

# Bose-Einstein Condensation in the Ionic Bose-Hubbard Model

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## 1 Introduction

The quantum phase transition from a Bose-Einstein condensate to a state with localized atoms can be experimentally realized by applying a periodic potential created by interfering laser light to a cold alkali gas. The Ionic Bose-Hubbard model (IBHM) has been proposed for studying the transition [1]. In this paper I will discuss the model and some possible applications of linked cluster expansions to study the associated quantum phase transition.

An exotic form of matter in which a macroscopic collection of bosons condenses into a single particle state was predicted long before it could be realized experimentally. The original prediction was for a non-interacting system, but after the observation of super-fluidity in liquid  $^4\text{He}$ , a system with strong interactions, London suggested that the  $^4\text{He}$  atoms were still condensing. Recent advances in laser cooling and magnetic traps have made it possible to observe Bose-Einstein condensation (BEC) in ultra-cold alkali gases. By applying a periodic potential, the strength of which can be varied, the BEC can be turned on or off. When the periodic potential is very strong at low temperatures the system is in a Mott insulator state, so the transition from the BEC to the Mott insulator state can be studied.

Linked cluster expansions provide a method of calculating numerically the presence or absence of a BEC. On a modern workstation, it is possible to calculate a series for an extensive quantity (in this case the reduced one particle density matrix) to higher than twelfth order. Using extrapolation techniques, the properties of the transition can be studied.

## 2 The Model

The cold alkali gas system is modeled as a lattice gas of hard core bosons with an imposed periodic potential. The Hamiltonian is written for a  $d$  dimensional hyper-cubic lattice with  $L^d$  sites. The Ionic Bose-Hubbard model has the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \alpha \sum_i (-1)^i a_i^\dagger a_i + U \sum_i a_i^\dagger a_i (a_i^\dagger a_i - 1) \quad (1)$$

where  $a_i^\dagger$  creates a boson on site  $i$ . The first term, the hopping term, allows for the “hopping” of a boson from site  $i$  to a neighboring site  $j$  (the angle bracket  $\langle i, j \rangle$  indicates nearest neighbors). In this paper, we will consider  $U = \infty$ , which restricts the occupation of a site to be 1 or 0 (hard-core bosons). The term with  $\alpha$  is a periodic potential that favors occupation of one sub-lattice of a bipartite lattice.

There is an exact mapping from the bosons to a spin model with

$$\begin{aligned} a_i^\dagger &= S_i^x + iS_i^y \equiv S_i^+ \\ a_i &= S_i^x - iS_i^y \equiv S_i^- \\ a_i^\dagger a_i &= S_i^z + \frac{1}{2} \end{aligned} \quad (2)$$

With a Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_j^+ S_i^-) + \alpha \sum_i \left[ \frac{1}{2} + (-1)^i S_i^z \right] \quad (3)$$

$$= - \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) + \alpha \sum_i \left[ \frac{1}{2} + (-1)^i S_i^z \right]$$

where a constant has been added to make the periodic potential positive.

We define the reduced one particle density matrix

$$\gamma(i, j) = \langle a_i^\dagger a_j \rangle = \langle S_i^+ S_j^- \rangle = \langle S_i^x S_j^x + S_i^y S_j^y \rangle \quad (4)$$

BEC occurs when the matrix  $\gamma(i, j)$  has an eigenvalue of the order of the number of particles in the thermodynamic limit. This definition of BEC is discussed in [2] and [3], and a more modern review of BEC in the alkali gases is presented in [4].

### 3 Phase Diagram

Recent work [1] proves that in three or higher dimensions, for sufficiently small  $\alpha$  and temperature, BEC occurs, while at sufficiently large  $\alpha$  or temperature there is no BEC. Figure 1 is a schematic phase diagram for dimensions  $d \geq 3$ . In two dimensions, the same proof holds for  $T = 0$ .

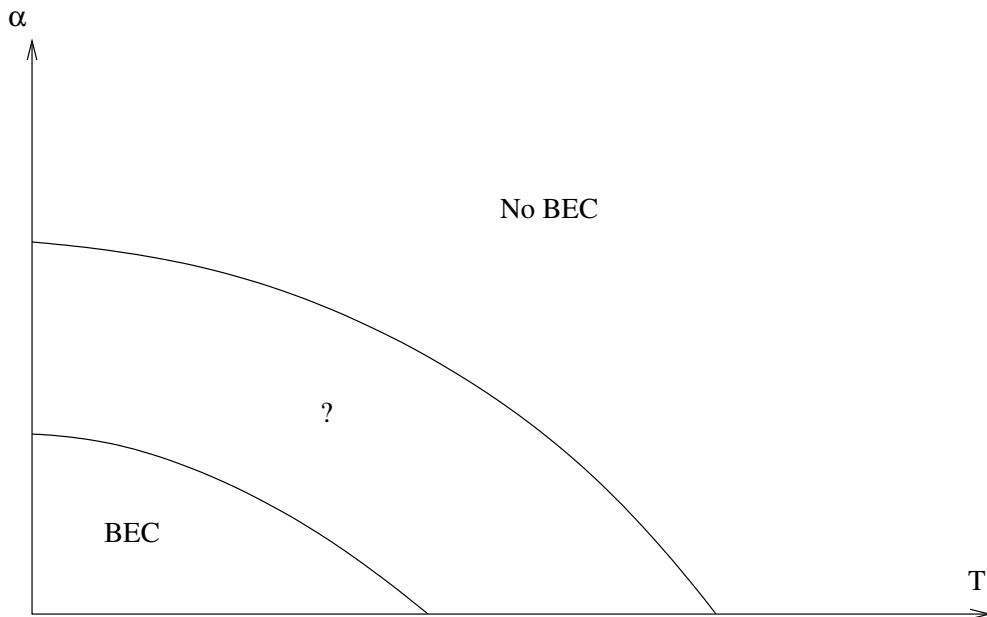


Figure 1: Phase diagram of the IBHM with  $d \geq 3$

This implies that in two dimensions, at  $T = 0$ , there is a critical  $\alpha_c \neq 0$  that marks the phase transition from a Mott insulator ( $\alpha > \alpha_c$ ) to a BEC ( $\alpha < \alpha_c$ ).

### 4 Linked Cluster Expansions

Linked cluster expansions allow us to calculate an extensive property on a lattice as a power series, exact to a given order, using a finite number of graphs [5],[6]. In the IBHM, this paper will focus on possibilities of calculating the reduced single particle density matrix ( $\gamma(i, j) = \langle a_i^\dagger a_j \rangle$ ) on a two dimensional square lattice.

For each cluster we construct the perturbation expansion for  $\gamma(i, j)$ . Then the results for the various clusters are combined via subgraph subtraction which yields the quantity per site on the infinite lattice, which will remain finite only if BEC occurs.

Since most of the embeddings will give the same weight calculation as other embeddings, we can save a lot of computation by performing a weight calculation on only one of a set of embeddings with the same

topology. For this, we can use our list of embeddings to generate a list of topologies, and a lattice constant for each topology.

Once we have the list of topologies, we can then construct a power series for the quantities on a finite cluster.

We begin by writing our Hamiltonian as

$$\mathcal{H} = \alpha \left( \mathcal{H}_0 + \frac{1}{\alpha} \mathcal{H}_1 \right) \quad (5)$$

where we know the ground state of the unperturbed Hamiltonian  $\mathcal{H}_0$ . The result of [1] show that the ground state at  $\alpha = \infty$  at half filling is a Mott insulator (i.e. the state with occupancy of all sites of the favored sub-lattice). So as one expansion, we can take

$$\begin{aligned} \mathcal{H}_0 &= \sum_i (-1)^i a_i^\dagger a_i \\ \mathcal{H}_1 &= -\frac{1}{2} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) \end{aligned} \quad (6)$$

where we are turning on the hopping as we increase  $\frac{1}{\alpha}$ . This expansion is shown as the dashed line in figure 2. We expect to see a critical  $\alpha_c$  where the correlation length diverges, after which the series expansion is no longer meaningful.

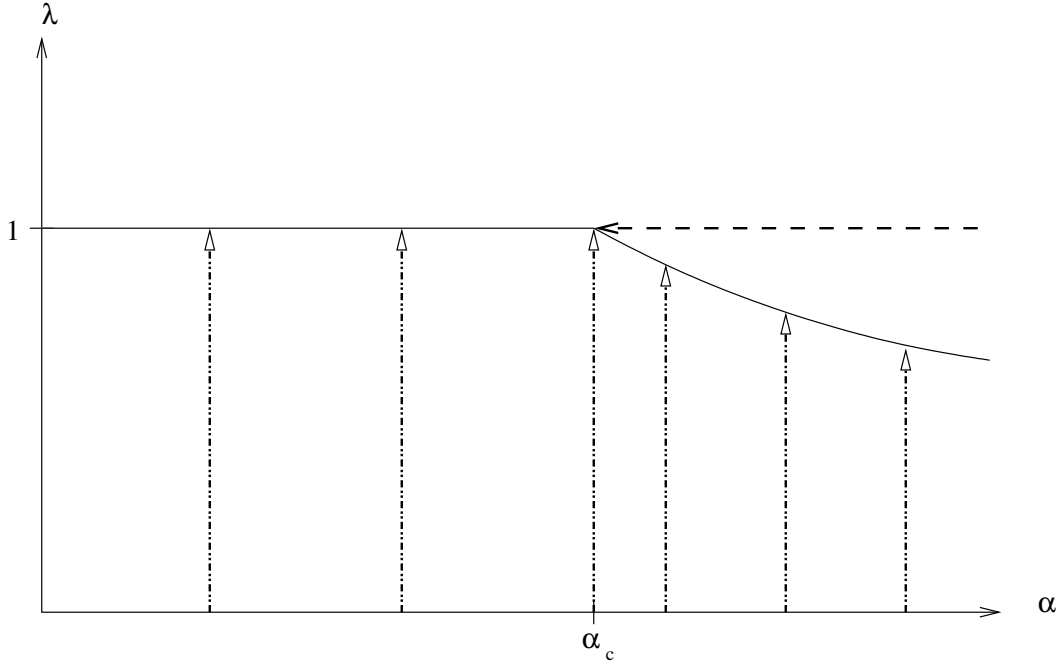


Figure 2: Possible expansions for the  $d = 2$  IBHM

Another expansion that is possible involves the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \lambda \mathcal{H}_1 \quad (7)$$

where

$$\mathcal{H} = - \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) + \alpha \sum_i (-1)^i S_i^z \quad (8)$$

with a spin rotation

$$\mathcal{H} = - \sum_{\langle i,j \rangle} (S_i^z S_j^z + S_i^y S_j^y) + \alpha \sum_i (-1)^i S_i^x \quad (9)$$

so that we can take

$$\begin{aligned}\mathcal{H}_0 &= - \sum_{\langle i,j \rangle} S_i^z S_j^z \\ \mathcal{H}_1 &= - \sum_{\langle i,j \rangle} S_i^y S_j^y - \alpha \sum_i (-1)^i S_i^x\end{aligned}\tag{10}$$

where now we recover our original model when  $\lambda = 1$ . The expansion should behave as long as  $\alpha < \alpha_c$ . When  $\alpha > \alpha_c$ , we should see a divergence of the correlation length for some  $\lambda < 1$ . These expansions are shown as the dot dot dash lines in figure 2.

## 5 Conclusion

This paper has discussed the Bose-Einstein condensate to Mott insulator transition in the Ionic Bose-Hubbard model. Recent work proves the occurrence of BEC for small enough periodic potential and temperature, and the absence of BEC at a large periodic potential at low temperature. Some possible applications of linked cluster expansions to the model have been proposed. It is also possible to perform the same calculations in one dimension, however, no true BEC can occur in one dimension.

## References

- [1] M. Aizenman, E.H. Lieb, R. Seiringer, J.P. Solovej, J. Yngvason  
Phys. Rev. A **70**, 023612 (2004)
- [2] O. Penrose, L. Onsager, Phys. Rev. **104**, 576 (1956)
- [3] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962)
- [4] A.J. Leggett, Rev. Mod. Phys. **73**, 307 (2001)
- [5] M.P. Gelfand, R.R.P. Singh, Adv. Phys. **49**, 93 (2000)
- [6] W.H. Zheng, C.J. Hamer, R.R.P. Singh, S. Trebst, and H. Monien,  
Phys. Rev. B **63**, 144410 (2001)