting up a quantum simulator experiment using dipolar dysprosium atoms.

References

[1] Feynman, R.P., Int J Theor Phys 21, 467–488 (1982)

[2] Maciej Lewenstein , Anna Sanpera , Veronica Ahufinger , Bogdan Damski , Aditi Sen(De) Ujjwal Sen (2007), Advances in Physics, 56:2, 243-379

[3] Rudolf Grimm, Matthias Weidemüller, Yurii B. Ovchinnikov, Advances In Atomic, Molecular, and Optical Physics, Academic Press, Volume 42, 2000, Pages 95-170,

[4] Cheng Chin, Rudolf Grimm, Paul Julienne, and Eite Tiesinga, Rev. Mod. Phys. 82, 1225

[5] J M Zhang and R X Dong, 2010 Eur. J. Phys. 31 591

[6] T. McIntosh, P. Pisarski, R. J. Gooding, and E. Zaremba, Phys. Rev. A 86, 013623

[7] Davide Rossini and Rosario Fazio 2012 New J. Phys. 14 065012

[8] S. Baier, M. J. Mark, D. Petter, K Aikawa, L. Chomaz, Z. Cai, M. Baranov, P. Zollerand, F. Ferlaino, Science, Vol 352, Issue 6282 pp. 201-205