Critical Phenomena of the Bose-Hubbard Model in Ultracold Atoms

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Ultracold bosons in optical lattices are interesting physical systems in which precision experiments meet theoretically tractable examples of strongly-correlated many-body states. The Bose-Hubbard model is a very successful theoretical treatment of many systems that have been realized experimentally to date. In this paper, we examine how the critical properties of the Bose-Hubbard model correspond to the properties of the Landau-Ginzburg free energy expansion studied extensively in class. With the correspondence of the two systems in hand, we examine the phase diagram of the model under the mean-field approximation and how coupling to a gauge potential affect the phase boundaries.

Starting with the realization of Bose-Einstein condensation[1, 2] and Fermi degeneracy[3] in atomic gases, one goal of atomic physics has been observing the emergent phenomena of complicated many-body physics in ultracold systems. This is a particularly attractive goal due the relative simplicity and tunability of atomic interactions, and the ability to realize calculable systems[4]. An important long-term goal of atomic physics is to make contributions to the microscopic understanding of many-body interactions and phase transitions beyond those described by Landau's symmetry-breaking theory. A particularly important model in both atomic physics experiments and condensed matter physics–one that manages to connect to both Landau-Ginzburg theory and physics beyond this approach–is the Bose-Hubbard model. This paper aims to develop a basic understanding of the predictions of this model and how they relate to both Landau-Ginzburg theory but also physics beyond this paradigm.

BOSE HUBBARD MODEL AND LANDAU-GINZBURG EXPANSION

The Landau-Ginzburg description of universal behavior across phase transitions is based on the statistics of a non-relativistic order parameter field[5]. In class, this description took the form of a phenomenological expansion of the free energy density in terms of the order-parameter. However, in experimental realizations of quantum phase transitions–especially in atomic physics where a major experimental goal is quantum simulation of many-body phenomena–the physics is instead motivated by a microscopic description of the interacting particles[6].

An important model of interacting many-body systems that is microscopically realizable in atomic physics experiments with ultracold bosons in optical lattices is the Bose-Hubbard model. We wish to examine the implications–specifically the phase diagram and critical properties of thermodynamic variables–of this model of interacting systems. To begin with, we wish to reconcile the microscopically-motivated, Bose-Hubbard description with the phenomenological description of Landau-Ginzburg theory covered in class.

The Bose-Hubbard model is commonly written in a second-quantized formalism that reads:

$$H = -t\sum_{\langle ij\rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i \quad (1)$$

Here we have the following free parameters determined by the microscopic details of the system–the hopping energy t, the interaction energy U; and the global chemical potential μ.

In optical lattice systems, this Hamiltonian is derived from the first-quantized equivalent that includes the trap and lattice potentials as well as kinetic energy and a two-body, s-wave contact interaction term[6, 7]:

$$H = \sum_i \left[\frac{\vec{p}_i^2}{2m} + V_0 \sin^2(\vec{k}\cdot\vec{x}_i) + V_{trap}(\vec{x}_i)\right] + \frac{1}{2}\frac{4\pi\hbar^2 a_s}{m}\sum_{i\neq j}\delta^3(\vec{x}_i - \vec{x}_j) \quad (2)$$

The second-quantized version is obtained by projecting this Hamiltonian onto bosonic field operators: $\hat{\psi}(\vec{x}) = \sum_i \hat{b}_i w_i(\vec{x} - \vec{x}_i)$,where $w_i(\vec{x} - \vec{x}_i)$ are Wannier functions of the i^{th} band, a basis wavefunction that diagonalizes the momentum and lattice contributions to the Hamiltonian[6]. The Bose-Hubbard model is obtained by restricting the sums to atoms in the lowest vibrational band of the lattice and to nearest neighbor interactions.

Since the trap potential usually has little curvature over over the separation of two lattice sites, and our interactions are local, we can combine the trap potential with the local chemical potential in (1) and thus represent the constants as:

$$t = \int d^3x\ w_1^*(\vec{x} - \vec{x}_j)\left(\frac{p^2}{2m} + V_0\sin^2(\vec{k}\cdot\vec{x})\right) w_1(\vec{x} - \vec{x}_i)$$

$$U = \frac{4\pi\hbar^2 a_s}{m}\int d^3x\ |w_1(\vec{x})|^4$$

$$\mu = \mu_{local} + V_{trap}$$

Now with microscopic justification of the terms in (1), we proceed with connecting this type of lattice model–different from the spin systems solved in class because of the non-local hopping contribution–to the Landau-Ginzburg free energy expansion in order to analyze the phase diagram of this model.

We begin as in [8] by noting the interaction and chemical potential parts of the Hamiltonian, H_0 below, are easily diagonalizable in the occupation number basis with eigenvalues:

$$\varepsilon(n) = \frac{U}{2}n(n-1) - \mu n \tag{3}$$

As a result, it is easiest to work in the interaction picture from time-dependent perturbation theory, but now introducing a Wick rotation from inverse temperature to a time-like parameter, τ as in, $\beta = i\tau/\hbar$. The interaction Hamiltonian now reads: $H_1 = e^{\tau H_0} H_1^t e^{-\tau H_0}$ where H_1^t is the hopping term of the Hubbard model. Thus, we can write down the partition function for (1) as:

$$Z = Tr\left[e^{-\beta H_0}\left\{\exp\left[i\int_0^\beta d\beta \; H_1(\beta)\right]\right\}\right]$$
$$Z = Z_0\left\langle T_\tau \exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \; H_1(\tau)\right]\right\rangle_0 \tag{4}$$

In addition, we enforce causality by adding the time-ordering to the integral. We can now relate this expression to that for the free energy of the system by:

$$\begin{aligned}\beta F &= -\ln Z \\ &= -\ln Z_0 - \ln\left\langle T_\tau \exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \; H_1(\tau)\right]\right\rangle_0\end{aligned} \tag{5}$$

This relation is now the starting point for all subsequent approaches to calculating critical properties of the Bose-Hubbard model. Equation (5) is, in general, not exactly solvable; the complicating feature of H_1 is that it is not localized to a single lattice site, but acts acts to couple two nearest-neighbor sites. This term can be approximated in several ways, using perturbation theory of field-theoretic treatments[9, 10], by variational methods[6, 11], by scaling relations[8], and by Monte-Carlo simulation[11]. In particular, this paper proceeds with a mean-field approach to the model that allows an initial understanding of the phases of the model and some predictions for thermodynamic behaviors.

MEAN-FIELD TREATMENT

We begin by looking at the operator H_1^t–the hopping Hamiltonian before transforming into the interaction picture. In the mean-field approximation, we define and assume a uniform order parameter in the ordered phase. Examining the Hamiltonian in the absence of hopping, we see that for $U > 0$ the system should have an ordered state where the number of atoms per site is minimized. Using this intuition, we define a complex order parameter, $\psi = \sqrt{n} = \langle a^\dagger \rangle = \langle a^\dagger \rangle$[10]. Using this order parameter, we can write:

$$\begin{aligned}H_1^t &= -t\sum_{\langle ij\rangle}\hat{a}_i^\dagger \hat{a}_j = -t\sum_{\langle ij\rangle}\left[\left(\langle\hat{a}_i^\dagger\rangle\hat{a}_j + \hat{a}_i^\dagger\langle\hat{a}_j\rangle\right) - \langle\hat{a}_i^\dagger\rangle\langle\hat{a}_j\rangle\right] \\ &= -t\sum_{\langle ij\rangle}\left[\left(\psi\hat{a}_i + \hat{a}_j^\dagger\psi\right) - \psi^2\right] \\ &= -2dt\sum_i\left[\left(\hat{a}_i^\dagger + \hat{a}_i\right)\psi - \psi^2\right]\end{aligned} \tag{6}$$

Since both terms generated by the substitution above are first order or greater in ψ, we first search for a zeroth order free energy per particle contribution. We see this in the constant first term on the right hand side of equation (5).

$$F_n = -\frac{1}{\beta}\ln Z_0 = \frac{U}{2}n(n-1) - \mu n \tag{7}$$

In addition, at zeroth order we have the stability condition $\delta F \leq 0$, so we can provide an estimate for the area in the μ-U parameter space where we have an ordered phase and equation (7) is non-zero.

$$\begin{aligned}&\delta F = F_n - F_{n\pm1} \leq 0, \text{ so:} \\ &\mu_+ \leq Un \\ &\mu_- \leq U(n-1)\end{aligned} \tag{8}$$

Thus, to zeroth order in the mean-field approximation we have an ordered phase with integer lattice fillings at all dimensions in the region: $U(n-1) \leq \mu \leq Un$. These regions are shown as the areas below the straight lines in figure 1 on the next page. Now let's examine higher order terms in ψ to see if this order persists.

We now extract terms of quadratic order in the order parameter from equation (5). Examining the interaction Hamiltonian, we notice one contribution of order ψ^2 that can be immediately calculated in the Landau-Ginzburg expansion because it is diagonal in the occupation number basis that H_0 is diagonal in.

$$\begin{aligned}&\beta F = -\ln Z_0 + 2dNt\psi^2 \ldots \\ &-\ln\left\langle \exp\left[\frac{2dt}{\hbar}\int_0^{\beta\hbar} d\tau \; \sum_i e^{\tau H_0}\left(\hat{a}_i^\dagger + \hat{a}_i\right)\psi e^{-\tau H_0}\right]\right\rangle_0\end{aligned}$$

Examining the third term above, we want to expand the interaction terms out to second order in ψ^2. Because we are expanding the cumulants of the interaction Hamiltonian, only connected (diagonal) terms will contribute to the expansion:

$$\left\langle H_1^2\right\rangle_0^c = (2dt)^2\beta\psi^2\sum_i\left\langle(\hat{a}_i^\dagger\hat{a}_i + \hat{a}_i\hat{a}_i^\dagger)\right\rangle_0 + O(\psi^4)$$

$$= (2dt)^2 N\beta\psi^2 \left(\frac{n}{F_n - F_{n-1}} + \frac{n+1}{F_{n+1} - F_n}\right) + O(\psi^4)$$
$$= (2dt)^2 N\beta\psi^2 \left(\frac{n}{U(n-1) - \mu} + \frac{n+1}{\mu - Un}\right) + O(\psi^4)$$

So the Landau-Ginzburg expansion of the free energy per particle for the Bose-Hubbard interaction reads:

$$F_n = \left(\frac{U}{2}n(n-1) - \mu n\right)$$
$$+2dt\left(1 + \frac{2dtn}{U(n-1) - \mu} + \frac{2dt(n+1)}{\mu - Un}\right)\psi^2 + O(\psi^4)$$

Now, we investigate how including such higher order terms of ψ changes the order we found in all dimensions at zeroth order approximation.

According to Landau-Ginzburg theory, minima in the free energy correspond to phase transitions so we look for a transition and find one corresponding to:

$$1 + \frac{2dtn}{U(n-1) - \mu} + \frac{2dt(n+1)}{\mu - Un} = 0 \qquad (9)$$

Solving the resulting quadratic equation for μ in terms of U:

$$\mu_\pm = \frac{1}{2}\left[U(2n-1) - 2dt\right] \pm \frac{1}{2}\sqrt{U^2 - 4dtU(2n+1) + 4d^2t^2} \qquad (10)$$

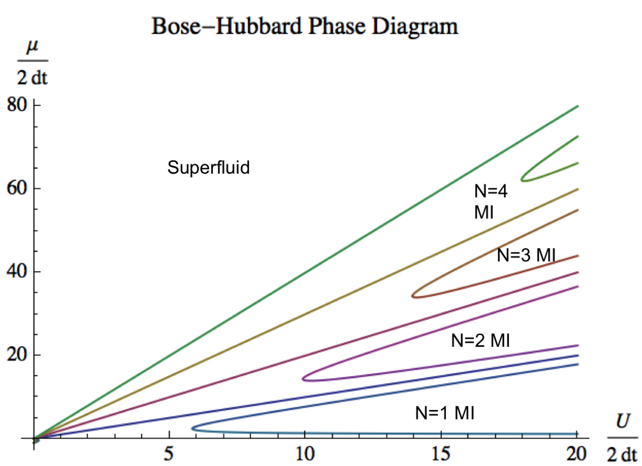

FIG. 1. Phase boundaries of the superfluid to insulator transition. The straight lines represent the zeroth order mean-field approximation, and the lobed structures the second-order approximation. The plateaus of different densities in the insulating phase are indicated.

The resulting mean-field prediction for the phase diagram of the Bose-Hubbard model is shown in Figure 1. In experiments with ultracold bosons in optical lattices, various radial distances from the trap center experience different local chemical potentials due to the definitions of this parameter on page one. Thus in an optical lattice at appropriate interaction energies, there can be several density plateaus that simultaneously exist in the trap. This structure has been experimentally verified both through precision spectroscopy of the lattice[12], and more recently directly observed in a quantum gas microscope[13]. In addition, notice that although we were able to map the Bose-Hubbard interaction onto a Landau-Ginzburg model, there is no lower critical dimension for this phase transition.

BOSE-HUBBARD MODEL COUPLED TO A VECTOR GAUGE FIELD

Now, we consider a simple generalization of the Bose-Hubbard model to one that is coupled to a vector gauge field. Engineered microscopically-varying gauge potentials are a recent addition to the many tools available to atomic physicists to simulate many-body physics in ultracold atomic gases[14]. In this section, we use the same microscopic formulation explained in the first section to derive a Bose-Hubbard model coupled to a gauge potential.

We include the addition of a gauge degree of freedom in our microscopic description of the system via the Hamiltonian:

$$H = \sum_i \left[\frac{(\vec{p}_i - q\vec{A})^2}{2m} + V_0 \sin^2(\vec{k}\cdot\vec{x}_i) + V_{trap}(\vec{x}_i)\right]$$
$$+\frac{1}{2}\frac{4\pi\hbar^2 a_s}{m}\sum_{i\neq j}\delta^3(\vec{x}_i - \vec{x}_j) \qquad (11)$$

As written, this addition has made the calculation of the tunneling matrix element much harder, but we can perform the so-called "Peierls substitution" by the transformation[15]:

$$\vec{k} \rightarrow \vec{k'} = \vec{k} - \frac{q\vec{A}}{\hbar} \qquad (12)$$

As discussed in ref. [15], this substitution modifies the time evolution of the system and gives rise to an additional phase factor in the direction in which $\vec{A}$ points. Following the argument in the appendix of ref. [7], we interpret this phase as a geometrical phase given by:

$$\gamma(C) = \frac{q}{\hbar}\oint_C \vec{A}\cdot d\vec{r} \qquad (13)$$

In view of the microscopic justification of the terms in the Bose-Hubbard Hamiltonian, we see that this additional phase factor does not effect the value of the interaction energy or chemical potential, but there is a non-zero contribution to the tunneling given by:

$$t = \int d^3x\ w_1^*(\vec{x} - \vec{x}_j)e^{-\frac{2\pi qi}{\hbar}\oint_C \vec{A}\cdot d\vec{x}}\left(\frac{p^2}{2m}\right.$$
$$\left.+V_0\sin^2(\vec{k}\cdot\vec{x})\right) w_1(\vec{x} - \vec{x}_i)e^{\frac{2\pi qi}{\hbar}\oint_C \vec{A}\cdot d\vec{x}}$$

$$t = e^{\frac{2\pi q i}{\hbar}\int_{\vec{x}_j}^{\vec{x}_i}\vec{A}\cdot d\vec{x}} \int d^3x \; w_1^*(\vec{x}-\vec{x}_j)\left(\frac{p^2}{2m} + V_0\sin^2(\vec{k}\cdot\vec{x})\right) w_1(\vec{x}-\vec{x}_i)$$

For simplicity, we restrict the problem now to two dimensions and assume the symmetric gauge for the vector potential. In addition, we define the phase factor to be $2\pi\gamma i$ as such to be uniform in two dimensions. With the given microscopic derivation of the new elements of the Bose-Hubbard model, we write out the Hamiltonian for the model coupled to a gauge degree of freedom:

$$H = -te^{2\pi\gamma i}\sum_{\langle ij\rangle}\hat{a}_i^\dagger\hat{a}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i \quad (14)$$

We see the gauge degree of freedom enters the Hamiltonian through the field, γ and luckily only modifies the part we were forced to handle perturbatively in the second section.

As a side note, it appears this Hamiltonian is the subject of current research and intense interest particularly in atomic and condensed matter physics because it is thought to describe states of the fractional quantum Hall type[14, 16–18]. We thus proceed to gain understanding for how the presence of the γ field modifies the order demonstrated in the second section.

Once again, since the phase factor only effects the hopping term, we can begin with the same zeroth-order prediction for the phase diagram as in the second term. The next step is to examine the interaction term and look for next-leading-order contributions. Begin with assuming γ is small so that we can expand the phase factor out to quadratic order. Then recalling equation (5) we see for zeroth-order in γ and second-order in ψ we recover the same phase diagram for the superfluid to insulator transition. The first order contribution in γ averages to zero, so to next order we have a term:

$$\left\langle H_1^2\right\rangle_0^c = (4t)^2\beta\psi^2\left(\frac{(2\pi\gamma i)^2}{2!}\right)\sum_i\left\langle(\hat{a}_i^\dagger\hat{a}_i + \hat{a}_i\hat{a}_i^\dagger)\right\rangle_0$$
$$= (4t)^2 N\beta\psi^2\left(-2\pi^2\gamma^2\right)\left(\frac{n}{U(n-1)-\mu} + \frac{n+1}{\mu - Un}\right)$$

Combining this leading order correction to the free energy expression in the last section we see up to order γ^2 and ψ^2:

$$F_n = \left(\frac{U}{2}n(n-1) - \mu n\right)$$
$$+4t\left(1 + \frac{4tn}{U(n-1)-\mu} + \frac{4t(n+1)}{\mu - Un}\right)(1 - 2\pi^2\gamma^2)\psi^2$$

We see that to this order the coupling to the gauge field does not change the shape of the μ-U phase diagram. However, we see that there is another way that this function can become singular:

$$\frac{\partial F}{\partial\psi} = 0 \Rightarrow \; \gamma = \frac{1}{4\pi^2} \quad (15)$$

Indicating possible interesting behavior at large γ corresponding to large flux per lattice site.

Examining the literature on such a topic[16, 19] we see that in high flux regimes the shape of the superfluid-insulator phase diagram does in fact change. However, the critical behavior observed in these systems is associated with topological structures such as vortices[14, 20], much like the phase transitions studied in class associated with the XY model, and two dimensional melting problems[5]. Theoretical and experimental studies of such transitions are ongoing because one of the most important outstanding problems in physics is the origin of a particular type of topological excitation, the $\nu = 5/2$ fractional quantum Hall state.

SUMMARY AND OUTLOOK

In conclusion, we have demonstrated the mean-field phase diagram of the Bose-Hubbard model, shown how such a model–with an interaction unlike the spin models covered extensively in class–corresponds to a Landau-Ginzburg description, and how to include effects in the Bose-Hubbard model like coupling to a gauge degree of freedom. In addition, we have discussed how the Bose-Hubbard model coupled to a gauge field also can lead to the interesting physics of topological charges, especially fractional quantum Hall states.

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