Effective Action Approach to Quantum Phase Transitions in Bosonic Lattices

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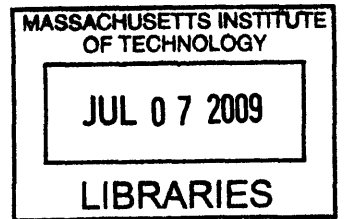in partial fulfillment of the requirements for the degree of

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Abstract

In this thesis, I develop a new, field-theoretic method for describing the quantum phase transition between Mott insulating and superfluid states observed in bosonic optical lattices. I begin by adding to the Hamiltonian of interest a symmetry breaking source term. Using time-dependent perturbation theory, I then expand the grand-canonical free energy as a double power series in both the tunneling and the source term. From here, an order parameter field is introduced, and the underlying effective action is derived via a Legendre transformation. After determining the Ginzburg-Landau expansion of the effective action to first order in the tunneling term, expressions for the Mott insulator–superfluid phase boundary, condensate density, average particle number, and compressibility are derived and analyzed in detail. Additionally, excitation spectra in the ordered phase are found by considering both longitudinal and transverse variations of the order parameter. Finally, these results are applied to the concrete case of the Bose-Hubbard Hamiltonian on a three dimensional cubic lattice, and compared with the corresponding results from mean-field theory. Although both approaches yield the same Mott insulator - superfluid phase boundary to first order in the tunneling, the predictions of the effective action theory turn out to be superior to the mean-field results deeper into the superfluid phase.

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Acknowledgments

Contents

Chapter 1

Introduction

Recent developments in the field of dilute ultracold quantum gasses [1, 2, 3, 4, 5] have led to the experimental investigation of atoms in periodic potentials [6]. They are a fascinating new generation of many-particle quantum systems as they allow for the study of a variety of solid-state phenomena under perfectly controlled conditions [4, 6, 7, 8, 9, 10, 11, 12]. For instance, bosonic lattice systems show a quantum phase transition for varying lattice depths. In deep lattices the tunneling between lattice sites is suppressed, and a Mott insulating state forms with a fixed number of bosons residing on each lattice site. For shallow lattices, however, the dominance of inter-site tunneling allows for bosons to spread coherently over the whole lattice, forming a superfluid. The occurrence of such a quantum phase transition between a Mott insulator and a superfluid is observable, for instance, in time-of-flight absorption pictures taken after switching off the lattice potential. They image momentum distributions integrated along one axis, and therefore by Heisenberg's uncertainty principle give information about the corresponding spatial distributions. Thus, the localization of atoms in the Mott phase results in diffuse absorption pictures, while the delocalized superfluid phase gives rise to Bragg-like interference patterns.

The theoretical analysis of this quantum phase transition is usually based on the

Bose-Hubbard model Hamiltonian [13, 14, 15, 16],

$$\hat{H}_{\mathrm{BH}} = \sum_{i} \left[\frac{1}{2} U \hat{a}_i^\dagger \hat{a}_i \left(\hat{a}_i^\dagger \hat{a}_i - 1 \right) - \mu \hat{a}_i^\dagger \hat{a}_i \right] - t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j, \qquad (1.1)$$

where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are bosonic annihilation and creation operators, μ is the chemical potential, and $\langle i, j \rangle$ signifies a sum over nearest neighbor sites i and j. Additionally, U parameterizes the on-site interaction energy between two atoms at a given site, and t characterizes the kinetic energy, in this case given by the tunneling of an atom between two neighboring lattice sites. The quartic on-site coupling term, however, makes an exact diagonalization of (1.1) impossible. Thus, while Monte-Carlo simulations have proven fruitful for obtaining numerical results [17, 18, 19], analytic descriptions of bosonic lattices near the quantum phase boundary have so far been typically limited to mean-field [13, 15] or strong-coupling approximations [20, 21]. Currently, the most precise analytic result for the whole Mott insulator-superfluid phase diagram in a three dimensional cubic lattice at zero temperature is found in Ref. [22]. Therein, a Landau expansion for an effective potential with a spatially and temporally global order parameter is derived. In this thesis, we generalize the results of Ref. [22] by allowing for a spatially and temporally varying order parameter, thus determining a Ginzburg-Landau expansion for the effective action. This allows us to obtain an approximate analytic description of bosonic lattice systems near the quantum phase boundary. This work is based primarily upon my previous paper, Ref [23]

To this end we proceed as follows. The remainder of this Chapter will present a derivation of the Bose-Hubbard model, and an overview of the Ginzburg-Landau theory of phase transitions. Then, In Chapter 2, we consider a very general type of Hamiltonian consisting of an arbitrary on-site interaction and an arbitrary tunneling term, of which the Bose-Hubbard Hamiltonian is a special case, and determine the grand-canonical free energy to first order in the tunneling term. This tunneling approximation is motivated by the fact that in three dimensions, the Mott insulator-superfluid quantum phase transition is observed to occur for small values of t/U (note that the tunneling expansion is related to the random-walk expansion of Refs.

[24, 25, 26]). Next, in Chapter 3 we introduce an order parameter field and derive a Ginzburg-Landau expansion of the effective action, allowing for the computation of physical quantities near the phase boundary in both the Mott insulator and the superfluid phase. Sections 3.1 and 3.2 present predictions of our effective-action theory for both static homogeneous and spatio-temporally varying order parameter fields, including expressions for the particle density, the compressibility, the superfluid density, and the excitation spectra. Finally, in Chapter 4, we specify our results to the Bose-Hubbard Hamiltonian, and compare them to the predictions of the standard mean-field theory. Although both approaches yield the same approximation for the location of the phase boundary, our effective action approach turns out to be superior to the mean-field theory for the following reasons. First, we demonstrate that the effective action approach leads to qualitatively better results deeper into the superfluid phase. Secondly, in contrast to the mean-field approximation, the effective action approach can be systematically extended to higher orders in the tunneling parameter in order to quantitatively improve the results, as has already been demonstrated for the case of the effective potential in Ref. [22].

1.1 Derivation of the Bose-Hubbard Model

We can see how Eq. (1.1) comes about by examining the setup of optical lattice experiments. bosons are confined using pairs of counter-propegating lasers aligned along all three spatial axes [4, 5, 6]. This establishes standing waves in all three dimensions, creating a cubic array of electric field intensity maxima. Due to the Stark effect. the bosonic atoms are attracted to these intensity maxima. as there electronic energy will be lower there due to level splitting. Thus. the effect of the laser beams is to establish a potential energy term in the Hamiltonian of the form

$$V_{\text{lattice}}(\vec{x}) = V_0 \sum_{\sigma} \sin^2\left(\frac{\pi \vec{x}_\sigma}{a}\right).$$ (1.2)

where $\sigma = 1, 2, 3$ is the spatial direction, and a is the laser wavelength. Additionally, we suppose that there is a hard-core repulsive interaction due to the presence of two atoms at the same point, parameterized by the coupling constant g. Putting these terms together, we can construct the second-quantized Hamiltonian for the lattice system as

$$\hat{H} = \int \mathrm{d}^3 x \, \hat{\psi}^\dagger(\vec{x}) \left[-\frac{\nabla^2}{2m} + V_{\text{lattice}}(\vec{x}) + g\hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x}) - \mu \right] \hat{\psi}(\vec{x}), \qquad (1.3)$$

where $\hat{\psi}(\vec{x})$ and $\hat{\psi}^\dagger(\vec{x})$ are the annihilation and creation operators for bosons at position $\vec{x}$. They satisfy the canonical commutation relations

$$\left[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}') \right] = \left[\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{x}') \right] = 0 \quad \left[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}') \right] = \delta(\vec{x} - \vec{x}'). \qquad (1.4)$$

Since the potential $V_{\text{lattice}}(\vec{x})$ is periodic in $\vec{x}$, we can identify each intensity maximum as a lattice site i and, via Bloch's theorem, switch to a basis of Wannier functions [27] $w_i(\vec{x})$ localized about i which satisfy

$$\int \mathrm{d}^3 x \, w_i^*(\vec{x}) w_j(\vec{x}) = \delta_{ij} \qquad (1.5)$$

In this basis. the bosonic field operators become

$$\hat{\psi}(\vec{x}) = \sum_i \hat{a}_i w_i(\vec{x}) \quad \hat{\psi}^\dagger(\vec{x}) = \sum_i \hat{a}_i^\dagger w_i^*(\vec{x}) \qquad (1.6)$$

where $\hat{a}_i^\dagger$ and $\hat{a}_i$ are bosonic creation and annihilation operators at site i obeying the standard commutation relations

$$\left[\hat{a}_i, \hat{a}_j \right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger \right] = 0, \quad \left[\hat{a}_i, \hat{a}_j^\dagger \right] = \delta_{ij}. \qquad (1.7)$$

For our analysis, the specific form of the Wannier functions is not important, but they can be found numerically if one is so inclined [28].

Up to now. our treatment has been exact. Now, however, we substitute the

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Wannier-function decomposition of the field operators into Eq. (1.3), and make the approximation that the Wannier functions are strongly localized enough that all but nearest neighbor overlap integrals can be neglected. With the definitions

$$t = -\int d^3x \, w_i^*(\vec{x}) \left[-\frac{\nabla^2}{2m} + V_{\text{lattice}}(\vec{x}) \right] w_j(\vec{x}) \tag{1.8}$$

and

$$U = g \int d^3x \, |w_i(\vec{x})|^4 \tag{1.9}$$

we recover the Bose-Hubbard Hamiltonian (1.1).

1.2   Ginzburg-Landau Theory

Our main tool for analyzing phase transitions in the Bose-Hubbard model will be the Ginzburg-Landau theory [29, 30]. The primary tenant of this framework is that different phases are characterized by different symmetry properties. In the case of the insulator-superfluid phase transition we will be examining, the relevant symmetry is the breaking of global $U(1)$ phase symmetry $\hat{a}_i \to \hat{a}_i e^{i\theta}$ in the superfluid ground state [30]. Clearly, from Eq. (1.1), this is a symmetry of the Hamiltonian, so that the breaking of it by the ground state of the system is referred to as *spontaneous symmetry breaking.*

The fundamental quantity of the Ginzburg-Landau theory is the order parameter, which quantifies the extent of the symmetry breaking. The order parameter should be 0 in the symmetric (in this case, the insulating state), and acquires a nonzero value at the phase boundary. Because we are interested in symmetry breaking of the creation and annihilation operator phases, we choose as our order parameter field

$$\psi_i = \langle \hat{a}_i \rangle \tag{1.10}$$

This quantity must acquire a nonzero value if the phase symmetry shown above is broken.

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To quantify the properties of the phase transition, a thermodynamic potential must be found which depends on the order parameter field. For us, this role will be served by the effective action Γ. Since the Hamiltonian does not break the phase symmetry, we expect the effective action to depend only on even powers of ψ_i. The standard Ginzburg-Landau theory proceeds by expanding the thermodynamic potential to fourth order in the order parameter. Since in equilibrium all thermodynamic potentials are stationary (i.e. their differentials are zero when the appropriate state variables are held fixed) [29], we can find the equilibrium value of the order parameter by setting the first derivative of Γ equal to 0. From there, many other thermodynamic quantities may be determined.

Chapter 2

The Grand-Canonical Free Energy

We consider bosons on a background lattice with lattice sites denoted by i. Suppose they are described by a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{2.1}$$

which depends on bosonic creation and annihilation operators $\hat{a}_i^\dagger$ and $\hat{a}_i$. We assume that $\hat{H}_0$ is a sum of local terms each diagonal in the occupation number basis, i.e.

$$\hat{H}_0 = \sum_i f_i(\hat{a}_i^\dagger \hat{a}_i) \tag{2.2}$$

so its energy eigenvalues are given by

$$E_{\{n_i\}} = \sum_i f_i(n_i). \tag{2.3}$$

As we will be working grand-canonically, we stipulate that the terms $f_i(\hat{a}_i^\dagger \hat{a}_i)$ include the usual $-\mu \hat{a}_i^\dagger \hat{a}_i$ dependence on the chemical potential μ. Also, we make the simplifying assumption that $\hat{H}_1$ is only a two-boson hopping term

$$\hat{H}_1 = -\sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j \tag{2.4}$$

with t_{ij} symmetric in i and j and $t_{ii} = 0$. As with the Bose-Hubbard model (1.1), $\hat{H}_0$ in Eq. (2.2) describes the bosonic on-site interaction, while $\hat{H}_1$ in Eq. (2.4) incorporates the tunneling of bosons between lattice sites. Note, however, that Eq. (2.1) with Eqs. (2.2) and (2.4) covers a significantly more general scenario than the Bose-Hubbard model. The on-site interaction in the Bose-Hubbard model (1.1) is a two-boson term with a global interaction strength, but in Eq. (2.2), however, we have allowed for the on-site interaction of any finite number of bosons. In addition, we have allowed the Hamiltonian to vary between lattice sites. Thus, our model is also capable of describing on-site disorder, which may arise from a local chemical potential, or from a local interaction [4, 13, 31]. Furthermore, Eq. (2.4) contains not only the tunneling of bosons between nearest neighbor sites as in Eq. (2.1), but also between arbitrarily distant sites.

As we are ultimately interested in investigating quantum phase transitions, we follow general field-theoretic considerations and add source terms to the Hamiltonian (2.1) in order to explicitly break any global symmetries [32, 33]

$$\hat{H}_1 \rightarrow \hat{H}_1' = -\sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left[j_i(\tau) \hat{a}_i^\dagger + j_i^*(\tau) \hat{a}_i \right]. \tag{2.5}$$

Since the source currents $j_i(\tau), j_i^*(\tau)$ depend explicitly upon the imaginary time variable τ, standard time-dependent perturbation theory may be used to find a perturbative expression for the grand-canonical free energy. To do this, we switch to the imaginary-time Dirac interaction picture [34], with operators given by

$$\hat{O}_D(\tau) = e^{\tau \hat{H}_0} \hat{O} e^{-\tau \hat{H}_0}, \tag{2.6}$$

where we have set $\hbar = 1$. In this representation, the Schrödinger initial value problem for the time-evolution operator takes the form

$$\frac{d}{d\tau} \hat{U}_D(\tau, \tau_0) = -\hat{H}_{1D}'(\tau) \hat{U}_D(\tau, \tau_0). \tag{2.7}$$

$$\hat{U}_D(\tau_0, \tau_0) = 1. \tag{2.8}$$

This is solved by the Dyson expansion

$$\hat{U}_{\mathrm{D}}(\tau, \tau_0) = 1 + \sum_{n=1}^{\infty} \hat{U}_{\mathrm{D}}^{(n)}(\tau, \tau_0), \tag{2.9}$$

$$\hat{U}_{\mathrm{D}}^{(n)}(\tau, \tau_0) = \frac{(-1)^n}{n!} \int_{\tau_0}^{\tau} \mathrm{d}\tau_1 \int_{\tau_0}^{\tau} \mathrm{d}\tau_2 \ldots \int_{\tau_0}^{\tau} \mathrm{d}\tau_n \hat{T} \left[\hat{H}'_{\mathrm{1D}}(\tau_1) \hat{H}'_{\mathrm{1D}}(\tau_2) \ldots \hat{H}'_{\mathrm{1D}}(\tau_n) \right], \tag{2.10}$$

where $\hat{T}$ is the standard imaginary-time ordering operator. The grand-canonical partition function for the system is defined as

$$\mathcal{Z} = \mathrm{tr} \left\{ \hat{T} e^{-\int_0^{\beta} \mathrm{d}\tau \hat{H}(\tau)} \right\}, \tag{2.11}$$

which can be rewritten as

$$\mathcal{Z} = \mathrm{tr} \left\{ e^{-\beta \hat{H}_0} \hat{U}_{\mathrm{D}}(\beta, 0) \right\}. \tag{2.12}$$

This gives the partition function $\mathcal{Z}$ as a functional of the currents. For brevity. we shall - in cases where no confusion may arise - suppress the arguments of functionals. Thus, by substituting Eqs. (2.9) and (2.10) into Eq. (2.12), we obtain

$$\mathcal{Z} = \mathcal{Z}^{(0)} + \sum_{n=1}^{\infty} \mathcal{Z}^{(n)}, \tag{2.13}$$

$$\mathcal{Z}^{(n)} = \mathcal{Z}^{(0)} \frac{(-1)^n}{n!} \int_0^{\beta} \mathrm{d}\tau_1 \int_0^{\beta} \mathrm{d}\tau_2 \ldots \int_0^{\beta} \mathrm{d}\tau_n \left\langle \hat{T} \left[\hat{H}'_{\mathrm{1D}}(\tau_1) \hat{H}'_{\mathrm{1D}}(\tau_2) \ldots \hat{H}'_{\mathrm{1D}}(\tau_n) \right] \right\rangle_0, \tag{2.14}$$

where

$$\mathcal{Z}_l^{(0)} = \mathrm{tr}\{ e^{-\beta \hat{H}_0} \} = \prod_l \sum_{n=0}^{\infty} e^{-\beta f_l(n)} \tag{2.15}$$

is the partition function of the unperturbed system, and

$$< \bullet >_0 = \frac{1}{\mathcal{Z}^{(0)}} \mathrm{tr} \left\{ \bullet \, e^{-\beta \hat{H}_0} \right\} \tag{2.16}$$

represents the thermal average with respect to the *unperturbed* Hamiltonian $\hat{H}_0$. This

can be expressed more compactly as

$$\mathcal{Z} = \mathcal{Z}^{(0)} \left\langle \hat{T} \exp\left(-\int_0^\beta d\tau \hat{H}'_{1D}(\tau)\right) \right\rangle_0 . \tag{2.17}$$

Inserting the explicit form of $\hat{H}'_{1D}(\tau)$ from Eqs. (2.5) and (2.6), we see that the expectation values appearing in Eq. (2.14) can be expanded in terms of Green's functions of the unperturbed system. Furthermore, since the grand-canonical free energy is given as a logarithm of the partition function

$$\mathcal{F} = -\frac{1}{\beta}\log\mathcal{Z}, \tag{2.18}$$

the Linked Cluster Theorem [35] tells us that $\mathcal{F}$ can be expanded diagrammatically in terms of *cumulants* defined as

$$C_{2n}^{(0)}(i'_1, \tau'_1; \ldots; i'_n, \tau'_n | i_1, \tau_1; \ldots; i_n, \tau_n) = \left.\frac{\delta^{2n} C_0^{(0)}[j, j^*]}{\delta j_{i'_1}(\tau'_1)\ldots\delta j_{i'_n}(\tau'_n)\delta j^*_{i_1}(\tau_1)\ldots\delta j^*_{i_n}(\tau_n)}\right|_{j=j^*=0} . \tag{2.19}$$

with the generating functional

$$C_0^{(0)}[j, j^*] = \log\left.\frac{\mathcal{Z}}{\mathcal{Z}^{(0)}}\right|_{t_{ij}\equiv 0} = \log\left\langle \hat{T}\exp\left\{-\left(\sum_i \int_0^\beta d\tau \left[j_i(\tau)\hat{a}_i^\dagger(\tau) + j_i^*(\tau)\hat{a}_i(\tau)\right]\right)\right\}\right\rangle_0 . \tag{2.20}$$

with only contributions from connected diagrams [36]. Note that this approach, rather than a decomposition of the Green's functions via Wick's theorem, must be used in our case as $\hat{H}_0$ is not necessarily quadratic in the creation and annihilation operators. Because $\hat{H}_0$ is local according to Eq. (2.2), the average in Eq. (2.20) factors into independent averages for each lattice site. It follows that $C_0^{(0)}[j, j^*]$ is a sum of local quantities, and thus the cumulants $C_{2n}^{(0)}(i'_1, \tau'_1; \ldots; i'_n, \tau'_n | i_1, \tau_1; \ldots; i_n, \tau_n)$ vanish unless

all site indices are equal. With this, we can write

$$C_{2n}^{(0)}(i_1', \tau_1'; \ldots; i_n', \tau_n' | i_1, \tau_1; \ldots; i_n, \tau_n) = {}_{i_1}C_{2n}^{(0)}(\tau_1', \ldots, \tau_n' | \tau_1, \ldots, \tau_n) \prod_{n,m} \delta_{i_n', i_m}, \quad (2.21)$$

so that it only remains to determine the local quantities ${}_iC_{2n}^{(0)}(\tau_1', \ldots, \tau_n' | \tau_1, \ldots, \tau_n)$. Using the definitions (2.19) and (2.20), we find that

$$_iC_2^{(0)}(\tau_1 | \tau_2) = \left\langle \hat{T}\left[\hat{a}_i^\dagger(\tau_1)\hat{a}_i(\tau_2)\right] \right\rangle_0 = G^{(0)}(i, \tau_1 | i, \tau_2), \quad (2.22)$$

where $G^{(0)}(i, \tau_1 | j, \tau_2) = \delta_{ij}G^{(0)}(i, \tau_1 | i, \tau_2)$ is the imaginary-time Green's function of the unperturbed system. Similarly,

$$\begin{aligned}
_iC_4^{(0)}(\tau_1, \tau_2 | \tau_3, \tau_4) = & \left\langle \hat{T}\left[\hat{a}_i^\dagger(\tau_1)\hat{a}_i^\dagger(\tau_2)\hat{a}_i(\tau_3)\hat{a}_i(\tau_4)\right] \right\rangle_0 \\
& - {}_iC_2^{(0)}(\tau_1 | \tau_3){}_iC_2^{(0)}(\tau_2 | \tau_4) - {}_i C_2^{(0)}(\tau_1 | \tau_4){}_iC_2^{(0)}(\tau_2 | \tau_3). \quad (2.23)
\end{aligned}$$

Note that local the quantity $_iC_4^{(0)}(\tau_1, \tau_2 | \tau_3, \tau_4)$ is symmetric under both the exchanges $\tau_1 \leftrightarrow \tau_2$ and $\tau_3 \leftrightarrow \tau_4$.

Because each power of the tunneling parameter t_{ij} is associated with a creation operator and an annihilation operator, and each power of $j_i(\tau)$ $(j_i^*(\tau))$ is associated with one creation (annihilation) operator, we can construct the connected diagrams which contribute to $\mathcal{F}$ according to the following rules [37]:

1. Each vertex with n lines entering and n lines exiting corresponds to a $2n$-th order cumulant $_iC_{2n}^{(0)}$.

2. Draw all topologically inequivalent connected diagrams.

3. Label each vertex with a site index, and each line with an imaginary-time variable.

4. Each internal line is associated with a factor of t_{ij}.

5. Each incoming (outgoing) external line is associated with a factor of $j_i(\tau)$ $(j_i^*(\tau))$.

6. Multiply by the multiplicity and divide by the symmetry factor.

7. Integrate over all internal time variables.

Each diagram is then multiplied by the appropriate factors of $j_i(\tau)$, $j_i^*(\tau)$, and t_{ij}, and all spacetime variables are integrated. Since $\hat{H}_0$ in Eq. (2.2) is diagonal in the occupation number basis and local, there can be no contributions from diagrams with one line. Thus, to first order in the tunneling t_{ij} and fourth order in the currents $j_i(\tau)$ we find

$$
\begin{aligned}
\mathcal{F} = F_0 - \frac{1}{\beta} \sum_i \Bigg\{ & \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \left[a_2^{(0)}(i,\tau_1|i,\tau_2) j_i(\tau_1) j_i^*(\tau_2) + \sum_j a_2^{(1)}(i,\tau_1|j,\tau_2) t_{ij} j_i(\tau_1) j_j^*(\tau_2) \right] \\
& + \frac{1}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \, a_4^{(0)}(i,\tau_1;i,\tau_2|i,\tau_3;i,\tau_4) j_i(\tau_1) j_i(\tau_2) j_i^*(\tau_3) j_i^*(\tau_4) \\
& + \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \sum_j t_{ij} \Big[a_4^{(1)}(i,\tau_1;i,\tau_2|j,\tau_3;i,\tau_4) j_i(\tau_1) j_i(\tau_2) j_j^*(\tau_3) j_i^*(\tau_4) \\
& + a_4^{(1)}(i,\tau_1;j,\tau_2|i,\tau_3;i,\tau_4) j_i(\tau_1) j_j(\tau_2) j_i^*(\tau_3) j_i^*(\tau_4) \Big] \Bigg\}.
\end{aligned}
\tag{2.24}
$$

where

$$
F_0 = -\frac{1}{\beta} \log \mathcal{Z}^{(0)} = -\frac{1}{\beta} \sum_i \log \left\{ \sum_{n=0}^\infty e^{-\beta f_i(n)} \right\}
\tag{2.25}
$$

is the grand-canonical free energy of the unperturbed system, and the respective

coefficients a_{2n} are given by the following diagrams and expressions:

$$a_2^{(0)}(i, \tau_1 | i, \tau_2) = \tau_1 \,\longrightarrow\!\!\bullet\!\!\longrightarrow\, \tau_2 = {}_iC_2^{(0)}(\tau_1 | \tau_2), \tag{2.26}$$

$$a_2^{(1)}(i, \tau_1 | j, \tau_2) = \tau_1 \,\longrightarrow\!\!\bullet\!\!\rightarrow\!\!\bullet\!\!\longrightarrow\, \tau_2 = \int_0^\beta d\tau_i C_2^{(0)}(\tau_1 | \tau)_j C_2^{(0)}(\tau | \tau_2), \tag{2.27}$$

$$a_4^{(0)}(i, \tau_1; i, \tau_2 | i, \tau_3; i, \tau_4) = \quad = {}_iC_4^{(0)}(\tau_1, \tau_2 | \tau_3, \tau_4), \tag{2.28}$$

$$a_4^{(1)}(i, \tau_1; i, \tau_2 | j, \tau_3; \imath, \tau_4) = \quad = \int_0^\beta d\tau_i C_4^{(0)}(\tau_1, \tau_2 | \tau, \tau_4)_j C_2^{(0)}(\tau | \tau_3). \tag{2.29}$$

In the next chapter, we will see how this expansion (2.24) of the grand-canonical free energy leads to the Ginzburg-Landau expansion of the effective action to first order in t_{ij}.

At this point, it is also worth making some observations about the two-particle Green's function $G(\imath, \tau_1 | j, \tau_2)$, defined in the standard way as

$$G(\imath, \tau_1 | j, \tau_2) = \left\langle \hat{T}\left[\hat{a}_i^\dagger(\tau_1)\hat{a}_j(\tau_2)\right] \right\rangle = -\beta \frac{\delta^2 \mathcal{F}}{\delta j_i(\tau_1)\delta j_j^*(\tau_2)} = \frac{1}{\mathcal{Z}} \mathrm{tr}\left\{ e^{-\beta \hat{H}_0} \frac{\delta^2 \hat{U}_D(\beta, 0)}{\delta j_i(\tau_1)\delta j_j^*(\tau_2)} \right\}. \tag{2.30}$$

This quantity can also be expanded diagrammatically in terms of cumulants, provided we realize that the effect of the prefactor $1/\mathcal{Z}$ in Eq. (2.30) is simply to cancel all disconnected diagrams [34], ensuring that the only diagrams that contribute are connected diagrams with two external lines [36, 37]. Thus, there is a natural corre-

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spondence between the Green's function and the coefficients $a_2^{(n)}$ defined above:

$$G(i, \tau_1 | j, \tau_2) = G^{(0)}(i, \tau_1 | j, \tau_2) + G^{(1)}(i, \tau_1 | j, \tau_2) + \ldots$$

$$= \delta_{ij} a_2^{(0)}(i, \tau_1 | i, \tau_2) + a_2^{(1)}(i, \tau_1 | j, \tau_2) + \ldots. \quad (2.31)$$

Chapter 3

The Effective Action

Evaluation of the diagrams shown in Eqs. (2.27) and (2.29) involve integration over the time variable associated with the internal line. Thus, their evaluation can be simplified by transforming to Matsubara space, where these integrals amount to simple multiplication. We use the following convention for the forward and inverse Matsubara transformations

$$g(\omega_m) = \frac{1}{\sqrt{\beta}} \int_0^{\beta} d\tau\, e^{i\omega_m \tau} g(\tau), \tag{3.1}$$

$$g(\tau) = \frac{1}{\sqrt{\beta}} \sum_{m=-\infty}^{\infty} g(\omega_m) e^{-i\omega_m \tau}, \tag{3.2}$$

with the Matsubara frequencies

$$\omega_m = \frac{2\pi m}{\beta} \ , \quad m \in \mathbb{Z}. \tag{3.3}$$

Since the unperturbed Hamiltonian (2.2) is time-translation invariant, it follows from Eqs. (2.19) and (2.20) that the cumulants - and thus the functions a_{2n} - must depend on time-differences only. In terms of Matsubara frequencies, this implies that one of

the frequency variables is restricted by a delta function, i.e. we have

$$a_2^{(0)}(i, \omega_{m1}|i, \omega_{m2}) = a_2^{(0)}(i, \omega_{m1})\delta_{\omega_{m1}, \omega_{m2}}, \tag{3.4}$$

$$a_4^{(0)}(i, \omega_{m1}; i, \omega_{m2}|i, \omega_{m3}; i, \omega_{m4}) = a_4^{(0)}(i, \omega_{m1}; i, \omega_{m2}|i, \omega_{m4})\delta_{\omega_{m1}+\omega_{m2}, \omega_{m3}+\omega_{m4}}. \tag{3.5}$$

Using this frequency conservation, we find from Eq. (2.27)

$$a_2^{(1)}(i, \omega_{m1}|j, \omega_{m2}) = a_2^{(0)}(i, \omega_{m1})a_2^{(0)}(j, \omega_{m1})\delta_{\omega_{m1}, \omega_{m2}}, \tag{3.6}$$

and correspondingly Eq. (2.29) implies

$$a_4^{(1)}(i, \omega_{m1}; i, \omega_{m2}|j, \omega_{m3}; i, \omega_{m4}) = a_4^{(0)}(i, \omega_{m1}; i, \omega_{m2}|i, \omega_{m4})a_2^{(0)}(j, \omega_{m3})\delta_{\omega_{m1}+\omega_{m2}, \omega_{m3}+\omega_{m4}}. \tag{3.7}$$

Thus, the first order corrections to the functions a_{2n} can be expressed entirely in terms of $a_2^{(0)}$ and the corresponding zeroth order terms. Using the expressions (2.26) and (2.28), along with the definitions (2.22) and (2.23), we find that these two coefficients are explicitly given by

$$a_2^{(0)}(i, \omega_m) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta f_i(n)}$$
$$\times \left[\frac{n+1}{f_i(n+1) - f_i(n) - i\omega_m} - \frac{n}{f_i(n) - f_i(n-1) - i\omega_m} \right], \tag{3.8}$$

and

$$a_4^{(0)}(i, \omega_{m1}; i, \omega_{m2} | i, \omega_{m4}) = \frac{1}{\beta \mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta f_i(n)}$$

$$\times \left\{ \frac{n(n-1)}{f_i(n-2) - f_i(n-1) + i\omega_{m4}} \left[\frac{1}{i(\omega_{m4} - \omega_{m2})} \left(\frac{e^{\beta(f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2}))} - 1}{f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2})} \right. \right. \right.$$

$$\left. - \frac{e^{\beta(f_i(n) - f_i(n-1) - i\omega_{m1})} - 1}{f_i(n) - f_i(n-1) - i\omega_{m1}} \right) - \frac{1}{f_i(n-1) - f_i(n-2) - i\omega_{m2}}$$

$$\times \left. \left(\frac{e^{\beta(f_i(n) - f_i(n-2) - i(\omega_{m1} + \omega_{m2}))} - 1}{f_i(n) - f_i(n-2) - i(\omega_{m1} + \omega_{m2})} - \frac{e^{\beta(f_i(n) - f_i(n-1) - i\omega_{m1})} - 1}{f_i(n) - f_i(n-1) - i\omega_{m1}} \right) \right]$$

$$+ \frac{n^2}{f_i(n) - f_i(n-1) - i\omega_{m2}} \left[\frac{1}{i(\omega_{m4} - \omega_{m2})} \left(\frac{e^{\beta(f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2}))} - 1}{f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2})} \right. \right.$$

$$\left. - \frac{e^{\beta(f_i(n) - f_i(n-1) - i\omega_{m1})} - 1}{f_i(n) - f_i(n-1) - i\omega_{m1}} \right)$$

$$\left. - \frac{1}{f_i(n-1) - f_i(n) + i\omega_{m4}} \left(\beta \delta_{\omega_{m1} \omega_{m4}} - \frac{e^{\beta(f_i(n) - f_i(n-1) - i\omega_{m1})} - 1}{f_i(n) - f_i(n-1) - i\omega_{m1}} \right) \right]$$

$$+ \frac{n(n+1)}{f_i(n) - f_i(n-1) - i\omega_{m2}} \left[\frac{1}{f_i(n+1) - f_i(n-1) - i(\omega_{m1} + \omega_{m2})} \right.$$

$$\times \left(\frac{e^{\beta(f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2}))} - 1}{f_i(n) - f_i(n-1) + i(\omega_{m4} - \omega_{m1} - \omega_{m2})} - \frac{e^{\beta(f_i(n) - f_i(n+1) + i\omega_{m4})} - 1}{f_i(n) - f_i(n+1) + i\omega_{m4}} \right)$$

$$\left. \left. - \frac{1}{f_i(n+1) - f_i(n) - i\omega_{m1}} \left(\beta \delta_{\omega_{m1} \omega_{m4}} - \frac{e^{\beta(f_i(n) - f_i(n+1) + i\omega_{m4})} - 1}{f_i(n) - f_i(n+1) + i\omega_{m4}} \right) \right] \right\}_{\omega_{m1} \leftrightarrow \omega_{m2}}$$

$$- \left\{ a_2^{(0)}(i, \omega_{m1} | i, \omega_{m4}) a_2^{(0)}(i, \omega_{m2}) \right\}_{\omega_{m1} \leftrightarrow \omega_{m2}}, \tag{3.9}$$

where we have introduced the notation $\{\bullet\}_{x \leftrightarrow y}$ to denote a symmetrization in the variables x and y. Hence the expansion of the grand-canonical free energy (2.24) can be compactly rewritten as

$$\mathcal{F} = F_0 - \frac{1}{\beta} \left[\sum_{ij} \sum_{\omega_{m1}, \omega_{m2}} M_{ij}(\omega_{m1}, \omega_{m2}) j_i(\omega_{m1}) j_j^*(\omega_{m2}) \right.$$

$$\left. + \sum_{ijkl} \sum_{\substack{\omega_{m1}, \omega_{m2} \\ \omega_{m3}, \omega_{m4}}} N_{ijkl}(\omega_{m1}, \omega_{m2}, \omega_{m3}, \omega_{m4}) j_i(\omega_{m1}) j_j(\omega_{m2}) j_k^*(\omega_{m3}) j_l^*(\omega_{m4}) \right],$$

$$\tag{3.10}$$

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where we have introduced the abbreviations

$$M_{ij}(\omega_{m1}, \omega_{m2}) \equiv \left[a_2^{(0)}(i, \omega_{m1})\delta_{ij} + a_2^{(0)}(i, \omega_{m1})a_2^{(0)}(j, \omega_{m1})t_{ij} \right] \delta_{\omega_{m1}\omega_{m2}} \qquad (3.11)$$

and

$$N_{ijkl}(\omega_{m1}, \omega_{m2}, \omega_{m3}, \omega_{m4}) \equiv \frac{\delta_{\omega_{m1}+\omega_{m2}, \omega_{m3}+\omega_{m4}}}{4} a_4^{(0)}(i, \omega_{m1}; i, \omega_{m2}|i, \omega_{m4}) \Big\{ \delta_{ij}\delta_{jk}\delta_{kl}$$
$$+ 2\delta_{il} \left[t_{ik}a_2^{(0)}(k, \omega_{m3})\delta_{ij} + t_{ij}a_2^{(0)}(j, \omega_{m2})\delta_{ik} \right] \Big\}. \qquad (3.12)$$

Use of the expansion given above is limited by the fact that the currents $j_i(\omega_m)$ are unphysical quantities. Therefore we desire a thermodynamic potential in terms of physically relevant observables. To this end, we define an order parameter field $\psi_i(\omega_m)$ in the standard field-theoretic way [32, 33] as

$$\psi_i(\omega_m) = \langle \hat{a}_i(\omega_m) \rangle = \beta \frac{\delta \mathcal{F}}{\delta j_i^*(\omega_m)}. \qquad (3.13)$$

To first order in the tunneling parameter t_{ij}, we find that the order parameter field is given by

$$\psi_i(\omega_m) = -\sum_p \sum_{\omega_{m1}} M_{pi}(\omega_{m1}, \omega_m)j_p(\omega_{m1})$$
$$- 2 \sum_{pjk} \sum_{\omega_{m1}, \omega_{m2}, \omega_{m3}} N_{pjki}(\omega_{m1}, \omega_{m2}, \omega_{m3}, \omega_m)j_p(\omega_{m1})j_j(\omega_{m2})j_k^*(\omega_{m3}).$$

$$(3.14)$$

This finding motivates the performance of a Legendre transformation of $\mathcal{F}$ to obtain the effective action which is a functional of the order parameter field.

$$\Gamma[\psi_i(\omega_m), \psi_i^*(\omega_m)] = \mathcal{F} - \frac{1}{\beta} \sum_i \sum_{\omega_m} [\psi_i(\omega_m)j_i^*(\omega_m) + \psi_i^*(\omega_m)j_i(\omega_m)]. \qquad (3.15)$$

The importance of the functional Γ is made clear with the following observation. The physical situation of interest is the case when the artificially introduced currents

vanish, i.e. when we set $j_i(\omega_m) \equiv j_i^*(\omega_m) \equiv 0$. Since ψ and j^* are conjugate variables, we have that

$$j_i(\omega_m) = -\beta \frac{\delta \Gamma}{\delta \psi_i^*(\omega_m)}, \tag{3.16}$$

and thus this physical situation corresponds to

$$\frac{\delta \Gamma}{\delta \psi_i^*(\omega_m)}\bigg|_{\psi=\psi_{eq}} \equiv \frac{\delta \Gamma}{\delta \psi_i(\omega_m)}\bigg|_{\psi=\psi_{eq}} \equiv 0. \tag{3.17}$$

This means that the equilibrium value of the square of the order parameter field $|\psi|^2_{eq}$ is determined by the condition that the effective action Γ is stationary with respect to variations about it. Furthermore, we have from Eq. (3.15) that the effective action Γ, evaluated at the equilibrium order parameter field, is equal to the physical grand-canonical free energy:

$$\Gamma|_{\psi=\psi_{eq}} = \lim_{j \to 0} \mathcal{F}. \tag{3.18}$$

Now, a Ginzburg-Landau expansion of the effective action can be obtained. First, using the fact that to first order in t_{ij}

$$M_{ij}^{-1}(\omega_{m1}, \omega_{m2}) = \frac{\delta_{\omega_{m1}\omega_{m2}}}{a_2^{(0)}(i, \omega_{m1})} \left[\delta_{ij} - a_2^{(0)}(i, \omega_{m1}) t_{ij} \right], \tag{3.19}$$

Eq. (3.14) can be inverted recursively to find $j_i(\omega_m)$ as a functional of the order parameter field, yielding

$$j_i(\omega_m) = - \sum_{p,\omega_{m1}} M_{ip}^{-1}(\omega_m, \omega_{m1}) \Bigg[\psi_p(\omega_{m1}) $$

$$-2 \sum_{qjk} \sum_{\omega_{m2},\omega_{m3}} N_{qjkp}(\omega_{m1}, \omega_{m2}, \omega_{m3}, \omega_m) J_q(\omega_{m1}) J_j(\omega_{m2}) J_k^*(\omega_{m3}) \Bigg], \tag{3.20}$$

where we have defined the abbreviation

$$J_i(\omega_m) = - \sum_{p,\omega_{m1}} M_{pi}^{-1}(\omega_{m1}, \omega_m) \psi_p(\omega_{m1}). \tag{3.21}$$

Inserting this expression for $j_i(\omega_m)$ into Eq. (3.15) together with the expansion (3.10), and keeping terms only up to first order in the tunneling t_{ij}, we find

$$\Gamma = F_0 + \frac{1}{\beta}\sum_i \Bigg\{ \sum_{\omega_m} \Bigg[\frac{|\psi_i(\omega_m)|^2}{a_2^{(0)}(i,\omega_m)} - \sum_j t_{ij}\psi_i(\omega_m)\psi_j^*(\omega_m)\Bigg] \tag{3.22}$$

$$- \sum_{\substack{\omega_{m1},\omega_{m2}\\ \omega_{m3},\omega_{m4}}} \frac{a_4^{(0)}(i,\omega_{m1};i,\omega_{m2}|i,\omega_{m3};i,\omega_{m4})}{4a_2^{(0)}(i,\omega_{m1})a_2^{(0)}(i,\omega_{m2})a_2^{(0)}(i,\omega_{m3})a_2^{(0)}(i,\omega_{m4})}\psi_i(\omega_{m1})\psi_i(\omega_{m2})\psi_i^*(\omega_{m3})\psi_i^*(\omega_{m4}) \Bigg\}.$$

Thus, after performing the Legendre transformation, it turns out that the tunneling parameter t_{ij} appears up to first order only in terms which are quadratic in the order parameter field. Furthermore, note that this result for the effective action is sufficiently general that it depends on only three quantities of the unperturbed system: the grand-canonical free energy (2.25) and the Matsubara transform of the zeroth-order coefficients (3.8) and (3.9). Finally, the condition for equilibrium (3.17) becomes

$$0 = \frac{\psi_i(\omega_m)}{a_2^{(0)}(i,\omega_m)} - \sum_j t_{ij}\psi_j(\omega_m)$$

$$- \sum_{\omega_{m1},\omega_{m2},\omega_{m3}} \frac{a_4^{(0)}(i,\omega_{m1};i,\omega_{m2}|i,\omega_{m3};i,\omega_m)}{2a_2^{(0)}(i,\omega_{m1})a_2^{(0)}(i,\omega_{m2})a_2^{(0)}(i,\omega_{m3})a_2^{(0)}(i,\omega_m)}\psi_i(\omega_{m1})\psi_i(\omega_{m2})\psi_i^*(\omega_{m3}).$$

$$\tag{3 23}$$

Due to the complexity introduced by allowing the functions f_i in the Hamiltonian (2.2) to be site-dependent, and the fact that many interesting physical scenarios can be modeled with a uniform on-site interaction, we restrict our attention in the rest of this paper to the homogeneous situation

$$f_i(\hat{a}_i^\dagger\hat{a}_i) = f(\hat{a}_i^\dagger\hat{a}_i). \tag{3 24}$$

In this case, the cumulants are no longer on-site quantities, and we may thus drop the site indices in the coefficients a_{2n}. In the next sections, we examine the physical implications of both a static and a dynamic order parameter field.

3.1 Physical Quantities in the Static Case

Consider first an order parameter field that is constant in both time and space, i.e. of the form

$$\psi_i(\omega_m) = \psi \sqrt{\beta} \delta_{\omega_m, 0}. \qquad (3.25)$$

With this, the effective action (3.22) simplifies to the effective potential

$$\Gamma = N_s \left[\frac{|\psi|^2}{a_2^{(0)}(0)} - \frac{\beta a_4^{(0)}(0,0|0,0)}{4\left[a_2^{(0)}(0)\right]^4} |\psi|^4 \right] - |\psi|^2 \gamma + F_0, \qquad (3.26)$$

where N_s denotes the total number of lattice sites, and $\gamma = \sum_{ij} t_{ij}$. In the case where

$$a_4^{(0)}(0,0|0,0) < 0 \qquad (3.27)$$

we have, according to the standard Landau theory, a phase transition of second order with a phase boundary given by the set of system parameters satisfying

$$0 = \frac{N_s}{a_2^{(0)}(0)} - \gamma. \qquad (3.28)$$

As this is the case of most interest, we will assume that such a phase transition exists. We also find that Eq. (3.23) takes the simple form

$$0 = \psi \left[\frac{N_s}{a_2^{(0)}(0)} - \gamma - |\psi|^2 \frac{\beta N_s a_4^{(0)}(0,0|0,0)}{2(a_2^{(0)}(0))^4} \right], \qquad (3.29)$$

from which we see that in the ordered phase the equilibrium value of $|\psi|^2$, and thus the condensate density, is given by

$$|\psi|_{eq}^2 = \frac{2(a_2^{(0)}(0))^3 \left[N_s - a_2^{(0)}(0)\gamma \right]}{\beta N_s a_4^{(0)}(0,0|0,0)}. \qquad (3.30)$$

Furthermore, due to Eq. (3.18), other physical quantities follow from evaluating derivatives of Γ at ψ_{eq}. For instance, the expectation value of the number of par-

ticles per lattice site $\langle n \rangle = -\frac{1}{N_s} \frac{\partial \mathcal{F}}{\partial \mu}$ in the ordered phase is given by

$$\langle n \rangle = -\frac{1}{N_s} \frac{\partial \Gamma}{\partial \mu} \bigg|_{\psi = \psi_{\text{eq}}}, \tag{3.31}$$

and correspondingly, the compressibility $\kappa = \frac{\partial \langle n \rangle}{\partial \mu}$ follows from

$$\kappa = -\frac{1}{N_s} \frac{\partial^2 \Gamma}{\partial \mu^2} \bigg|_{\psi = \psi_{\text{eq}}}. \tag{3.32}$$

In general, any thermodynamic quantity expressible as a function of derivatives of the grand-canonical free energy $\mathcal{F}$ can be expressed as the same function of derivatives of Γ with respect to the same variables, evaluated at $\upsilon = \psi_{\text{eq}}$.

Relaxing the condition of spatial homogeneity of the order parameter, we are able to determine the superfluid density of the system. The superfluid density is defined as the effective fluid density that remains at rest when the entire system is moved at a constant velocity [38, 39]. As is well known in quantum mechanics, such a uniform velocity corresponds to imposing twisted boundary conditions. Equivalently, we introduce Peierls phase factors

$$\hat{a}_i \rightarrow \hat{a}_i e^{i \frac{\vec{x}_i}{L} \cdot \vec{\phi}} \tag{3.33}$$

in the original Hamiltonian (2.1). Here $\vec{\phi}$ is related to the velocity of the system according to $\vec{v} = \vec{\phi}/m^* L$ where m^* is the effective particle mass, $\vec{x}_i$ are the lattice vectors, and L is the extent of the system in the direction of $\vec{v}$. Equating the kinetic energy of the superfluid with the free energy difference $\mathcal{F}(\vec{\phi}) - \mathcal{F}(\vec{0})$, we see that the superfluid density ρ is given by

$$\rho = \lim_{|\vec{\phi}| \rightarrow 0} \frac{2m^* L^2}{N_s |\vec{\phi}|^2} \left[\mathcal{F}(\vec{\phi}) - \mathcal{F}(\vec{0}) \right]. \tag{3.34}$$

Examining the form of $\hat{H}_0$ and $\hat{H}_1$ in Eqs. (2.2) and (2.4), we see that the effect of introducing the phase factors in Eq. (3.33) is simply to redefine the tunneling

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parameter t_{ij} as

$$t_{ij}(\vec{\phi}) = t_{ij} e^{i\frac{\vec{x}_j - \vec{x}_i}{L}\cdot\vec{\phi}}.$$ (3.35)

Thus, using Eq. (3.18) we can express ρ in terms of the effective action as

$$\rho = \lim_{|\vec{\phi}|\to 0} \frac{2m^* L^2}{N_s |\vec{\phi}|^2} \left[\Gamma(\vec{\phi})\Big|_{\psi=\psi_{\text{eq}}(\vec{\phi})} - \Gamma(\vec{0})\Big|_{\psi=\psi_{\text{eq}}(\vec{0})} \right],$$ (3.36)

which, with the aid of Eq. (3.22) reduces to

$$\rho = \lim_{|\vec{\phi}|\to 0} \frac{2m^* L^2}{N_s |\vec{\phi}|^2} \left\{ \sum_{ij} \left[t_{ij} \left(\left|\psi_{\text{eq}}(\vec{\phi})\right|^2 e^{i\frac{\vec{x}_j - \vec{x}_i}{L}\cdot\vec{\phi}} - \left|\psi_{\text{eq}}(\vec{0})\right|^2 \right) \right] \right.$$ (3.37)

$$\left. + N_s \left[\frac{1}{a_2^{(0)}(0)} \left(\left|\psi_{\text{eq}}(\vec{\phi})\right|^2 - \left|\psi_{\text{eq}}(\vec{0})\right|^2 \right) - \frac{\beta a_4^{(0)}(0,0|0,0)}{4(a_2^{(0)}(0))^4} \left(\left|\psi_{\text{eq}}(\vec{\phi})\right|^4 - \left|\psi_{\text{eq}}(\vec{0})\right|^4 \right) \right] \right\}.$$

Thus, the superfluid density is determined explicitly once a definite form of the tunneling parameter t_{ij} is specified.

3.2 Physical Quantities in the Dynamic Case

By allowing the order parameter to vary in imaginary time, we can also use the effective action to obtain an analytic form for the Matsubara Green's function. To do so, we note that the Legendre transformation (3.13), (3.15), (3.16) implies

$$\beta \frac{\delta^2 \Gamma}{\delta\psi_i(\omega_{m1})\delta\psi_j^*(\omega_{m2})}\Bigg|_{\psi=\psi_{\text{eq}}} = -\frac{\delta j(\psi_j(\omega_{m2}))}{\delta\psi_i(\omega_{m1})}\Bigg|_{\psi=\psi_{\text{eq}}} = \left(-\beta\frac{\delta^2 \mathcal{F}}{\delta j_i^*(\omega_{m1})\delta j_j(\omega_{m2})} \right)^{-1}\Bigg|_{j\equiv 0}.$$ (3.38)

We recognize immediately from Eq. (2.30) that this is precisely the inverse of the Matsubara Green's function $\mathcal{G}(i,\omega_{m1}|j,\omega_{m2})$. Next, we consider Γ expanded to arbitrary order in t_{ij}.

$$\Gamma = F_0 + \frac{1}{\beta} \sum_i \left(\sum_{\omega_m} \frac{|\psi_i(\omega_m)|^2}{a_2^{(0)}(\omega_m)} + \sum_{n=1}^{\infty} \sum_j \alpha_2^{(n)}(\omega_m)[(t)^n]_{ij}\psi_i(\omega_m)\psi_j^*(\omega_m) + \dots \right),$$ (3.39)

where the expansion coefficients $\alpha_2^{(n)}$ are determined by methods like those described above. We then find from Eq. (3.38) that the Matsubara Green's function is given by

$$[\mathcal{G}(j, \omega_{m2}|i, \omega_{m1})]^{-1} = \delta_{\omega_{m1}, \omega_{m2}} \left(\frac{\delta_{ij}}{a_2^{(0)}(\omega_{m1})} + \sum_{n=1}^{\infty} \alpha_2^{(n)}(\omega_{m1})[(t)^n]_{ij} + \dots \right). \quad (3.40)$$

Recognizing that $\delta_{\omega_{m1}, \omega_{m2}} \delta_{ij} / a_2^{(0)}(\omega_{m1})$ is simply the inverse of the unperturbed Matsubara Green's function, we see that the power series in t_{ij} in Eq. (3.40) gives a series expansion of the self-energy Σ:

$$\Sigma(i, \omega_{m1}|j, \omega_{m2}) = \left[\mathcal{G}^{(0)}(i, \omega_{m1}|j, \omega_{m2})\right]^{-1} - [\mathcal{G}(i, \omega_{m1}|j, \omega_{m2})]^{-1} = -\delta_{\omega_{m1}, \omega_{m2}} \sum_{n=1}^{\infty} \alpha_2^{(n)}(\omega_{m1})[(t)^n]_{ij}.$$
$$(3.41)$$

Thus, we conclude that our effective action gives an expansion for the Green's function in terms of the self-energy in powers of t_{ij}. In the non-ordered phase, this is the same as if we had computed the corrections to the unperturbed Green's function directly from our perturbative expansion of $\mathcal{F}$ and performed a resummation [37]. Specifying Eq. (3.40) to our present first-order case, we hence find

$$\left[\mathcal{G}^{(0)}(j, \omega_{m2}|i, \omega_{m1})\right]^{-1} - \Sigma^{(1)}(j, \omega_{m2}|i, \omega_{m1})$$

$$= \delta_{ij} \left[\frac{1}{a_2^{(0)}(\omega_{m1})} + \frac{2\delta_{\omega_{m1} \omega_{m2}} a_4^{(0)}(\omega_{m1}, 0|0, \omega_{m2})(a_2^{(0)}(0))^2 \left(\frac{\gamma}{N_s} - \frac{1}{a_2^{(0)}(0)} \right)}{(a_2^{(0)}(\omega_{m1}))^2 a_4^{(0)}(0, 0|0, 0)} \right] - t_{ij}.$$

$$(3.42)$$

Denoting by $t_{\vec{k}\vec{k}'}$ the Fourier transform of the tunneling parameter,

$$t_{\vec{k}\vec{k}'} = \sum_{ij} t_{ij} e^{i\left(\vec{k}' \, \vec{x}_j - \vec{k} \, \vec{r}_i\right)}. \quad (3.43)$$

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we find that Eq. (3.42) can be rewritten in Fourier space as

$$\left[\mathcal{G}(\vec{k}', \omega_{m2} | \vec{k}, \omega_{m1}) \right]^{-1}$$

$$= \frac{1}{a_2^{(0)}(\omega_{m1})} + \frac{2\delta_{\omega_{m1}\omega_{m2}} a_4^{(0)}(\omega_{m1}, 0 | 0, \omega_{m2})(a_2^{(0)}(0))^2 \left(\frac{\gamma}{N_s} - \frac{1}{a_2^{(0)}(0)} \right)}{(a_2^{(0)}(\omega_{m1}))^2 a_4^{(0)}(0, 0 | 0, 0)} - t_{\vec{k}\vec{k}'}. \quad (3.44)$$

We see that the second term above is a contribution to the Green's function due completely to the existence of a non-vanishing order parameter. This correction can thus be exploited to improve analytical time-of-flight calculations for bosonic lattice systems in the superfluid phase [40].

Next, we can examine excitations of the system at zero temperature by looking for spatio-temporal variations of the order parameter field about $\psi_{\text{eq}} = \sqrt{|\psi|^2_{\text{eq}}} e^{i\theta_0}$ which preserve the equilibrium condition (3.17), where θ_0 is an arbitrary global phase. To this end, we first must specify to the case where our system is translationally invariant, such that

$$t_{\vec{k}\vec{k}'} = t_{\vec{k}} \delta_{\vec{k}\vec{k}'}. \quad (3.45)$$

Next, we add to the equilibrium value of the order parameter field a small variation $\delta\psi(\vec{x}_i, \omega_m)$. We then Taylor expand the effective action Γ about ψ_{eq} in terms of these variations. The first order term vanishes due to the equilibrium condition (3.17), leaving

$$\Gamma = \Gamma[\psi_{\text{eq}}] + \sum_{\substack{i,j \\ \omega_{m1}, \omega_{m2}}} \frac{\delta^2 \Gamma}{\delta(\delta\psi_i(\omega_{m1}))\delta(\delta\psi_j^*(\omega_{m2}))} \Bigg|_{\delta\psi \equiv 0} \delta\psi_i(\omega_{m1})\delta\psi_j^*(\omega_{m2}) + \dots. \quad (3.46)$$

Demanding that in equilibrium the effective potential is stationary with respect to the variations $\delta\psi$ in the standard way gives the equation of motion

$$\sum_{i,\omega_{m1}} \frac{\delta^2 \Gamma}{\delta(\delta\psi_i(\omega_{m1}))\delta(\delta\psi_j^*(\omega_{m2}))} \Bigg|_{\delta\psi \equiv 0} \delta\psi_i(\omega_{m1}) = 0. \quad (3.47)$$

This equation can be satisfied in two distinct ways. The trivial solution $\delta\psi(\vec{r}_i, \omega_m) \equiv 0$ corresponds to the static homogeneous equilibrium examined in the previous section.

The second solution is given by

$$\frac{\delta^2 \Gamma}{\delta(\delta\psi_i(\omega_{m1}))\delta(\delta\psi_j^*(\omega_{m2}))}\bigg|_{\delta\psi \equiv 0} = 0 \tag{3.48}$$

and describes the excitation spectrum of the system. In particular, by analytically continuing Eq. (3.48) to real frequencies and transforming to Fourier space, we are able to identify the dispersion relation of low-lying excitations as those curves $\omega(\vec{k})$ which make the equation valid. The standard method of performing this analytic continuation is to find the equations of motion in imaginary-time and perform an inverse Wick rotation. Because of the complexity of the coefficient $a_4^{(0)}(\omega_{m1}, \omega_{m2}|\omega_{m3}, \omega_{m4})$, however, this is ill-suited to our present needs. Therefore, we note that our imaginary time evolution operator $\exp\left(-\hat{H}\tau\right)$ can be mapped to the real-time evolution operator $\exp\left(-i\hat{H}t\right)$ by the formal substitution $\hat{H} \rightarrow i\hat{H}$. To maintain the reality of the grand-canonical free energy, we must also perform the substitution $\mathcal{F} \rightarrow -i\mathcal{F}$. We thus find that in terms of real frequencies the effective action is given by

$$\Gamma_{\mathrm{R}} = F_0 + \frac{1}{\beta}\sum_i \left\{ \int d\omega \left[-i\frac{|\psi_i(\omega)|^2}{a_{2\mathrm{R}}^{(0)}(\omega)} - \sum_j t_{ij}\psi_i(\omega)\psi_j^*(\omega) \right] \right. \tag{3.49}$$

$$\left. + i\int d\omega_1 \int d\omega_2 \int d\omega_3 \int d\omega_4 \frac{a_{4\mathrm{R}}^{(0)}(\omega_1, \omega_2|, \omega_3, \omega_4)}{4a_{2\mathrm{R}}^{(0)}(\omega_1)a_{2\mathrm{R}}^{(0)}(\omega_2)a_{2\mathrm{R}}^{(0)}(\omega_3)a_{2\mathrm{R}}^{(0)}(\omega_4)}\psi_i(\omega_1)\psi_i(\omega_2)\psi_i^*(\omega_3)\psi_i^*(\omega_4) \right\}.$$

where $a_{2\mathrm{R}}^{(0)}$ and $a_{4\mathrm{R}}^{(0)}$ are obtained from Eqs. (3.8) and (3.9) respectively by the replacement $f_i(n) \rightarrow if_i(n)$. Thus, the real-time continuation of the condition (3.48) is given by

$$\frac{\delta^2 \Gamma_{\mathrm{R}}}{\delta(\delta\psi_i(\omega_1))\delta(\delta\psi_j^*(\omega_2))}\bigg|_{\delta\psi \equiv 0} = 0. \tag{3.50}$$

In general, the function $\omega(\vec{k})$ will have a positive and a negative frequency branch Because we determined these curves by expanding the effective action Γ_{R} about a minimum, however, only the positive frequency branch of $\omega(\vec{k})$ are to be considered as physically relevant.

Since the order parameter is complex. we examine separately variations of both

the magnitude and of the phase. First, we consider excitations in the amplitude of the order parameter. To this end, we replace ψ in Eq. (3.22) by $\psi_{\text{eq}}\sqrt{\beta}\delta_{\omega_m,0} + \delta\psi_i(\omega_m)$, where $\delta\psi_i(\omega_m)$ is an arbitrary infinitesimal function of the lattice site i and ω_m, with fixed phase θ_0. Carrying out the functional derivative in Eq. (3.50) and performing the continuation outlined above and transforming to Fourier space yields the equation

$$0 = \frac{-i}{a_{2R}^{(0)}(\omega_A)} + \frac{2a_{4R}^{(0)}(\omega_A, 0|0, \omega_A)(a_{2R}^{(0)}(0))^2 \left[\frac{\gamma}{N_s} + \frac{i}{a_{2R}^{(0)}(0)}\right]}{(a_{2R}^{(0)}(\omega_A))^2 a_{4R}^{(0)}(0, 0|0, 0)} - t_{\vec{k}}. \qquad (3.51)$$

This gives a constraint equation which can be solved for the dispersion relation of amplitude excitations $\omega_A(\vec{k})$. By comparing Eq. (3.51) with the Matsubara Green's function (3.44), we notice that the dispersion relation $\omega_A(\vec{k})$ coincides with the poles of the translationally invariant real-time Green's function.

To treat the phase degree of freedom, we note first that adding a small time-varying phase to ψ_{eq} amounts to the transformation

$$\psi \to \psi_{\text{eq}} e^{i\theta_i(\tau)} \approx \psi_{\text{eq}} \left[1 + i\theta_i(\tau) - \frac{1}{2}\theta_i(\tau)^2\right]. \qquad (3.52)$$

Expressing this in Matsubara space, we have

$$\psi \to \psi_{\text{eq}} \left[1 + i\theta_i(\omega_m) - \frac{1}{2}\sum_{\omega_n}\theta_i(\omega_n)\theta_i(\omega_m - \omega_n)\right]. \qquad (3.53)$$

Inserting the transformation (3.53) into the real-time effective action (3.49) and performing the derivative (3.50) yields the condition

$$0 = \frac{-i}{a_{2R}^{(0)}(\omega_\theta)} + \frac{i}{a_{2R}^{(0)}(0)} - \frac{2a_{2R}^{(0)}(0)^4 \left(\frac{\gamma}{N_s} + \frac{i}{a_{2R}^{(0)}(0)}\right)}{a_{4R}^{(0)}(0, 0|0, 0)} \left[2b(0, 0, 0, 0) + b(\omega_\theta, -\omega_\theta, 0, 0)\right.$$
$$\left. + b(0, 0, \omega_\theta, -\omega_\theta) - 2b(\omega_\theta, 0, \omega_\theta, 0) - 2b(\omega_\theta, 0, 0, \omega_\theta)\right] + \frac{\gamma}{N_s} - t_{\vec{k}}, \qquad (3.54)$$

where we have defined

$$b(\omega_1, \omega_2 | \omega_3, \omega_4) = \frac{a_{4R}^{(0)}(\omega_1, \omega_2 | \omega_3, \omega_4)}{a_{2R}^{(0)}(\omega_1) a_{2R}^{(0)}(\omega_2) a_{2R}^{(0)}(\omega_3) a_{2R}^{(0)}(\omega_4)}.$$

(3.55)

This determines the dispersion relation $\omega_\theta(\vec{k})$ of the phase excitations. We note that since $t_{\vec{0}} = \gamma/N_s$, $\omega_\theta(\vec{0}) = 0$ is a solution to the constraint (3.54) in accordance with Goldstone's theorem [32, 33].

Lastly, we investigate the phenomenon of second sound. As is well known, the observed elementary excitations of a superfluid are given by phonons. To obtain their corresponding dispersion relation $\omega_s(\vec{k})$, we must examine the phase excitations in the presence of the amplitude variations, i.e. $\psi \rightarrow [\psi_{\text{eq}} + \delta\psi_i(\omega_m)] e^{i\theta_i(\omega_m)}$. This has been considered, for example, in Refs. [41, 42], leading to the result

$$\omega_s(\vec{k}) = \sqrt{\omega_A(\vec{k})\omega_\theta(\vec{k})}.$$

(3.56)

Chapter 4

An Application: The Bose-Hubbard Hamiltonian

Having developed the field-theoretic approach for the general Hamiltonian (2.1), (2.2), (2.4) in the preceding chapters, we are now in a position to apply it to the specific case of the Bose-Hubbard Hamiltonian on a 3-dimensional cubic lattice defined by Eq. (1.1). As is well known, this model exhibits a quantum phase transition between a Mott insulating phase and a superfluid phase [13, 14, 15, 16]. The Hamiltonian (1.1) has exactly the form assumed in Chapter 2 when the following identifications are made:

$$f(n) = E_n = \frac{1}{2}Un(n-1) - \mu n \tag{4.1}$$

$$t_{ij} = t \sum_{\sigma} \left(\delta_{\vec{x}_i.\vec{x}_j + \vec{d}_\sigma} + \delta_{\vec{x}_i.\vec{x}_j - \vec{d}_\sigma} \right). \tag{4.2}$$

where $\vec{d}_\sigma$ denotes the lattice basis vectors with $k = 1, 2, 3$. Additionally, we see that the quantity γ introduced above simplifies to

$$\gamma = \sum_{ij} t_{ij} = 6N_s t. \tag{4.3}$$

Thus, we can apply all previously derived formulas to extract physical information about the Bose-Hubbard system. In the $\omega_m \to 0$ limit, we find that $a_2^{(0)}(0)$ becomes

$$a_2^{(0)}(0) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta E_n} \left(\frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}} \right). \tag{4.4}$$

The expression for $a_4^{(0)}(0,0|0,0)$ must be calculated via a more careful limiting procedure. Making use of the limit

$$\lim_{x \to 0} \frac{e^{bx} - 1}{x} = b, \tag{4.5}$$

we find that

$$\begin{aligned}
a_4^{(0)}(0,0|0,0) = \frac{2}{\beta \mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta E_n} & \left\{ n(n-1) \frac{-2}{(E_n - E_{n-1})^2 (E_n - E_{n-2})} \right. \\
& + n^2 \left[\frac{2}{(E_n - E_{n-1})^3} + \frac{\beta}{(E_n - E_{n-1})} \right] - n(n+1) \left[\frac{2(E_{n+1} - 2E_n + E_{n-1})}{(E_n - E_{n-1})^2 (E_n - E_{n+1})^2} \right. \\
& \left. + \frac{2\beta}{(E_{n+1} - E_n)(E_n - E_{n-1})} \right] - (n+1)^2 \left[\frac{2}{(E_{n+1} - E_n)^3} - \frac{\beta}{(E_{n+1} - E_n)^2} \right] \\
& \left. + (n+1)(n+2) \left[\frac{2}{(E_{n+1} - E_n)^2 (E_{n+2} - E_n)} \right] \right\} - 2(a_2^{(0)}(0))^2. \tag{4.6}
\end{aligned}$$

4.1 Effective Action Predictions in the Static Case

Before examining the physical implications of our effective action approach, we first introduce the standard mean-field treatment of the Bose-Hubbard Hamiltonian for comparison. The mean-field Hamiltonian is found by performing a Hartree-Fock expansion of the hopping term in the Hamiltonian (1.1) [13, 15]. Keeping in mind that the order parameter is defined according to $\psi = \langle \hat{a}_i \rangle$, this yields

$$\hat{H}_{\mathrm{MF}} = \hat{H}_0 - 6t \sum_i \left(\psi \hat{a}_i^{\dagger} + \psi^* \hat{a}_i - |\psi|^2 \right). \tag{4.7}$$
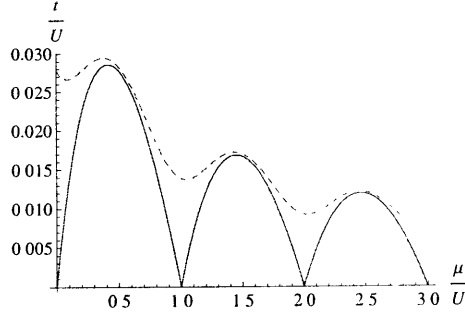
Figure 4-1: Plot of the critical value of the hopping parameter t versus the chemical potential μ, both scaled by the interaction energy U. The phase boundaries for two different temperatures are shown. The solid blue curve is $T/U = 0$, and the dashed red curve is $T/U = 0.1/k_B$.

The methods of Chapter 2 can be adapted to give an expansion of the mean-field free energy in powers of the order parameter, since

$$\hat{H}_{\mathrm{MF}} = \hat{H}_0 + \hat{H}_1'|_{t=0} + 6tN_s \, |\psi|^2 \,, \tag{4.8}$$

when we make the formal identification $j_i(\tau) = -6t\psi$. Thus, an expansion of $\mathcal{F}$ to zeroth order in t gives an expansion of the mean-field free energy $\mathcal{F}_{\mathrm{MF}}$ in powers of the order parameter, provided we recognize that the constant term in Eq. (4.8) contributes a term of order $|\psi|^2$ to $\mathcal{F}_{\mathrm{MF}}$. With these considerations in mind, we find the explicit result

$$\mathcal{F}_{\mathrm{MF}} = F_0 - N_s \left(a_2^{\mathrm{MF}} \, |\psi|^2 + \frac{\beta}{4} a_4^{\mathrm{MF}} \, |\psi|^4 \right), \tag{4.9}$$

where the mean-field Landau coefficients a_2^{MF} and a_4^{MF} are given by

$$a_2^{\mathrm{MF}} = a_2^{(0)}(0)(6t)^2 - 6t. \tag{4.10}$$

$$a_4^{\mathrm{MF}} = a_4^{(0)}(0.0|0,0)(6t)^4. \tag{4.11}$$

Thus, the mean-field result can also be expressed in terms of the same three quantities (2.25), (3.8), and (3.9) as our effective action approach.

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We now compare the predictions of our mean field theory with our effective action theory. First, we find that the mean-field phase boundary is given by the curve [13, 31, 43, 44]

$$t_c^{\text{MF}} = \frac{1}{6a_2^{(0)}(0)} = \frac{\mathcal{Z}^{(0)}}{6 \sum\limits_{n=0}^{\infty} e^{-\beta E_n} \left(\dfrac{n+1}{E_{n+1} - E_n} - \dfrac{n}{E_n - E_{n-1}} \right)}, \tag{4.12}$$

which turns out to be identical to the phase boundary found from Eq. (3.28). A plot of the phase boundary in Fig. 4-1 reveals that increasing thermal fluctuations destroy quantum coherence, as the superfluid phase shrinks with increasing temperature. Note that the main advantage of the field-theoretic method over the mean-field approach is in the fact that the phase boundary can be improved by carrying the expansion out to higher orders in t. The phase boundary to second tunneling order has already been calculated for $T = 0$ in Ref. [22] and for $T > 0$ in Ref. [37], and proves to be a considerable improvement over the mean-field result.

We next look now at the condensate density $|\psi|^2_{\text{eq}}$. From Eq. (3.30), we find

$$|\psi|^2_{\text{eq}} = \frac{2(a_2^{(0)}(0))^3}{\beta a_4^{(0)}(0)} \left[1 - 6t a_2^{(0)}(0) \right]. \tag{4.13}$$

while standard Landau-theory yields

$$|\psi|^2_{\text{MF}} = \frac{-2a_2^{\text{MF}}}{\beta a_4^{\text{MF}}} = \frac{2}{(6t)^3 \beta a_4^{(0)}(0)} \left[1 - 6t a_2^{(0)}(0) \right] \tag{4.14}$$

via the minimization of $\mathcal{F}_{\text{MF}}$.

Turning to the superfluid density, we see from Eq (3.35) that for the Bose-Hubbard model,

$$t(\vec{\phi}) = 2t \sum_{\sigma} \cos \left(\frac{\vec{d}_\sigma \cdot \vec{\varphi}}{L} \right). \tag{4.15}$$

where $\vec{d}_\sigma$ are the nearest neighbor lattice vectors in the σ direction. Therefore, in the Bose-Hubbard model we have $t = 1/(2m^*)$ [45]. Thus. from Eqs. (3.34) and (3.37) we find that for both the mean-field theory and the effective action theory to first order
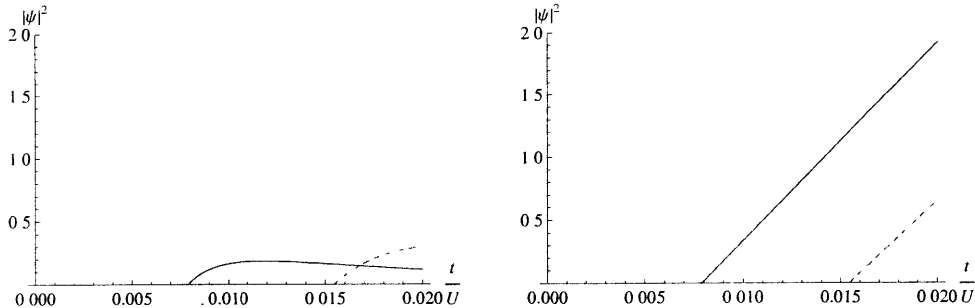
Figure 4-2: Plot of the condensate density as a function of the hopping parameter t/U for both the mean-field theory (left) and the effective action theory (right), with fixed $\mu/U = 0.9$. The solid blue curves are $T/U = 0$, and the dashed red curves are $T/U = 0.1/k_B$.

in t,

$$\rho = \frac{|\psi_{\text{eq}}|^2}{|\vec{\phi}|^2} \sum_\sigma (\hat{x}_\sigma \cdot \vec{\phi})^2. \tag{4.16}$$

Taking $\vec{\phi}$ to be in a lattice direction, we see that the superfluid and condensate densities are equal at this level of approximation.

A plot of the condensate/superfluid density as a function of the tunneling parameter t at a fixed value of the chemical potential μ for each theory can be seen in Fig. 4-2. It is interesting to note that while the superfluid density from the field-theoretic approach increases linearly with t, the mean-field superfluid density quickly begins to fall off as t increases, a behavior which is at odds with the notion of a superfluid [13]. Furthermore, it can be seen that Eq. (4.13) is simply a first order series expansion of Eq. (4.14) about $t = t_c$, meaning $|\psi|^2_{\text{eq}}$ is the tangent line to $|\psi|^2_{\text{MF}}$ at $t = t_c$. Thus, although the two results agree near the phase boundary, the mean-field prediction quickly begins to exhibit an unphysical behavior, suggesting that our field-theoretic result has a larger range of validity.

Next, we compare the average number of particles per lattice site $\langle n \rangle$ as computed in the two theories. In the ordered phase, the field theoretic prediction for $\langle n \rangle$ is given
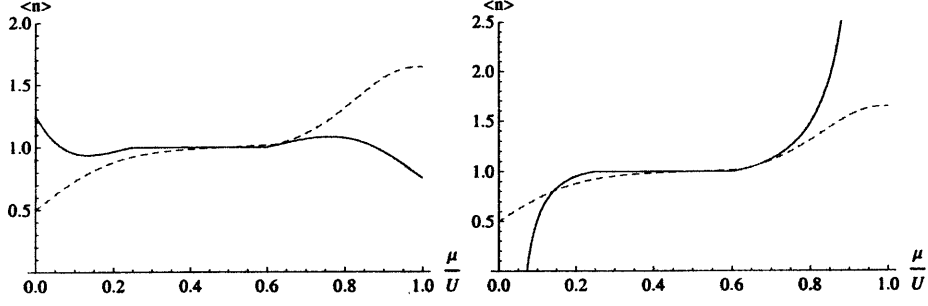
Figure 4-3: Plot of the average number of particles per site as a function of the chemical potential μ/U with fixed $t/U = 0.025$. Left shows the mean-field prediction, while right shows the field-theoretic prediction. The solid blue curves are $T/U = 0$, and the dashed red curves are $T/U = 0.1/k_B$.
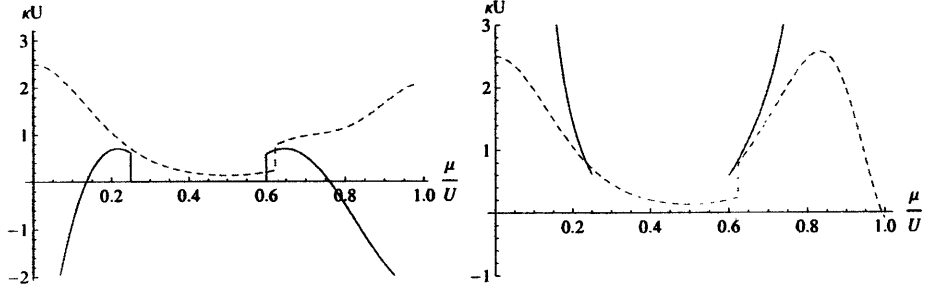

Figure 4-4: Plot of the compressibility κU as a function of the chemical potential μ/U with fixed $t/U = 0.025$. Left shows the mean-field prediction, while right shows the field-theoretic prediction. The solid blue curves are $T/U = 0$, and the dashed red curves are $T/U = 0.1/k_B$.

by Eq. (3.31) above, while the mean-field result is given by

$$\langle n \rangle_{\mathrm{MF}} = -\frac{1}{N_s} \frac{\partial \mathcal{F}_{\mathrm{MF}}}{\partial \mu}\bigg|_{|\psi|^2 = |\psi|^2_{\mathrm{MF}}}. \tag{4.17}$$

In the Mott phase, $|\psi|^2_{\mathrm{eq}} = |\psi|^2_{\mathrm{MF}} = 0$, and both theories predict

$$\langle n \rangle = \langle n \rangle_{\mathrm{MF}} = -\frac{1}{N} \frac{\partial F_0}{\partial \mu}, \tag{4.18}$$

which is simply $\langle n \rangle_0$. Plots of these two quantities as a function of the chemical potential at a fixed value of the hopping parameter are shown in Fig. 4-3. Although the predictions of both theories agree in the immediate vicinity of the phase boundary,
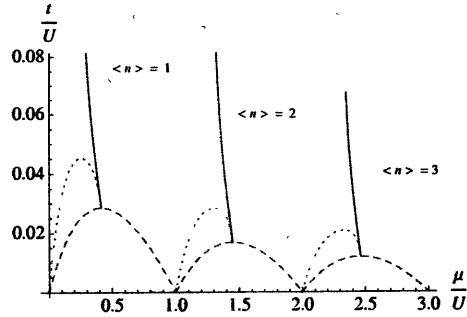
Figure 4-5: Contours of constant $\langle n \rangle$ in parameter space for both the mean-field and effective action theories at $T = 0$. The dotted blue curve shows the first three lobes of the phase boundary. The solid blue curves are the predictions of the effective action theory, while the dotted red curves show the predictions of the mean-field theory.

we see that at low temperatures $\langle n \rangle_{\mathrm{MF}}$ is not a monotonically increasing function of μ. In fact, the plot shows that away from the phase boundary, $\langle n \rangle_{\mathrm{MF}}$ actually decreases with increasing μ, i.e. the compressibility is predicted to be negative in the superfluid phase. This is directly at odds with the fact that a superfluid has, by definition, a positive compressibility [42]. The behavior of $\langle n \rangle$ as derived from the effective action, on the other hand, fits well with expectation further away from the phase boundary. This is highlighted in Fig. 4-4, which shows the compressibility κ for each case.

As a final point of comparison, we specify to the zero temperature case and examine contours in parameter space along which the average number density $\langle n \rangle$ is constant. Inside each Mott lobe, we know that the number density is fixed at the quantum number n of the lobe. In the superfluid phase, for fixed t we expect $\langle n \rangle$ to increase monotonically with increasing chemical potential. This implies that contours of constant $\langle n \rangle$ should be monotonic in μ. Such contours for $\langle n \rangle = 1, 2, 3$ are shown in Fig. 4-5. Although the mean-field and effective action contours agree close to the lobe tip, the mean-field result exhibits a non-monotonic behavior farther away from the lobe tip. Given the non-monotonic behavior of $\langle n \rangle_{\mathrm{MF}}$ discussed above, this is not wholly surprising. From these considerations, we conclude that the effective action theory has a larger range of validity than the mean field theory and, furthermore, we expect an increase in quantitative accuracy when higher powers of t are considered.

4.2 Effective Action Predictions in the Dynamic Case

We now turn our attention to the Green's function and the zero-temperature excitation spectra of the Bose-Hubbard model. Using Eq. (3.44), we see that to first order in t the Green's function of the system in the ordered phase can be written as

$$\mathcal{G}(\omega_m, \vec{k}) = \cfrac{a_2^{(0)}(\omega_m)}{1 + \cfrac{2a_4^{(0)}(\omega_m, 0|0, \omega_m)(a_2^{(0)}(0))^2 \left[6t - \frac{1}{a_2^{(0)}(0)}\right]}{(a_2^{(0)}(\omega_m))a_4^{(0)}(0,0|0,0)} - 2ta_2^{(0)}(\omega_m)\sum_\sigma \cos(k_\sigma d)}, \qquad (4.19)$$

where d is the lattice spacing, and $\vec{k}$ is restricted to the first Brillouin zone. At the phase boundary we have $6t - 1/a_2^{(0)}(0) = 0$, and the Green's function reduces to

$$\mathcal{G}(\omega_m, \vec{k}) = \frac{a_2^{(0)}(\omega_m)}{1 - 2ta_2^{(0)}(\omega_m)\sum_\sigma \cos(k_\sigma d)}. \qquad (4.20)$$

This is precisely the result obtained in the Mott phase via a resummation of zero loop diagrams [37].

From Eq. (3.51), we see that the zero-temperature dispersion relation for amplitude excitations $\omega_A(\vec{k})$ satisfies

$$0 = \frac{-\imath}{a_{2R}^{(0)}(\omega_A)} + \frac{2a_{4R}^{(0)}(\omega_A, 0|0, \omega_A)(a_{2R}^{(0)}(0))^2 \left[6t + \frac{\imath}{a_{2R}^{(0)}(0)}\right]}{(a_{2R}^{(0)}(\omega_A))^2 a_{4R}^{(0)}(0.0|0.0)} - 2t\sum_\sigma \cos(k_\sigma d), \quad (4.21)$$

which we recognize also as the condition for poles in Eq. (4.19) continued to real time. While too complicated to solve exactly. Eq. (4.21) can be inverted numerically to yield the dispersion relation $\omega_A(\vec{k})$. A plot of $\omega_A(\vec{k})$ taken along the $(1, 1, 1)$ direction in the first Brillouin zone is shown in Fig. 4-6. We observe that in the superfluid phase. $\omega_A(\vec{k})$ is gapped and quadratic,

$$\omega_A(\vec{k}) \approx \Delta + \eta k^2. \qquad (4.22)$$

Furthermore, at the phase boundary, we find that the dispersion becomes gapless and linear.

Next, we consider the zero-temperature dispersion relation $\omega_\theta(\vec{k})$ of phase excitations. For the Bose-Hubbard model, Eq. (3.54) takes the form

$$
0 = \frac{-i}{a_{2R}^{(0)}(\omega_\theta)} + \frac{i}{a_{2R}^{(0)}(0)} - \frac{2a_{2R}^{(0)}(0)^3 \left(i + 6ta_{2R}^{(0)}(0) \right)}{a_{4R}^{(0)}(0,0|0,0)} \bigg[2b(0,0,0,0) + b(\omega_\theta, -\omega_\theta, 0, 0)
$$
$$
+ b(0,0,\omega_\theta, -\omega_\theta) - 2b(\omega_\theta, 0, \omega_\theta, 0) - 2b(\omega_\theta, 0, 0, \omega_\theta) \bigg] + 2t \left[3 - \sum_\sigma \cos{(k_\sigma d)} \right].
$$
$$
\tag{4.23}
$$

We can numerically solve this equation for $\omega_\theta(\vec{k})$. A plot of $\omega_\theta(\vec{k})$ along the $(1,1,1)$ direction in the first Brillouin zone is shown in the right of Fig. 4-6. We see that in the superfluid phase the dispersion is quadratic with

$$
\omega_\theta(\vec{k}) \approx \zeta k^2. \tag{4.24}
$$

Finally, by comparing Eqs. (4.21) and (4.23), we find that at the phase boundary ω_A and ω_θ are degenerate. Lastly, using the result (3.56), we can investigate the behavior of superfluid second sound excitations. From our observations above, we find a linear dispersion for small k,

$$
\omega_s(\vec{k}) \approx ck \tag{4.25}
$$

with the velocity of sound

$$
c = \sqrt{\Delta \zeta}. \tag{4.26}
$$

Thus, the velocity of second sound at any point near the phase boundary can be found from the above numerical inversions. With this, we plot the sound velocity c as a function of the tunneling t/U in Fig. 4-7. We observe that, since near the phase boundary a large quadratic term suddenly appears in the phase dispersion relation, the sound velocity jumps immediately inside the superfluid phase. This jump must
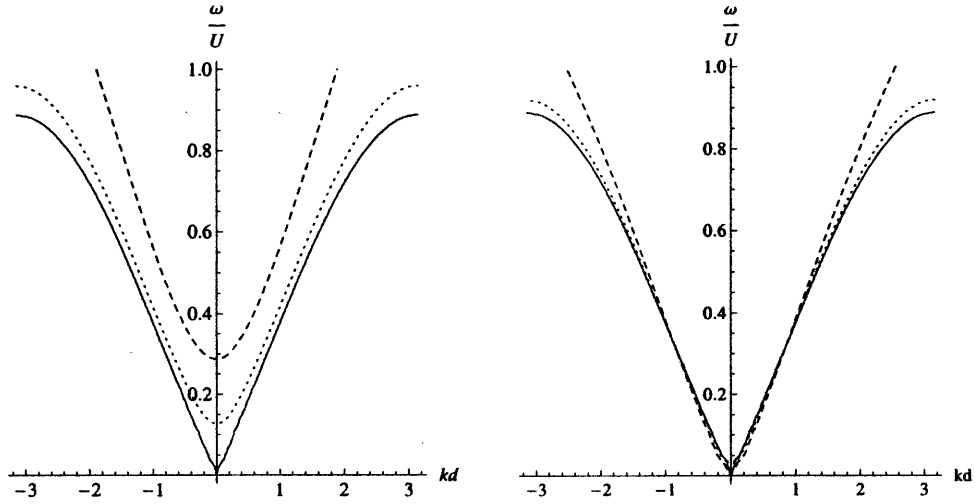
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Figure 4-6: Plots of the zero-temperature dispersion relations $\omega_A(\vec{k})$ (Left) and $\omega_\theta(\vec{k})$ (Right) for various values of the hopping t with fixed $n = 1$, $\mu/U = \sqrt{2} - 1$ and with $\vec{k} = (1,1,1)k/\sqrt{3}$. The solid blue lines corresponds to $t = t_c \approx 0.028\,U$, which for these values of μ and n is at the tip of the first Mott lobe. The dotted yellow lines corresponds to $t = 0.03\,U$, and the dashed red lines corresponds to $t = 0.035\,U$. Note that amplitude excitations exhibit a t-dependent energy gap, while the phase excitations are gapless in accordance with Goldstone's theorem.
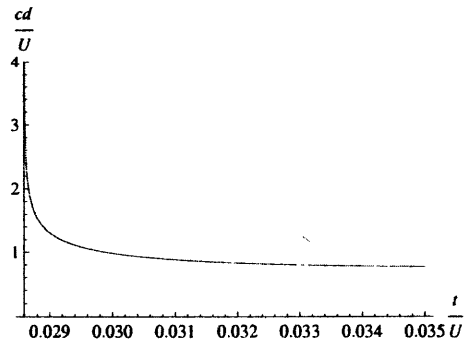

Figure 4-7: Plot of the second sound velocity c as a function of t/U for $t > t_c \approx 0.028\,U$ with $n{=}1$ and $\mu/U = \sqrt{2} - 1$.

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be viewed cautiously, however, as the Ginzburg-Landau expansion is incapable of accurately describing critical behavior in the immediate vicinity of the phase boundary [32, 33, 46, 47]. As the mass of the phase excitations begins to increase faster than the gap in the amplitude excitations, we see that the sound velocity begins to decrease. Far from the phase boundary, however, we know from the seminal Bogoliubov theory that the sound velocity must increase as $\sqrt{t}$ [41, 48], confirming that our theory is not valid in the deep superfluid phase.

Chapter 5

Summary and Conclusion

In this thesis we derived, to first order in the tunneling, the Ginzburg-Landau expansion of the effective action for a very general bosonic lattice Hamiltonian. From the effective action we calculated many static and dynamic system properties of experimental interest. In specifying these results to the Bose-Hubbard model, we compared them with the corresponding findings of the standard mean-field theory. Although both approaches yield – up to first order in the tunneling – the same phase boundary, our method gives qualitatively better results deeper in the superfluid phase. Additionally, we were able to find the dispersion relation for superfluid excitations, which cannot readily be done in the mean-field approach. The primary advantage of our effective-action theory, however, lies in its extensibility. It is straightforward to generalize the derivation given in Chapters 2 and 3 by calculating diagrams beyond the tree level in order to include higher-order tunneling corrections. As seen in Section 3.2, this gives a systematic hopping expansion of the self-energy function *in both the ordered and non-ordered phases*, providing an arbitrarily precise description of the system dynamics near the phase boundary. This should allow, for instance, for the calculation of time-of-flight absorption pictures and their corresponding visibilities for the whole phase diagram [40]. Furthermore, given the generality of the formalism, our effective action theory can, in principle, incorporate a variety of interesting effects, such as disordered lattices [4, 31], vortex dynamics [41], and tunneling beyond nearest neighbor sites. In particular, an effective action for the disordered Bose-Hubbard

model could give new insight into the nature of the Bose glass phase as a state of short-range order [13].

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