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Effective field theory for the Bose-Hubbard model

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# Introduction

The purpose of this thesis is to study the analytic properties of the Bose-Hubbard model, which describes a lattice gas of interacting bosons. Historically, however, the Hubbard model was introduced to describe electrons in transition metals by Hubbard et al in 1963 [1]. It later had an enormous success in many fields, such as the study of superconductivity [2] and the heavy fermions [3]. This model described interacting fermions in a periodic lattice. The same year the fermionic model was introduced, the Bose-Hubbard model was developed by Gersch and Kollmann [4] in a study on granular superconductors. However, it was only in the 1980s that it began to have more success [5, 6, 7]. After that time the model was used to study, among other things, Josephson arrays and ultracold atoms trapped in an optic potential [8, 9]. Recently, the model has been used also in the quantum communication and information field [10] and in the context of quantum chaos [11]. The model predicts a quantum phase transition between a Mott insulating phase and a superfluid phase. Various studies have been devoted to investigate the analytic properties of the model, and in recent times also some experimental works have been done to verify theoretical predictions [12, 16]. In particular, to go beyond mean-field results some authors use a variational approach [7, 24, 25], while others, like the present study uses a random phase approximation (RPA) approach [8, 13, 26].

The thesis is organized as follows. Chapter 1 starts with a derivation of the Bose-Hubbard model Hamiltonian, followed by the introduction of convenient effective theories used to study the fully superfluid regime and the regime near the Mott-superfluid phase transition. Chapter 2 is devoted to the computation of the excitation spectra and the grand canonical potential in both regimes, following a procedure described in [14, 15]. After that there is a study of the properties of the elementary excitations and a comparison of the predictions of the theories introduced for the study of the phase transition with experimental results found in [16] for a bosonic atomic gas trapped in a quasi-2D optical lattice. Chapter 3 begins as an analytic study of the properties of the equation of state (which can be obtained by the grand canonical potential) and its derivatives with the respect to a control parameter for a generic theory of the same form as the theories introduced to study the near-transition regime. A similar study for the case of non-relativistic weakly interacting gas can be found at [27]. Then, numerical predictions for the Bose-Hubbard in that regime are presented. Finally, also, analytic predictions for the fully superfluid regime for the same quantities are given. Regarding the appendices, Appendix A is a brief introduction on the concept of spontaneous symmetry breaking [17, 18] which is used in condensed matter physics to study the phase transitions [19]. Appendix B is an interesting study of both relativistic and non-relativistic weakly interacting gas, by studying the Klein-Gordon [20, 21] and the Gross-Pitaevskii [22, 23] actions. As mentioned in the thesis, there is a formal analogy between the results obtained for these systems and the predictions for the Bose-Hubbard model in both the regimes studied. A similar comparison and a fuller description of the properties of the weakly-interacting gas can be found at [28]. Appendix C shows how to compute Green functions in a quantum field theory. These technical results are necessary for the computation of effective field theories for the regime near the transition. Appendix D introduces the dimensional regularization technique, introduced by t'Hooft and Veltman [29] for renormalization of gauge fields, a regularization method used to treat divergent integrals encountered in the study of the equation of state. Finally Appendix E is a comparison between classical and quantum systems. In particular some formal analogies between the predictions of our theory and classical statistical physics [30, 31] are highlighted.



# Chapter 1

## Analysis of Bose-Hubbard model

### 1.1 Derivation of Bose-Hubbard Hamiltonian

In order to study the properties of the Bose-Hubbard model we need to introduce an external periodic potential in the shifted Hamiltonian of a weakly interacting gas of bosons, given by Equation (B.1). Let us call it  $V_{lat}(\vec{r})$ . Its minima are in correspondence to the positions of the sites. The shifted Hamiltonian of the model is given by:

$$\hat{H} = \int d^D \vec{r} \left\{ \hat{\psi}^\dagger \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{lat}(\vec{r}) - \mu \right) \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right\} \quad (1.1)$$

where  $m$  is the mass of the particles of the gas,  $\psi(\vec{r})$  is the matter field,  $\mu$  is the chemical potential. Finally, we assume that there is a contact interaction between the atoms. We have indicated its coupling by  $g$ . In Appendix B, the weakly-interacting gas is studied in more detail. Let us now define the coordinate vectors of the minima of the lattice potential as:

$$\vec{r} = \vec{r}_i \quad (1.2)$$

In order to study the properties of the model we expand the bosonic field in the Wannier functions (which are peaked in the position of lattice sites and fall rapidly):

$$\hat{\psi}(\vec{r}) = \sum_{ni} w_{ni}(\vec{r}) \hat{a}_{ni} \quad (1.3)$$

where  $w_{ni}$  are the Wannier functions. At ultra-cold temperatures, however, the bosons are in the lowest-energy states, namely the one with  $n = 0$ . Thus we can re-write the expansion as follows (ignoring the  $n = 0$  subscript):

$$\hat{\psi}(\vec{r}) = \sum_i w_i(\vec{r}) \hat{a}_i \quad (1.4)$$

Using this expansion in the shifted Hamiltonian:

$$\begin{aligned} \hat{H} = \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \int d^D \vec{r} \quad w_i^*(\vec{r}) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{lat}(\vec{r}) - \mu \right) w_j(\vec{r}) \\ + \frac{1}{2} \sum_{ii'jj'} \hat{a}_i^\dagger \hat{a}_{i'}^\dagger \hat{a}_j \hat{a}_{j'} g \int d^D \vec{r} \quad w_i^*(\vec{r}) w_{i'}^*(\vec{r}) w_j(\vec{r}) w_{j'}(\vec{r}) \end{aligned} \quad (1.5)$$

We can notice that this expression still contains interactions between atoms of different sites of the lattice. However, these interactions depend on the product of Wannier functions peaked at different sites which fall rapidly. For this reason we neglect all the terms involving products between Wannier functions relative to different sites except in the case of the kinetic term and the lattice potential term, where we consider also the products relative to nearest-neighbor sites. The shifted Hamiltonian becomes:

$$\hat{H} = \sum_{\langle ij \rangle} J_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_i (\varepsilon_i - \mu) \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_i U_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i \quad (1.6)$$

where  $\langle ij \rangle$  denotes the sum over the nearest-neighbor and

$$J_{ij} = \int d^D \vec{r} \quad w_i^*(\vec{r}) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{lat}(\vec{r}) \right) w_j(\vec{r}) \quad (1.7)$$

$$\varepsilon_i = \int d^D \vec{r} \quad w_i^*(\vec{r}) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{lat}(\vec{r}) \right) w_i(\vec{r}) \quad (1.8)$$

$$U_i = g \int d^D \vec{r} \quad w_i^*(\vec{r}) w_i^*(\vec{r}) w_i(\vec{r}) w_i(\vec{r}) \quad (1.9)$$

Assuming now the symmetry of the lattice, we have:

$$\begin{aligned} J_{ij} &= J \quad \forall i, j \\ U_i &= U \quad \forall i \\ \varepsilon_i &= \varepsilon \quad \forall i \end{aligned}$$

We can now write the Boson-Hubbard shifted Hamiltonian, using the number operators, in its usual form:

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j - (\mu - \varepsilon) \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad (1.10)$$

From now on we will drop, for simplicity, the ‘‘shifted’’ qualifier since we will always use the shifted Hamiltonian. Note that, we can consider  $(\mu - \varepsilon)$  as an effective chemical potential for this system.

## 1.2 Coherent State Approximation

The Bose-Hubbard Hamiltonian defined at the end of the previous Section as:

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j - (\mu - \varepsilon) \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad (1.11)$$

involves a phase transition between an insulating phase (i.e. a fixed number of atoms in each site) and a superfluid phase, as we will see in the next Section. Briefly, in the Mott insulating phase, the constant density implies that:

$$\langle \hat{a}_i \rangle = 0 \quad (1.12)$$

i.e. the mean-value of the destruction (and, therefore, creation operator) vanishes. In the superfluid phase, however this is not true, anymore. Hence, the mean-value of the annihilation operator can serve as our order parameter, which is non-zero in the ordered, i.e. superfluid, phase and zero in the disordered phase, i.e. Mott insulating. We now use an approximation that can be used to study the system when it is in the superfluid phase, far from the transition. The approximation involves the choice of time-dependent coherent states<sup>1</sup> as the ground state of the system, namely:

$$|\Phi(t)\rangle = \bigotimes_i |\alpha_i(t)\rangle \quad (1.13)$$

i.e. a tensor product of coherent states relative to each sites (  $|\alpha_i(t)\rangle$  ). The coherent states are eigenvectors of the annihilation operator:

$$\hat{a}_i |\alpha_i(t)\rangle = \psi_i(t) |\alpha_i(t)\rangle \quad (1.14)$$

where  $\psi_i$  is the eigenvalue. We now compute the expectation value of the action in space-time as:

$$\begin{aligned} S_R^{(CS)} &= \langle \Phi(t) | \int dt \left\{ \hat{a}_i^\dagger \left( i\hbar \frac{\partial}{\partial t} \right) \hat{a}_i - \hat{H} \right\} | \Phi(t) \rangle \Rightarrow \\ &= \int dt \left\{ \sum_i \psi_i^* i\hbar \frac{\partial}{\partial t} \psi_i + J \sum_{\langle ij \rangle} \psi_i^* \psi_j + (\mu - \varepsilon) \sum_i |\psi_i|^2 - \frac{U}{2} \sum_i |\psi_i|^4 \right\} \end{aligned} \quad (1.15)$$

<sup>1</sup>We need time-dependent states because we want to study the dynamics of the system. Note also that we are using the Schrödinger picture.

where the superscript ‘‘CS’’ stands for ‘‘Coherent State’’ and the subscript ‘‘R’’ stands for ‘‘real time’’ as opposed to the imaginary time that we will use to compute the thermodynamics. We can now perform the continuum approximation as follows. For the terms involving single-site summations we have:

$$\sum_i \Rightarrow \int d^D \vec{r} \frac{1}{l^D} \quad (1.16)$$

$$\psi_i \Rightarrow \psi(\vec{r}) \quad (1.17)$$

where  $l$  is the lattice constant. For the ‘‘hopping’’ term, i.e. the term involving nearest-neighbor interactions, we can proceed in the following way:

$$\psi_j \Rightarrow \psi(\vec{r} + l\vec{\hat{r}}) = \psi(\vec{r}) + l\vec{\hat{r}} \cdot \frac{\partial}{\partial \vec{r}} \psi(\vec{r}) + \frac{l^2}{2} \left( \vec{\hat{r}} \cdot \frac{\partial}{\partial \vec{r}} \right)^2 \psi(\vec{r}) \quad (1.18)$$

where  $\vec{\hat{r}}$  is a unit vector. In D-dimensions there are D linearly independent unit vectors and we can choose the canonical basis. For each direction there are two neighbors to a given site at the center. So, we have, for example, for the direction parallel to the x-axis:

$$\psi(\vec{r})(\psi(\vec{r} + l\vec{\hat{x}}) + \psi(\vec{r} - l\vec{\hat{x}})) = \psi^*(\vec{r}) \left( 2\psi(\vec{r}) + l^2 \frac{\partial^2}{\partial x^2} \psi(\vec{r}) \right) \quad (1.19)$$

where  $\vec{\hat{x}}$  is the unit-vector parallel to the x-axis. Doing this for every direction:

$$\psi(\vec{r})(\psi(\vec{r} + \vec{\hat{x}}) + \psi(\vec{r} - l\vec{\hat{x}})) = \psi^*(\vec{r})(2D\psi(\vec{r}) + l^2 \nabla^2 \psi(\vec{r})) \quad (1.20)$$

The action therefore now becomes a functional of  $\psi$ :

$$S_R^{(CS)}[\psi, \psi^*] = \int dt d^D \vec{r} \frac{1}{l^D} \left\{ \psi^* \left( i\hbar \frac{\partial}{\partial t} + J l^2 \nabla^2 + 2DJ + (\mu - \varepsilon) \right) \psi - \frac{U}{2} |\psi|^4 \right\} \quad (1.21)$$

For simplicity from now make a choice of units where all quantities are adimensional, namely<sup>2</sup>:

$$J = l = \hbar = 1 \quad (1.22)$$

the action now reads:

$$S_R^{(CS)}[\psi, \psi^*] = \int dt d^D \vec{r} \left\{ \psi^* \left( i \frac{\partial}{\partial t} + \nabla^2 + (\mu - \varepsilon + 2D) \right) \psi - \frac{U}{2} |\psi|^4 \right\} \quad (1.23)$$

We note that in order to describe a superfluid, we must have  $(\mu - \varepsilon + 2D) > 0$ , i.e:

$$\mu > -2D + \varepsilon \quad (1.24)$$

So, in general, we can have a negative chemical potential and still be in the superfluid phase. Note also that we are in units of  $J = 1$  and, therefore, the constraint on the chemical potential depends on  $J$ . To study the thermodynamics of the system we need to work in the Euclidean space, i.e. we have to perform a Wick rotation to convert the real time to the imaginary time, as follows:

$$\tau = it \quad (1.25)$$

We obtain the action in the Euclidean space:

$$S^{(CS)}[\psi, \psi^*] = \int d\tau d^D \vec{r} \left\{ \psi^* \left( \frac{\partial}{\partial \tau} - \nabla^2 - (\mu - \varepsilon + 2D) \right) \psi + \frac{U}{2} |\psi|^4 \right\} \quad (1.26)$$

This action now can be used to compute the partition function, let us call it  $Z^{(CS)}$  and the grand canonical potential density,  $\Omega^{(CS)}$ , for the system for a generic temperature  $T$  and volume  $V$  as follows:

$$Z^{(CS)} = \int D[\psi, \psi^*] \exp(-S^{(CS)}[\psi, \psi^*]) \quad (1.27)$$

$$\Omega^{(CS)} = -\frac{1}{\beta} \ln(Z^{(CS)}) \quad (1.28)$$

where  $D[\psi, \psi^*]$  is the functional measure. These calculations will be performed in detail in the Chapter 2.

<sup>2</sup>alternatively we can say that we measure lengths in units of the lattice spacing, energies in units of  $J$  and finally time in unit of  $\hbar/J$



## 1.3 The Local Limit and the Decoupling Approximation

### 1.3.1 The Local Limit

Using the same conventions as Section 1.2<sup>3</sup> we can write the Bose-Hubbard Hamiltonian as:

$$\hat{H} = - \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j - (\mu - \varepsilon) \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \quad (1.29)$$

A quite different approach to study the properties of this Hamiltonian is to consider the ‘‘hopping’’ term as a small perturbation of the Local Limit, i.e. when the hopping between different sites is neglected<sup>4</sup>. In this limit, clearly, the Hamiltonian becomes a sum over terms relative to each site:

$$\hat{H}_{loc} = \sum_i \left\{ -(\mu - \varepsilon) \hat{n}_i + \frac{U}{2} [\hat{n}_i(\hat{n}_i - 1)] \right\} = \sum_i \hat{h}_{loc,i} \quad (1.30)$$

where now we can define the single-site Hamiltonian as:

$$\hat{h}_{loc} = (\mu - \varepsilon) \hat{n} + \frac{U}{2} [\hat{n}(\hat{n} - 1)] \quad (1.31)$$

This Hamiltonian is diagonal in the Fock states basis<sup>5</sup>. Let call  $|n\rangle$  the Fock state that has eigenvalue  $n$ . In this case the expectation value of the Hamiltonian is given by:

$$\mathcal{E}_{loc}^{(n)} = \langle n | \hat{h}_{loc} | n \rangle = -(\mu - \varepsilon)n + \frac{U}{2}n(n - 1) \quad (1.32)$$

The ground state is defined as follows:

$$\mathcal{E}_{loc}(U, \mu, \varepsilon) = \min_n \mathcal{E}_{loc}^{(n)} = [-(\mu - \varepsilon)n + \frac{U}{2}n(n - 1)] \quad (1.33)$$

with  $n$  given by:

$$\begin{cases} n = 0 & \text{if } \mu - \varepsilon < 0 \\ U(n - 1) < \mu - \varepsilon < Un & \text{if } \mu - \varepsilon > 0 \end{cases}$$

In the Local Limit, this result is true for all sites due to the symmetry of the lattice. We note also that for  $\mu < \varepsilon$  the ground state energy is exactly zero for each site. The total ground state is the tensor product of Fock states relative to every site and since  $U$ ,  $\mu$  and  $\varepsilon$  are the same for every site the total energy is simply:

$$\mathcal{E}_0 = M\mathcal{E}_{loc} \quad (1.34)$$

where  $M$  is the total number of sites in the lattice.

### 1.3.2 Decoupling Approximation

We saw that when the hopping term is negligible the total Hamiltonian is a sum of single-site terms. The introduction of the hopping term, however, produces a non-diagonal Hamiltonian in the Fock states basis. To overcome this difficulty let us write the annihilation operator as the sum of its expectation value, let us call it  $\psi_i$ :

$$\psi_i = \langle \hat{a}_i \rangle \quad (1.35)$$

and the fluctuations around it<sup>6</sup>. If we consider expand up to the linear terms in the fluctuations:

$$\sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j \simeq \sum_{\langle ij \rangle} (\psi_i^* \hat{a}_j + \hat{a}_i^\dagger \psi_j - \psi_i^* \psi_j) \quad (1.36)$$

<sup>3</sup> $\hbar = J = l = 1$

<sup>4</sup>This is valid when  $\mu \gg J$  and  $U \gg J$ .

<sup>5</sup>The ground state for the whole system is the tensor product of Fock states

<sup>6</sup>We need fluctuations to explain the phase transition, as it will be more clear later. To arrive to Equation (1.36) we have to proceed in the following way:

$$\sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j \simeq \sum_{\langle ij \rangle} (\psi_i^* \psi_j + \delta_i^\dagger \psi_j + \psi_i^* \delta_j)$$

where  $\delta_i$  are the fluctuations around the expectation value. Now if we use the definition of the fluctuations we obtain Equation (1.36).

this expression, though, is still problematic since it is not a sum over single-sites terms. However, the lattice is symmetric and we can reasonably assume that the value of  $\psi_i$  does not depend on the index  $i$  and therefore we now take it to be homogeneous on the lattice. Note that  $\psi$  will be used as the order parameter of the phase transition. Its value will be fixed by minimizing the energy of the system. We will see that it is zero in the disordered (Mott insulating) phase and non-vanishing in the ordered (superfluid) phase. The hopping term becomes:

$$\sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j = 2D \sum_i (\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2) \quad (1.37)$$

The Hamiltonian now is a sum over single-site terms. For every site it reads (having removed the now unnecessary  $i$  index):

$$\hat{h} = \hat{h}_{loc} - 2D(\psi^* \hat{a} + \psi \hat{a}^\dagger - |\psi|^2) \quad (1.38)$$

We can divide the entire single-site Hamiltonian by  $2D$ , obtaining:

$$\hat{h} = -(\bar{\mu} - \bar{\varepsilon})\hat{n} + \frac{\bar{U}}{2}[\hat{n}(\hat{n} - 1)] - (\psi^* \hat{a} + \psi \hat{a}^\dagger - |\psi|^2) \quad (1.39)$$

where:

$$\begin{aligned} \bar{U} &= \frac{U}{2D} \\ \bar{\mu} &= \frac{\mu}{2D} \\ \bar{\varepsilon} &= \frac{\varepsilon}{2D} \\ \hat{h} &= \frac{\hat{h}}{2D} \end{aligned}$$

In this Hamiltonian we separate the ‘‘unperturbed’’ Hamiltonian from the perturbation. We take the modulus of the expectation value as our perturbation parameter, i.e.  $|\psi|$  as in the following definition:

$$\psi = |\psi|e^{i\theta} \quad (1.40)$$

The perturbation is given by:

$$|\psi|V = -(\psi^* \hat{a} + \psi \hat{a}^\dagger) = -|\psi|(e^{-i\theta} \hat{a} + e^{i\theta} \hat{a}^\dagger) \quad (1.41)$$

The Bose-Hubbard Hamiltonian has a global  $U(1)$  symmetry being invariant under a phase redefinition of the annihilation operator: our mean-field theory, therefore, must follow the same property, i.e. it must be invariant under a phase redefinition of  $\psi$ . Hence, odd-powered polynomial terms in the expansion are not allowed. Let the normalized ground-state energy of the local Hamiltonian be:

$$\bar{\mathcal{E}}_{loc} = \frac{\mathcal{E}_{loc}}{2D} \quad (1.42)$$

The total normalized energy given by the expansion has the form:

$$\bar{\mathcal{E}} = \bar{\mathcal{E}}_{loc} + \bar{c}_2 |\psi|^2 + \bar{c}_4 |\psi|^4 + O(|\psi|^6) \quad (1.43)$$

Phase transitions take place when  $\bar{c}_2$ , the quadratic coefficient vanishes<sup>7</sup>. We note that the term in the normalized Hamiltonian<sup>8</sup>  $|\psi|^2$  is already quadratic, so we will not use it in the perturbative approach. Our perturbation is given solely by the  $V$  term and only at the end of the calculations of second order-correction we will add the  $|\psi|^2$  contribution. We can now proceed with our expansion, namely:

$$\left( \hat{h}_{loc} + |\psi| \hat{V} \right) (|n\rangle + |\psi| |s^{(1)}\rangle) = \bar{\mathcal{E}}_{loc} |n\rangle + |\psi| \bar{\mathcal{E}}^{(1)} |s^{(1)}\rangle \quad (1.44)$$

<sup>7</sup>Note that if we did not include the fluctuations  $\bar{c}_2$  would be always positive and therefore it would not be possible to study a phase transition.

<sup>8</sup>From now on we will omit the term ‘‘normalized’’.

where  $|s^{(1)}\rangle$  is the state at the first-order perturbation,  $\bar{\mathcal{E}}^{(1)}$  is the contribution to the energy eigenvalue at first-order and  $\bar{\mathcal{E}}_0$  is the eigenvalue of the free Hamiltonian relative to the ground state  $|n\rangle$ . The first order equation is (after the simplification of the factor  $|\psi\rangle$ ):

$$\hat{V}|n\rangle + \hat{h}_{loc}|s^{(1)}\rangle = \bar{\mathcal{E}}_{loc}|s^{(1)}\rangle + \bar{\mathcal{E}}^{(1)}|n\rangle \quad (1.45)$$

At the first order in the perturbation parameter we can write:

$$(\langle n| + \langle s^{(1)}|\psi\rangle)(|n\rangle + |\psi\rangle|s^{(1)}\rangle) = 1 \quad \Rightarrow \langle s^{(1)}|n\rangle + \langle n|s^{(1)}\rangle = 0 \quad (1.46)$$

Therefore, multiplying by  $\langle n|$  the first-order eigenvalue equation of the Hamiltonian we obtain:

$$\langle n|\hat{V}|n\rangle + \langle n|\hat{h}_{loc}|s^{(1)}\rangle = \bar{\mathcal{E}}^{(1)} + \langle n|\bar{\mathcal{E}}_{loc}|s^{(1)}\rangle \quad \Rightarrow \bar{\mathcal{E}}^{(1)} = \langle n|\hat{V}|n\rangle \quad (1.47)$$

We found the first-order correction to the energy. This is zero since the states form an orthonormal basis and  $\hat{V}$  is linear in annihilation and creation operators, confirming the symmetry reasoning mentioned before. However, we will not use this result explicitly in the calculations (when unnecessary for our purposes) to show a more general procedure. To find the perturbed state we now use the completeness relation in the following way:

$$\hat{V}|n\rangle = \sum_{s \neq n} |s\rangle \langle s|\hat{V}|n\rangle + |n\rangle \langle n|\hat{V}|n\rangle \quad \Rightarrow \hat{V}|n\rangle = \sum_{s \neq n} |s\rangle \langle s|\hat{V}|n\rangle + \bar{\mathcal{E}}^{(1)}|n\rangle \quad (1.48)$$

the first order equation can be thus written as:

$$(\bar{\mathcal{E}}_{loc} - \hat{h}_{loc})|s^{(1)}\rangle = \sum_{s \neq n} |s\rangle \langle s|\hat{V}|n\rangle \quad (1.49)$$

from which finally we get the expression of the perturbed state:

$$\sum_{s'} \langle s'|(\bar{\mathcal{E}}_{loc} - \hat{h}_{loc})|s^{(1)}\rangle = \sum_{s'} \langle s'| \sum_{s \neq n} |s\rangle \langle s|\hat{V}|n\rangle \quad \Rightarrow |s^{(1)}\rangle = \sum_{s \neq n} \frac{\langle s|\hat{V}|n\rangle}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}} \quad (1.50)$$

where  $\bar{\mathcal{E}}_{loc,s}$  is the energy of an eigenstate  $|s\rangle$  of the perturbed Hamiltonian<sup>9</sup>. So, we can now proceed to find the second-order correction. In particular we have, for the states:

$$(\langle n| + |\psi\rangle\langle s^{(1)}| + |\psi|^2\langle s^{(2)}|)(|n\rangle + |\psi\rangle|s^{(1)}\rangle + |\psi|^2|s^{(2)}\rangle) = 1 \quad \Rightarrow 2\langle n|s^{(2)}\rangle + \langle s^{(1)}|s^{(1)}\rangle = 0 \quad (1.51)$$

The full expression of the second-order eigenvalue equation is given by:

$$(\hat{h}_{loc} + |\psi\rangle\hat{V})(|n\rangle + |\psi\rangle|s^{(1)}\rangle + |\psi|^2|s^{(2)}\rangle) = (\bar{\mathcal{E}}_{loc} + |\psi|\bar{\mathcal{E}}^{(1)} + |\psi|^2\bar{\mathcal{E}}^{(2)})(|n\rangle + |\psi\rangle|s^{(1)}\rangle + |\psi|^2|s^{(2)}\rangle) \quad (1.52)$$

the second-order part is given by:

$$\hat{h}_{loc}|s^{(2)}\rangle + \hat{V}|s^{(1)}\rangle = \bar{\mathcal{E}}_{loc}|s^{(2)}\rangle + \bar{\mathcal{E}}^{(1)}|s^{(1)}\rangle + \bar{\mathcal{E}}^{(2)}|n\rangle \quad (1.53)$$

now we multiply both sides of the equation by  $\langle n|$ :

$$\langle n|\hat{h}_{loc}|s^{(2)}\rangle + \langle n|\hat{V}|s^{(1)}\rangle = \langle n|\bar{\mathcal{E}}_{loc}|s^{(2)}\rangle + \langle n|\bar{\mathcal{E}}^{(1)}|s^{(1)}\rangle + \bar{\mathcal{E}}^{(2)} \quad (1.54)$$

we can therefore find  $\bar{\mathcal{E}}^{(2)}$ :

$$\bar{\mathcal{E}}^{(2)} = \langle n|\hat{V}|s^{(1)}\rangle - \langle n|\bar{\mathcal{E}}^{(1)}|s^{(1)}\rangle \quad (1.55)$$

$$\bar{\mathcal{E}}^{(2)} = \sum_{s \neq n} \langle n|\hat{V}|s\rangle \frac{\langle s|\hat{V}|n\rangle}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}} - \langle n|\bar{\mathcal{E}}^{(1)}|s\rangle \frac{\langle s|\hat{V}|s\rangle}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}} \quad (1.56)$$

which gives (the second term is zero since  $\bar{\mathcal{E}}^{(1)} = 0$ ):

$$\bar{\mathcal{E}}^{(2)} = \sum_{s \neq n} \frac{|\langle n|\hat{V}|s\rangle|^2}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}} \quad (1.57)$$

<sup>9</sup>For  $s = n$  we have  $\bar{\mathcal{E}}_{loc,s} = \bar{\mathcal{E}}_{loc}$

The total energy  $\bar{\mathcal{E}}$  at the second-order of expansion is therefore given by:

$$\bar{\mathcal{E}}(\psi) = \bar{\mathcal{E}}_{loc} + |\psi|^2 \mathcal{E}^{(2)} + |\psi|^2 = \bar{\mathcal{E}}_{loc} + \bar{c}_2 |\psi|^2 \quad (1.58)$$

therefore  $\bar{c}_2$  is given by:

$$\bar{c}_2 = 1 + \bar{\mathcal{E}}^{(2)} = 1 + \sum_{s \neq n} \frac{|\langle n | \hat{V} | s \rangle|^2}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}} \quad (1.59)$$

The numerator of  $\frac{|\langle n | \hat{V} | s \rangle|^2}{\bar{\mathcal{E}}_{loc} - \bar{\mathcal{E}}_{loc,s}}$  is nonzero only when  $s = n + 1$  and  $s = n - 1$  because  $\hat{V}$  is linear in the annihilation and creation operators and we have chosen an orthonormal basis for unperturbed states. In particular since  $\hat{V} = -(e^{-i\theta} \hat{a} + \hat{a}^\dagger e^{i\theta})$  we have only these following nonvanishing terms (and their complex conjugates):

$$\langle n | \hat{V} | n + 1 \rangle = -e^{-i\theta} \sqrt{n+1} \quad (1.60)$$

$$\langle n - 1 | \hat{V} | n \rangle = -e^{+i\theta} \sqrt{n} \quad (1.61)$$

it follows therefore that:

$$\bar{c}_2 = 1 + \left( \frac{n+1}{(\bar{\mu} - \bar{\varepsilon}) - \bar{U}n} - \frac{n}{(\bar{\mu} - \bar{\varepsilon}) - \bar{U}(n-1)} \right) \quad (1.62)$$

The transition line is at  $\bar{c}_2 = 0$ . Imposing this condition in the expression of the parameter we obtain:

$$1 + \left( \frac{(n+1)((\bar{\mu} - \bar{\varepsilon}) - \bar{U}(n-1)) - n((\bar{\mu} - \bar{\varepsilon}) - \bar{U}n)}{[(\bar{\mu} - \bar{\varepsilon}) - \bar{U}n][(\bar{\mu} - \bar{\varepsilon}) - \bar{U}(n-1)]} \right) = 0 \quad (1.63)$$

$$(\bar{\mu} - \bar{\varepsilon})^2 + \bar{U}^2 n^2 - \bar{U}^2 n - 2(\bar{\mu} - \bar{\varepsilon})\bar{U}n + \bar{U}(\bar{\mu} - \bar{\varepsilon}) + (\bar{\mu} - \bar{\varepsilon} + \bar{U}) = 0 \quad (1.64)$$

This equation can be rewritten as:

$$(\bar{\mu} - \bar{\varepsilon})^2 - 2(\bar{\mu} - \bar{\varepsilon}) \left( \bar{U} \left( n - \frac{1}{2} \right) - \frac{1}{2} \right) + \bar{U} + \bar{U}^2 n(n-1) = 0 \quad (1.65)$$

i.e. an second-order equation in  $\bar{\mu} - \bar{\varepsilon}$  in function of  $\bar{U}$ . Its solutions are:

$$(\bar{\mu} - \bar{\varepsilon})^\pm = \bar{U} \left( n - \frac{1}{2} \right) - \frac{1}{2} \pm \frac{1}{2} \sqrt{\bar{U}^2 - 2\bar{U}(2n+1) + 1} \quad (1.66)$$

These solutions describe a curve in the  $(\bar{U}, \bar{\mu} - \bar{\varepsilon})$  plane of the phase-space which correspond to the transition lines. Being a Landau mean-field theory, we know that the transition occurs when  $\bar{c}_2$  changes sign [32, 33]. The regions enclosed by the lines describe the ‘‘Mott Insulator Phase’’ ( $\bar{c}_2 > 0$ ) instead the region outside the ‘‘lobes’’ corresponds to a superfluid phase, characterized by  $\bar{c}_2 < 0$ . In Figure 1.1 we plotted the solutions of equation (1.66) in the  $(\bar{U}, \bar{\mu} - \bar{\varepsilon})$  plane for  $n = 1, 2, 3$ . We can see that for small values of  $\bar{U}$  and high values of  $\bar{\mu} - \bar{\varepsilon}$  we are in the superfluid phase. The regions inside the ‘‘lobes’’ are relative to the Mott phase, characterized by high  $\bar{U}$ , i.e. strong interaction. If we now divide by  $\bar{U}$  Equation (1.66) we obtain:

$$\frac{(\bar{\mu} - \bar{\varepsilon})^\pm}{\bar{U}} = \left( n - \frac{1}{2} \right) - \frac{1}{2\bar{U}} \pm \frac{1}{2} \sqrt{\left( \frac{1}{\bar{U}} \right)^2 - 2\frac{1}{\bar{U}}(2n+1) + 1} \quad (1.67)$$

which solutions are plotted in Figure 1.2. Here it is more evident the fact that the ‘‘lobes’’ are fully separated from each other and from the superfluid phase region.

The tips of the lobes instead describe a transition characterized by critical values of  $\bar{U}$  and  $\bar{\mu} - \bar{\varepsilon}$ , i.e. when the solutions coincide. Hence, they are multicritical points. We have:

$$\bar{U}^c = (2n+1) + \sqrt{(2n+1)^2 - 1} \quad (1.68)$$

$$(\bar{\mu} - \bar{\varepsilon})^c = \bar{U}^c \left( n - \frac{1}{2} \right) - \frac{1}{2} \quad (1.69)$$

In Figure 1.3, we plot  $\bar{c}_2$  for  $D = 2$  and  $n = 1$  at  $(\bar{\mu} - \bar{\varepsilon}) = (\bar{\mu} - \bar{\varepsilon})^c$ . To better study the features of the perturbed energy we also need the fourth-order correction<sup>10</sup>. In particular we will have:

$$\bar{\mathcal{E}}(\psi) = \bar{\mathcal{E}}_{loc} + \bar{c}_2 |\psi|^2 + \bar{c}_4 |\psi|^4 \quad (1.70)$$

<sup>10</sup>We do not consider higher-order corrections.

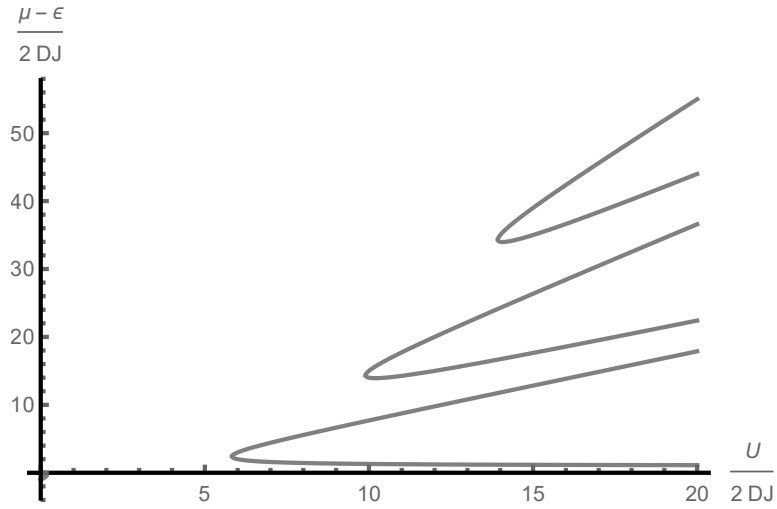


Figure 1.1: The solutions for  $n = 1, 2, 3$  of Equation (1.66) are plotted. On the x-axis we have the ratio  $U/2DJ$ , while on the y-axis we have the ratio  $(\mu - \epsilon)/2DJ$ . This phase diagram can be obtained, for example by fixing the coupling of the hopping term,  $J$ . Inside the lobes we are in the disordered Mott phase, characterized by vanishing mean-value of the annihilation operator. Outside the lobes we are in the ordered superfluid phase, where, instead, the mean-value of annihilation operator is non-vanishing.

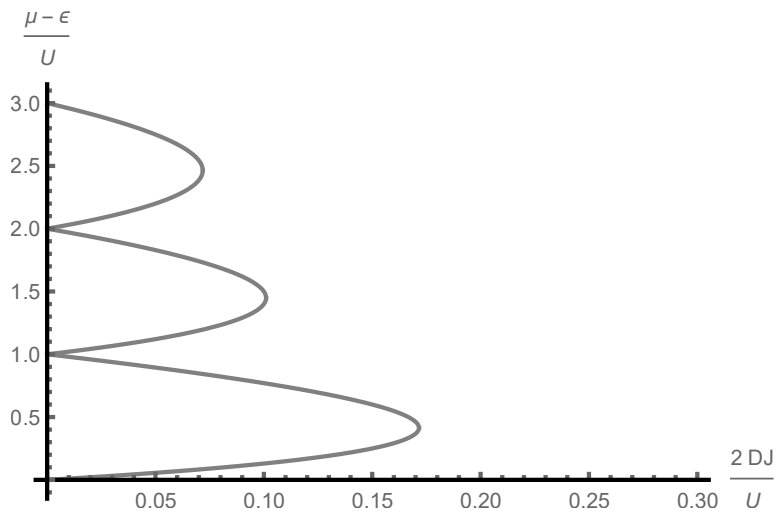


Figure 1.2: The solutions for  $n = 1, 2, 3$  of Equation (1.67) are plotted. On the x-axis we have the ratio  $2DJ/U$ , while on the y-axis we have the ratio  $(\mu - \epsilon)/U$ . This phase diagram can be obtained by fixing the on-site interaction (hence by fixing  $U$ ). Inside the lobes we are in the disordered Mott phase, characterized by vanishing mean-value of the annihilation operator. Outside the lobes we are in the ordered superfluid phase, where, instead, the mean-value of annihilation operator is non-vanishing.

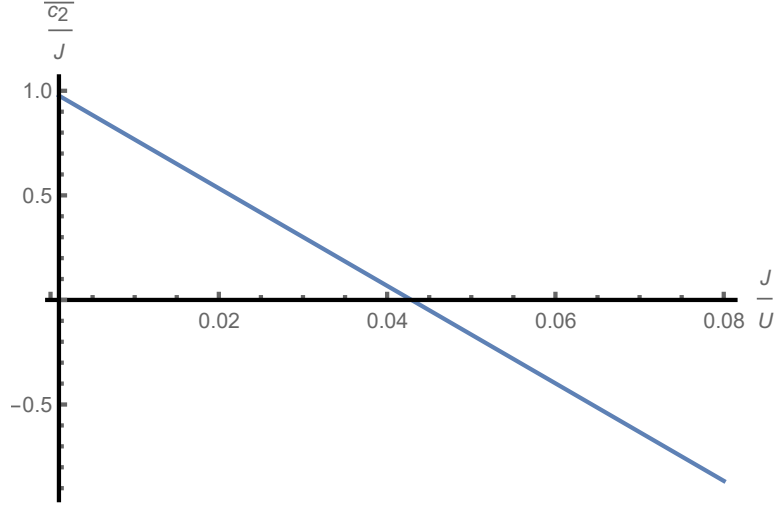


Figure 1.3: Here the parameter  $\bar{c}_2$  is plotted for  $D = 2$ ,  $n = 1$  and  $\frac{\mu-\varepsilon}{U} = \frac{(\mu-\varepsilon)^c}{U^c}$  defined at Equations (1.68) and (1.69). From the properties of Landau theories [32, 33], we know that the transition occurs when  $\bar{c}_2 = 0$ .

In particular, as it is shown in [13],  $\bar{c}_4$  is given by:

$$\bar{c}_4 = \frac{n(n-1)}{(\bar{U}(n-1) - \bar{\mu} - \bar{\varepsilon})^2(\bar{U}(2n-3) - 2(\bar{\mu} - \bar{\varepsilon}))} + \frac{(n+1)(n+2)}{[(\bar{\mu} - \bar{\varepsilon}) - \bar{U}n]^2(2(\bar{\mu} - \bar{\varepsilon}) - \bar{U}(2n+1))} - \left( \frac{n}{\bar{U}(n-1) - (\bar{\mu} - \bar{\varepsilon})} + \frac{n+1}{(\bar{\mu} - \bar{\varepsilon}) - \bar{U}n} \right) \left( \frac{n}{[\bar{U}(n-1) - (\bar{\mu} - \bar{\varepsilon})]^2} + \frac{n+1}{[(\bar{\mu} - \bar{\varepsilon}) - \bar{U}n]^2} \right) \quad (1.71)$$

This parameter is always positive. Therefore the energy of a generic site becomes:

$$\bar{\mathcal{E}}(\psi) = \bar{\mathcal{E}}_0 + \bar{c}_2|\psi|^2 + \bar{c}_4|\psi|^4 \quad (1.72)$$

Note that this function is proportional to the free-energy of Landau mean-field theory [32, 33], where we have expanded up to the fourth-order in the order parameter (for more details see Appendix A). The total energy is given by:

$$\bar{\mathcal{E}}^{(DA)}(\psi) = \sum_i \bar{\mathcal{E}}(\psi) = M\bar{\mathcal{E}}(\psi) \quad (1.73)$$

where “DA” stands for “Decoupling Approximation”. Now let us redefine the “unbarred” quantities given by the multiplication of the  $2D$  factor:

$$c_{2,4} = 2D\bar{c}_{2,4} \quad (1.74)$$

$$\mathcal{E} = 2D\bar{\mathcal{E}} = \mathcal{E}_{loc} + c_2|\psi|^2 + c_4|\psi|^4 \quad (1.75)$$

$$\mathcal{E}^{(DA)} = 2D\bar{\mathcal{E}}^{(DA)} = M\mathcal{E} \quad (1.76)$$

We also note that  $\mathcal{E}$  is, in this approximation, the value of the grand-canonical potential density:

$$\frac{\Omega^{(DA)}}{M} = -\frac{1}{M\beta} \ln[\exp(-\beta\mathcal{E}^{(DA)})] = \mathcal{E} \quad (1.77)$$

where we have used  $M$ , the number of sites, instead of  $V$ , the volume, because in our choice of units ( $l = 1$ ) they are equivalent. If we compute the stationarity condition of  $\mathcal{E}$  with the respect to  $\psi$ , we obtain:

$$\frac{\partial}{\partial \psi} \mathcal{E}(\psi, \psi^*) = 0 \quad \Rightarrow \quad |\psi| = \begin{cases} 0 & \text{if } c_2 > 0 \\ \sqrt{\frac{-c_2}{2c_4}} & \text{if } c_2 < 0 \end{cases} \quad (1.78)$$

In the Mott (disordered) phase ( $c_2 > 0$ ) the order parameter  $\psi$  vanishes, while it is nonvanishing in the superfluid (ordered) phase ( $c_2 < 0$ ) is nonzero. Note that while the energy of the system, given by (1.75), is invariant under a phase transformation, this is not true anymore for the minimum when we are in the

superfluid (ordered) phase. We have a spontaneous symmetry breaking<sup>11</sup>. When  $c_2 > 0$  we are in the Mott phase and the potential density reduces to the local term:

$$\mathcal{E}(\psi = 0) = \mathcal{E}_{loc} = -(\mu - \varepsilon)n + \frac{U}{2}n(n - 1) \quad (1.79)$$

The particle density,  $\rho$  is, in general, given by:

$$\rho = -\frac{\partial \Omega}{\partial \mu \bar{V}} \quad (1.80)$$

where  $\Omega$  is a generic grand canonical potential. In our case, for the Mott phase we have:

$$\rho = n \quad (1.81)$$

i.e. the particle density is the same of the number of particles in each site. On the other hand, for the superfluid phase we have:

$$\mathcal{E}(\psi, \psi^*) = \mathcal{E}_{loc} + c_2|\psi|^2 + c_4|\psi|^4 = \mathcal{E}_{loc} - \frac{c_2^2}{4c_4} \quad (1.82)$$

where we have substituted the value of the order parameter which extremize the potential for the superfluid phase, i.e. the value found at Equation (1.78) for  $c_2 < 0$ . If we now compute the particle density we find:

$$\rho = n + \frac{c_2 \partial_\mu c_2}{2c_4} - \frac{c_2^2 \partial_\mu c_4}{4c_4^2} \quad (1.83)$$

The non-zero value of the order parameter, in the superfluid phase, causes the arising of an additional contribution to the density. We stress, however, another interesting feature. If we take the derivative of  $\rho$  with the respect to  $c_2$  we get (we treat  $\partial_\mu c_2$  as independent of  $c_2$ ):

$$\frac{\partial}{\partial c_2} \rho = +\frac{\partial_\mu c_2}{2c_4} - \frac{c_2 \partial_\mu c_4}{2c_4} \quad (1.84)$$

At the transition, where  $c_2 = 0$  the second term vanishes. This is not true, in general for the first term. The first term vanishes only at the tips of the lobes, when  $\partial_\mu c_2$  goes to zero. If we take a fixed value of  $\mu$  at the transition a change in  $c_2$  is connected to a change in  $J/U$ . Therefore by changing the value of  $J/U$  a transition is only possible at the tips, i.e. the multicritical points, when we have a transition at constant density. For all other points, we need to fix the value of  $J/U$  and change the effective chemical potential, i.e.  $(\mu - \varepsilon)$ . Finally, let us now see if this approximation at an appropriate limit recovers the quadratic and quartic coefficients of the Coherent State one, introduced in the previous Section. This, unfortunately, is not the case. In fact if we consider the limit  $\bar{U} \ll \bar{\mu} - \bar{\varepsilon}$  which corresponds to the fully superfluid regime we obtain:

$$c_2 = 2D + (2D)^2 \frac{1}{\mu - \varepsilon} \quad (1.85)$$

$$c_4 = (2D)^4 \frac{U}{2(\mu - \varepsilon)^4} (4n + 1) \quad (1.86)$$

where  $c_2$  and  $c_4$  are clearly different to respectively  $(\mu - \varepsilon + 2D)$ , which was the coefficient of the second-order term in the order parameter for the Coherent State Approximation, and  $U$ , which was the coefficient of the fourth-order term<sup>12</sup>. The analogy therefore is purely formal. Let us, however, compute the constraint on  $\mu - \varepsilon$  in order to see the values of  $\mu$  which are compatible with both the approximations. In order to have a superfluid state we must have:

$$c_2 = 2D + (2D)^2 \frac{1}{\mu - \varepsilon} < 0 \quad (1.87)$$

which can be rewritten as:

$$1 < -\frac{2D}{\mu - \varepsilon} \quad (1.88)$$

<sup>11</sup>For a fuller discussion of the spontaneous symmetry breaking mechanism, see Appendix A

<sup>12</sup>In the limit  $U \ll \mu - \varepsilon$  the zeroth-order term of  $c_4$  in  $\bar{U}$  is zero.

From the Coherent state approximation we have found the constraint:

$$\mu - \varepsilon > -2D \quad (1.89)$$

It is evident that for  $\mu - \varepsilon > 0$  the constraints are mutually exclusive. It is maybe quite surprising that the two constraints instead are exactly the same when  $\mu - \varepsilon$  is negative. So the constraint on  $\mu - \varepsilon$  in order to use both the models is given by:

$$-2D < \mu - \varepsilon < 0 \quad (1.90)$$

We stress two interesting features: the first is that since  $\mu - \varepsilon < 0$  the constant term in the expression of the total energy,  $\mathcal{E}_0$ , vanishes in the region of allowed value of chemical potential for both approximation. Secondly that if  $J = 0$  there is no region where both approximations are possible. This because we have worked in units with  $J = 1$  and therefore the  $2D$  term in reality is proportional to  $J$ . This however should not be too surprising: at  $J = 0$  there is no nearest-neighbors interaction and therefore we are in a “perfect” Mott phase, i.e. the Local Limit, whereas we have assumed to be in the superfluid region.

## 1.4 Beyond mean field

In order to study better the properties of the system near the quantum phase transition we need to go beyond mean-field. To do this we need to introduce terms in space and time derivative in order to study the dynamics and thermodynamics of the system. We will use a strong coupling random phase approximation as in [26], characterized by  $U/J \gg 1$ . In order to do so let us reconsider the action in the Bose-Hubbard model in the imaginary time formalism:

$$S = \int d\tau \left\{ \sum_i \left[ a_i^* \left( \frac{\partial}{\partial \tau} - (\mu - \varepsilon) \right) a_i + \frac{U}{2} a_i^* a_i^* a_i a_i \right] - \sum_{\langle ij \rangle} a_i^* a_j \right\} \quad (1.91)$$

Let us separate the hopping term from the rest of the action in the following way:

$$S = S_0 - \int d\tau \sum_{\langle ij \rangle} a_i^* a_j \quad (1.92)$$

where  $S_0$  is the sum of all single-site terms:

$$S_0 = \int d\tau \left[ \sum_i a_i^* \left( \frac{\partial}{\partial \tau} - \mu \right) + \frac{U}{2} a_i^* a_i^* a_i a_i \right] \quad (1.93)$$

We can define the total partition function as:

$$Z = \int D[a, a^*] \exp \left\{ -S_0 + \int d\tau \sum_{\langle ij \rangle} a_i^* a_j \right\} \quad (1.94)$$

We can now write the hopping term as:

$$\sum_{\langle ij \rangle} a_i^* a_j = \sum_{ij} a_i^* J_{ij} a_j \quad (1.95)$$

where  $J_{ij}$  is the (i,j) element of a matrix  $J$  which is characterized by:

$$J_{ij} = \begin{cases} 1 & \text{if } i, j \text{ nearest neighbor} \\ 0 & \text{otherwise} \end{cases}$$

performing now a Hubbard-Stratonovich transformation on the hopping term we obtain:

$$Z = \int D[a, a^*, \psi, \psi^*] \exp \left\{ -S_0 - \int d\tau \sum_{ij} \psi_i^* J_{ij}^{-1} \psi_j + \int d\tau \sum_i (\psi_i^* a_i + c.c) \right\} \quad (1.96)$$



where  $J_{ij}^{-1}$  is the (i,j) element of the inverse matrix of  $J$ , which exact form is not of our interest, as we will see later. Now we can multiply and divide  $Z$  by:

$$Z_0 = \int D[a, a^*] \exp\{-S_0\} \quad (1.97)$$

i.e. the partition function of the sum of all the single-site terms, obtaining:

$$Z = Z_0 \int D[\psi, \psi^*] \left[ \exp\left\{ \int d\tau \sum_{ij} \psi_i^* J_{ij}^{-1} \psi_j \right\} \frac{\int D[a, a^*] \exp\{-S_0 + \int d\tau \sum_i (\psi_i^* a_i + c.c.)\}}{Z_0} \right] \quad (1.98)$$

But we have that:

$$\frac{\int D[a, a^*] \exp\{-S_0 - \int d\tau \sum_i (\psi_i^* a_i + c.c.)\}}{Z_0} = \left\langle \exp \left\{ + \int d\tau \sum_i (\psi_i^* a_i + c.c.) \right\} \right\rangle_0 \quad (1.99)$$

i.e. it is the mean value of the linear terms. The generator functional of connected Green functions, let us call it  $W_0[\psi, \psi_*]$  can be written as an expansion of that functions as follows:

$$W_0 = - \sum_N \frac{1}{(N!)^2} \int d\tau_1 \cdots d\tau_N d\tau'_1 \cdots d\tau'_N \sum_i G_{2N}^{(0)}(\tau_1, \dots, \tau_N, \tau'_1, \dots, \tau'_N) \psi_i^*(\tau_1) \cdots \psi_i^*(\tau_N) \cdots \psi_i(\tau'_1) \cdots \psi_i(\tau'_N) \quad (1.100)$$

where  $G_0^{(2N)}$  is the 2N-points connected correlation function and we used the fact that the action  $S_0$  contains a sum of local, i.e. single lattice, terms. For clarification about this point, we suggest to read Appendix C. It can be shown that is given by:

$$\left\langle \exp \left\{ + \int d\tau \sum_i (\psi_i^* a_i + c.c.) \right\} \right\rangle_0 = \exp\{-W_0[\psi, \psi_*]\} \quad (1.101)$$

Therefore our partition function at the fourth order of expansion of  $W_0$  can be written as:

$$Z = Z_0 \int D[\psi, \psi^*] \exp \left\{ \int d\tau \sum_{ij} \psi_i^* J_{ij}^{-1} \psi_j - \int d\tau \int d\tau' \sum_i \psi_i^* G_0^{(2)}(\tau - \tau') \psi_i + \int d\tau \tilde{G}_4 \psi_i^* \psi_i^* \psi_i \psi_i \right\} \quad (1.102)$$

where we have approximated the four-point Green function to its static value<sup>13</sup>,  $\tilde{G}_4$ . We can now define an effective action as:

$$S_{eff} = - \int d\tau \sum_{ij} \psi_i^* J_{ij}^{-1} \psi_j + \int d\tau \int d\tau' \sum_i \psi_i^* G_0^{(2)}(\tau - \tau') \psi_i - \int d\tau \tilde{G}_4 \psi_i^* \psi_i^* \psi_i \psi_i \quad (1.103)$$

If we perform a Fourier Transform for the quadratic term we obtain:

$$S_{eff} = \sum_n \sum_{\vec{q}} \psi_{n,\vec{q}}^* \left( \frac{1}{2 \sum_{k=1}^D \cos(q_k)} + G_0^{(2)}(i\omega_n) \right) \psi_{n,\vec{q}} - \int d\tau \tilde{G}_4 \psi_i^* \psi_i^* \psi_i \psi_i \quad (1.104)$$

where  $\vec{q}$  are the momenta,  $\omega_n$  are the Matsubara frequencies,  $\psi_{n,\vec{q}}$  is the Fourier Transform of the auxiliary field, the first term in the parenthesis is the Fourier Transform of  $J^{-1}$  calculated as the reciprocal of the Fourier Transform of  $J$  and finally  $G_0^{(2)}(i\omega_n)$  is the Fourier Transform of the two-point Green function given by:

$$\tilde{G}_0^{(2)}(i\omega_n) = \frac{n+1}{i\omega_n + (\mu - \varepsilon) - Un} - \frac{n}{i\omega_n + (\mu - \varepsilon) - U(n-1)} \quad (1.105)$$

Expanding now the coefficients of the quadratic terms up to the second order in  $\omega_n$  and  $\vec{q}$ , the action can be written as:

$$S_{eff} = \sum_n \sum_{\vec{q}} \psi_{n,\vec{q}}^* \left( \tilde{G} + \frac{1}{2D} + \frac{\partial}{\partial \mu} \tilde{G} i\omega_n - \frac{1}{2} \frac{\partial^2}{\partial \mu^2} \tilde{G} \omega_n^2 - \frac{1}{4D^2} q^2 \right) \psi_{n,\vec{q}} + \int d\tau \tilde{G}_4 \psi_i^* \psi_i^* \psi_i \psi_i \quad (1.106)$$

<sup>13</sup>Approximation justified for high values of  $U$ . In fact, we are assuming that the coupling is strong.

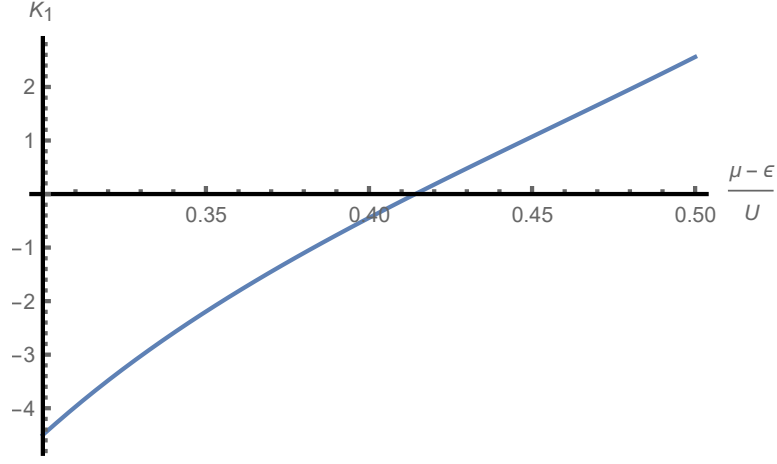


Figure 1.4: In this Figure we plot the behavior of  $K_1$  for  $n = 1$  and  $\frac{J}{U} = 0.04$ . Note that at  $\frac{\mu-\epsilon}{U} = \frac{(\mu-\epsilon)^c}{U^c}$  the parameter vanishes.

Performing now the continuum approximation and the following redefinition of fields:

$$\psi'_{n,\vec{q}} = 2D\psi_{n,\vec{q}} \quad (1.107)$$

$$\psi'_i = 2D\psi_i \quad (1.108)$$

we obtain:

$$S_{eff} = \sum_n \int d\vec{q} \psi_{n,\vec{q}}^* (c_2 + K_1 i\omega_n - K_2 \omega_n^2 + K_3 q^2) \psi_{n,\vec{q}} + \int d\tau c_4 \psi_i^* \psi_i^* \psi_i \psi_i \quad (1.109)$$

where:

$$K_1 = -\frac{\partial}{\partial \mu} c_2 \quad (1.110)$$

$$K_2 = -\frac{1}{2} \frac{\partial}{\partial \mu} c_2 \quad (1.111)$$

$$K_3 = 1 \quad (1.112)$$

We note that  $c_4$  and  $K_2$  are always positive and nonzero.  $K_3$  is a positive constant.  $c_2$  is positive in the Mott lobes and negative in the superfluid phase and finally  $K_1$  has an interesting behavior: at fixed  $n$ , for  $\frac{\mu-\epsilon}{U} < \frac{(\mu-\epsilon)^c}{U^c}$  is negative, it is positive with the opposite inequality and zero at when the equality is satisfied. In particular we plot  $K_1$  in Figure 1.4 for  $n = 1$ ,  $D = 2$  and at  $J/U = 0.04$ .

Returning finally to the Euclidean space:

$$S_{eff}[\psi, \psi^*] = \int d\tau \int d\vec{r} \left\{ K_1 \psi^* \frac{\partial}{\partial \tau} \psi + K_2 \left| \frac{\partial}{\partial \tau} \psi \right|^2 + K_3 |\vec{\nabla} \psi|^2 + c_2 |\psi|^2 + c_4 |\psi|^4 \right\} \quad (1.113)$$

and therefore the total partition function is:

$$Z = Z_0 \int D[\psi, \psi^*] \exp\{-S_{eff}[\psi, \psi^*]\} \quad (1.114)$$

Note the strong similarity between the action (1.113) and the action of the relativistic gas (B.33). In fact the two actions have the same form, if we do the following identifications:

$$\begin{aligned} K_1 &\leftrightarrow 2\hbar \frac{\mu_r}{mc^2} \\ K_2 &\leftrightarrow \frac{\hbar^2}{mc^2} \\ K_3 &\leftrightarrow \frac{\hbar^2}{m} \\ c_2 &\leftrightarrow \frac{\mu_r^2}{mc^2} - mc^2 \\ c_4 &\leftrightarrow \frac{g}{2} \end{aligned}$$

Hence, we can infer that the two actions share many properties. In fact, we expect that the form of the spectrum and the grand canonical potential is the same, after having done the identification above. The action we have found, however, has some problems. After all the field  $\psi$  is an auxiliary field and in fact has no direct physical meaning. As we will see, however, this model can still be used to make predictions near the transition line.

The problem of the physical meaning of the fields can be avoided if we perform a second Hubbard-Stratonovich transformation. Let us rewrite the partition function after the first transformation:

$$Z = Z_0 \int D[\psi, \psi^*] \exp\{-W_0[\psi, \psi^*] + \sum_{ij} \psi_i^* J_{ij}^{-1} \psi_j\} \quad (1.115)$$

if we introduce another auxiliary field, let us call it  $\phi$  we obtain:

$$Z = Z_0 \int D[\phi, \phi^*, \psi, \psi^*] \exp\{-\int d\tau \sum_{ij} \phi_i^* J_{ij} \phi_j + \sum_i (\phi_i^* \psi_i + c.c) - W_0[\psi, \psi^*]\} \quad (1.116)$$

As it is explained in [26] the new auxiliary fields we will introduce now have the same correlation functions of the original fields and therefore they have the same physical meaning as the fields  $a_i$ . The partition function can be rewritten as:

$$Z = Z_0 Z_1 \int D[\phi, \phi^*] \exp\{-\int d\tau \sum_{ij} \phi_i^* J_{ij} \phi_j\} \frac{\int D[\psi, \psi^*] \exp\{\sum_i (\phi_i^* \psi_i + c.c) - W_0[\psi, \psi^*]\}}{Z_1} \quad (1.117)$$

where  $Z_1$  is the partition function given by:

$$Z_1 = \int D[\psi, \psi^*] \exp\{-W_0[\psi, \psi^*]\} \quad (1.118)$$

It can be shown that integrating out  $\psi$  and  $\psi^*$ <sup>14</sup> and proceeding in the same way as the previous case, without however redefining the fields, we obtain  $\phi$ :

$$S_{EFF}[\psi, \psi^*] = \int d\tau \int d\vec{r} \left\{ \tilde{K}_1 \phi^* \frac{\partial}{\partial \tau} \phi + \tilde{K}_2 \left| \frac{\partial}{\partial \tau} \phi \right|^2 + \tilde{K}_3 |\vec{\nabla} \phi|^2 + \tilde{c}_2 |\phi|^2 + \tilde{c}_4 |\phi|^4 \right\} \quad (1.119)$$

where now the parameters are:

$$\tilde{K}_1 = \frac{\partial}{\partial \mu} \tilde{G} \quad (1.120)$$

$$\tilde{K}_2 = \frac{\partial^2}{\partial \mu^2} \tilde{G} \quad (1.121)$$

$$\tilde{K}_3 = 2D \quad (1.122)$$

$$\tilde{c}_2 = -2D + \frac{1}{\tilde{G}} \quad (1.123)$$

$$\tilde{c}_4 = \frac{\tilde{G}_4}{4\tilde{G}^4} \quad (1.124)$$

Despite the difference in their expressions, these parameters have similar behavior to the other ones found before.  $\tilde{c}_2$  is greater than zero in the Mott phase, negative in the superfluid and vanishes at the transition line (which coincides to the one calculated by imposing  $c_2 = 0$ ).  $\tilde{K}_1$  is positive (negative) for  $\frac{(\mu-\varepsilon)}{U} > \frac{(\mu-\varepsilon)_c}{U_c}$  ( $\frac{(\mu-\varepsilon)}{U} < \frac{(\mu-\varepsilon)_c}{U_c}$ ) and vanishes when the equality is satisfied.  $\tilde{K}_3$  is a positive constant and finally  $\tilde{K}_2$  and  $\tilde{c}_4$  are always positive. In Figure 1.5  $\tilde{c}_2$  is plotted at  $(\mu - \varepsilon) = (\mu - \varepsilon)_c$  for varying  $J/U$ . This plot can be compared with the one of  $\bar{c}_2 = c_2/2D$  for  $D = 2$  at Figure 1.3. In Figure 1.6, instead, by fixing  $J/U = 0.04$  we plotted  $\tilde{K}_1$  as a function of the ratio  $\frac{(\mu-\varepsilon)}{U}$ . Notice the strikingly similarity between the behavior of this coupling and that of  $K_1$  plotted in Figure 1.4. Finally,  $\tilde{K}_3$  is a positive constant like  $K_3$  while both  $\tilde{K}_2$  and  $\tilde{c}_4$  are always positive as were  $K_2$  and  $c_4$ .

<sup>14</sup>The procedure is very complicated since involves the elimination of anomalous contributions in the perturbative approach and it is beyond the scope of the present work.

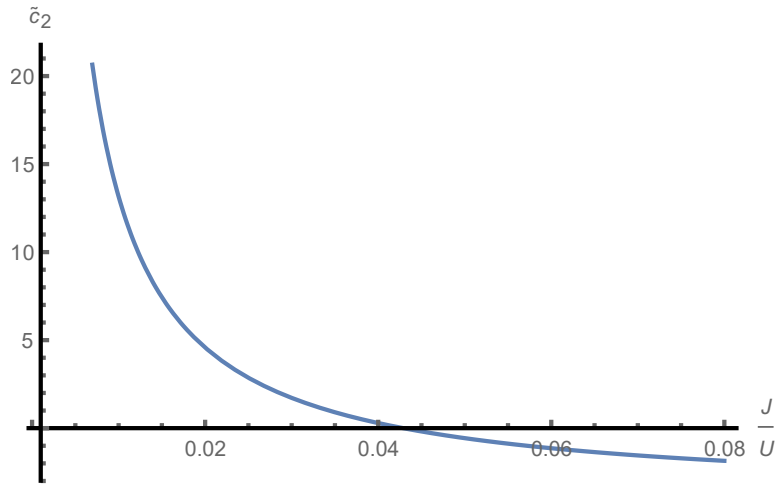


Figure 1.5: In this Figure we plot the behavior of  $\tilde{c}_2$  for  $n = 1$  and  $(\mu - \varepsilon) = (\mu - \varepsilon)^c$ . Note that at the critical value of the effective chemical potential  $\frac{U_c}{J}$  the parameter vanishes.

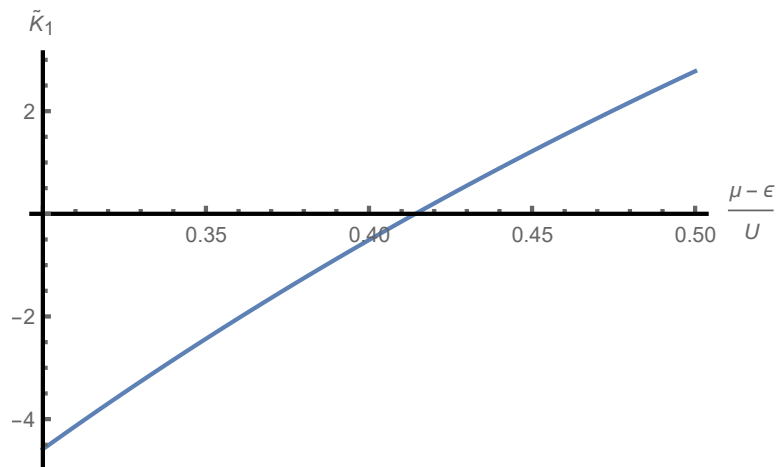


Figure 1.6: In this Figure we plot the behavior of  $\tilde{K}_1$  for  $n = 1$  and  $\frac{J}{U} = 0.04$ . Note that at  $\frac{(\mu - \varepsilon)}{U} = \frac{(\mu - \varepsilon)^c}{U^c}$  the parameter vanishes.



## Chapter 2

# Dynamics and thermodynamics of the Bose-Hubbard model

### 2.1 Fully superfluid regime

In the fully superfluid regime (i.e. in a region of phase-space far from the transition lines) we need to use the Coherent State Approximation. Let us now call  $V$  the total volume and  $T$  its temperature. Following the choice of units used in the Chapter 1 <sup>1</sup> we have that both the volume and the temperature are adimensional. The action in this approximation of the system at temperature  $T$  and volume  $V$  is given by:

$$S^{(CS)}[\psi, \psi^*] = \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ \psi^* \left( \frac{\partial}{\partial \tau} - \nabla^2 - (\mu - \varepsilon + 2D) \right) \psi + \frac{U}{2} |\psi|^4 \right\} \quad (2.1)$$

We can now define a partition function,  $Z^{(CS)}$ , and a grand canonical potential,  $\Omega^{(CS)}$  as follows:

$$Z^{(CS)} = \int D[\psi, \psi^*] \exp \left\{ S^{(CS)}[\psi, \psi^*] \right\} \quad (2.2)$$

$$\Omega^{(CS)} = -\frac{1}{\beta} \ln(Z^{(CS)}) \quad (2.3)$$

In order to find the dynamical and thermodynamical properties of the system we write  $\psi$  as:

$$\psi(\vec{r}, \tau) = \psi_0 + \chi(\vec{r}, \tau) \quad (2.4)$$

where  $\psi_0$  is the mean-field contribution, independent of space and time, and  $\chi$  is the fluctuation field. In order to find the value of  $\psi_0$  we need to minimize the mean-field contribution to the action (which is the same as minimizing the mean-field contribution to the grand-canonical potential). This can be done by considering the effective potential:

$$V_{eff}^{(CS)} = -(\mu - \varepsilon + 2D)|\psi_0|^2 + U|\psi_0|^4 \quad (2.5)$$

by imposing the stationarity condition to  $V_{eff}^{(CS)}$ :

$$\frac{\partial V_{eff}^{(CS)}}{\partial \psi_0} = 0 \quad (2.6)$$

we find that the modulus of the minimum is given by:

$$|\psi_0| = \begin{cases} 0 & \text{if } \mu - \varepsilon + 2D < 0 \\ \sqrt{\frac{\mu - \varepsilon + 2D}{U}} & \text{if } \mu - \varepsilon + 2D > 0 \end{cases} \quad (2.7)$$

Since we are working in the superfluid regime it is the lower case that is of ours interest. We choose the real-valued minimum:

$$\psi_0 = \psi_0^* = \sqrt{\frac{\mu - \varepsilon + 2D}{U}} \quad (2.8)$$

---

<sup>1</sup> $J = \hbar = l = 1$

We can now write the expression of the action expanded up to the second-order (i.e. Gaussian) in the fluctuations:

$$S^{(CS)}[\chi, \chi^*] = \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ -(\mu - \varepsilon + 2D)\psi_0^2 + \frac{1}{2}U\psi_0^4 + \psi_0 \frac{\partial}{\partial \tau} \psi - (\mu - \varepsilon + 2D)\psi_0(\chi + \chi^*) + \right. \\ \left. U\psi_0^3(\chi + \chi^*) + \chi^* \left( \frac{\partial}{\partial \tau} - \nabla^2 - (\mu - \varepsilon + 2D) + 2U\psi_0 \right) \chi + \frac{U}{2}(\chi\chi + \chi^*\chi^*) \right\} \quad (2.9)$$

where in the first line we have the constant and linear term in the fluctuation whereas in the second line we have, instead, the second-order one. The linear terms were written for the sake of completeness but they do not contribute<sup>2</sup>. If we use the expression of  $\psi_0$  we find that the expression of the action simplifies to:

$$S^{(CS)}[\chi, \chi^*] = \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ -\frac{(\mu - \varepsilon + 2D)^2}{2U} + \chi^* \left( \frac{\partial}{\partial \tau} - \nabla^2 + (\mu - \varepsilon + 2D) \right) \chi + \frac{(\mu - \varepsilon + 2D)}{2}(\chi\chi + \chi^*\chi^*) \right\} \quad (2.10)$$

In order to find the excitation spectrum of the system we can now proceed in two ways. We can find it by writing down the equation of motion in the Fourier space and then expressing the angular velocities as a function of the wavenumbers,  $\vec{q}$ . This procedure has the advantage to be more simple and intuitive but at the same time does not offer also an expression of the grand canonical potential density. Instead, we now will calculate the elementary excitations as an intermediate step in the calculation of the grand potential itself. The first step is to expand the fluctuation fields in the Fourier space as:

$$\chi = \sqrt{\frac{1}{V\beta}} \sum_{n, \vec{q}} \chi_{n, \vec{q}} e^{i(\omega_n \tau - \vec{q} \vec{r})} \quad (2.11)$$

where  $\omega_n$  are the Matsubara frequencies:

$$\omega_n = \frac{2\pi n}{\beta} \quad (2.12)$$

Let  $S^{(MF, CS)}$  be the part of the action which is constant in  $\chi$  and  $\chi^*$ . The grand canonical potential for the constant term results:

$$\Omega^{(MF, CS)} = V \frac{(\mu - \varepsilon + 2D)^2}{2U} \quad (2.13)$$

For the quadratic (Gaussian) part instead,  $S^{(G, CS)}$ , we will use the Fourier Transform defined above and the fact that:

$$\int_V d^D \vec{r} \frac{1}{V} e^{i(\vec{q} - \vec{q}') \vec{r}} = \delta_{\vec{q}, \vec{q}'} \quad (2.14)$$

$$\int_0^\beta d\tau \frac{1}{\beta} e^{i(\omega_n - \omega_{n'}) \tau} = \delta_{n, n'} \quad (2.15)$$

where  $\delta_{\vec{q}, \vec{q}'}$  is the Kroenecker delta. We can write  $S^{(G, CS)}$  as:

$$S^{(G, CS)}[\chi, \chi^*] = \frac{1}{2} \sum_{n, \vec{q}} \sum_{n', \vec{q}'} \frac{1}{V\beta} \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ e^{i(\omega_n - \omega_{n'}) \tau + i(\vec{q} - \vec{q}') \vec{r}} \chi_{n', \vec{q}'}^* [i\omega_n + q^2 - (\mu - \varepsilon + 2D) + 2g\psi_0^2] \chi_{n, \vec{q}} + \right. \\ \left. e^{-i(\omega_n - \omega_{n'}) \tau - i(\vec{q} - \vec{q}') \vec{r}} \chi_{-n', -\vec{q}'}^* [-i\omega_n + q^2 - (\mu - \varepsilon + 2D) + 2g\psi_0^2] \chi_{-n, -\vec{q}} + \right. \\ \left. \frac{g}{2} \psi_0^2 (e^{i(\omega_n + \omega_{n'}) \tau + i(\vec{q} + \vec{q}') \vec{r}} \chi_{n, \vec{q}} \chi_{n', \vec{q}'} + e^{-i(\omega_n + \omega_{n'}) \tau - i(\vec{q} + \vec{q}') \vec{r}} \chi_{-n, -\vec{q}} \chi_{-n', -\vec{q}'} + \right. \\ \left. e^{i(\omega_n + \omega_{n'}) \tau + i(\vec{q} + \vec{q}') \vec{r}} \chi_{n, \vec{q}}^* \chi_{n', \vec{q}'}^* + e^{-i(\omega_n + \omega_{n'}) \tau - i(\vec{q} + \vec{q}') \vec{r}} \chi_{-n, -\vec{q}}^* \chi_{-n', -\vec{q}'}^*) \right\} \quad (2.16)$$

<sup>2</sup>The linear terms in the fluctuations cancel out. Instead the linear terms in the derivatives give no contribution to the equation of motion.

Hence using the relations involving the Kroenecker deltas written above we can write the precedent equation in a different (and far more simple) formalism, namely involving a matrix formalism:

$$S^{(G,CS)}[\chi, \chi^*] = \frac{1}{2} \sum_{n, \vec{q}} \begin{bmatrix} \chi_{n, \vec{q}}^* & \chi_{-n, -\vec{q}} \end{bmatrix} M^{(CS)} \begin{bmatrix} \chi_{n, \vec{q}} \\ \chi_{-n, -\vec{q}}^* \end{bmatrix} \quad (2.17)$$

where  $M^{(CS)}$  is the matrix given by:

$$M^{(CS)} = \begin{bmatrix} i\omega_n + q^2 + \mu - \varepsilon + 2D & \mu - \varepsilon + 2D \\ \mu - \varepsilon + 2D & -i\omega_n + q^2 + \mu - \varepsilon + 2D \end{bmatrix} \quad (2.18)$$

The second-order correction contribution to the partition function is given by:

$$Z^{(G,CS)} = \int D[\chi, \chi^*] e^{-S^{(G,CS)}[\chi, \chi^*]} \quad (2.19)$$

and the second-order correction to the grand canonical potential density is given by:

$$\Omega^{(G,CS)} = -\frac{1}{\beta} \ln Z_2^{(CS)} = \frac{1}{2\beta} \sum_{n, \vec{q}} \ln(\det M^{(CS)}) = \frac{1}{2\beta} \sum_{n, \vec{q}} \ln[\omega_n^2 + (E_{\vec{q}}^{(CS)})^2] \quad (2.20)$$

where  $E_{\vec{q}}^{(CS)}$  is given by:

$$E_{\vec{q}}^{(CS)} = \sqrt{q^2[q^2 + 2(\mu - \varepsilon + 2D)]} \quad (2.21)$$

which has the same form as the Bogoliubov spectrum, given by Equation (B.32). Summing now over the Matsubara frequencies:

$$\Omega^{(G,CS)} = \sum_{\vec{q}} \left\{ \frac{E_{\vec{q}}^{(CS)}}{2} + \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}}^{(CS)}}) \right\} \quad (2.22)$$

Putting all parts of the grand canonical potential density together we get:

$$\Omega = \Omega^{(MF,CS)} + \Omega_0^{(G,CS)} + \Omega_T^{(G,CS)} \quad (2.23)$$

where  $\Omega_0^{(G,CS)}$ , the zero-point energy, and  $\Omega_T^{(G,CS)}$ , the thermodynamic fluctuation term, are given by:

$$\Omega_0^{(G,CS)} = \sum_{\vec{q}} \frac{E_{\vec{q}}^{(CS)}}{2} \quad (2.24)$$

$$\Omega_T^{(G,CS)} = \sum_{\vec{q}} \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}}^{(CS)}}). \quad (2.25)$$

Finally for completeness we also write the equation of motion for the fluctuations, using the Euler-Lagrangian Equations:

$$\frac{\partial}{\partial \tau} \chi - \nabla^2 \chi + (\mu - \varepsilon + 2D)(\chi + \chi^*) = 0 \quad (2.26)$$

$$\frac{\partial}{\partial \tau} \chi^* - \nabla^2 \chi^* + (\mu - \varepsilon + 2D)(\chi + \chi^*) = 0 \quad (2.27)$$

## 2.2 Regime near the transition

We now study the system near the transition between the Mott and superfluid phases. We found two effective theories with different order parameters and different couplings, but characterized by the same form of the action. The following calculations are independent of the particular set of couplings and order parameter. Thus, we will use the symbol  $\psi$  to denote our order parameter and letters without a “tilde”



to denote the couplings. We will re-insert the “tilde” only when necessary. As we have in Chapter 1 the system is described by an action of the form<sup>3</sup>:

$$S[\psi, \psi^*] = \beta \mathcal{E}_0 + \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ K_1 \psi^* \frac{\partial}{\partial \tau} \psi + K_2 \left| \frac{\partial}{\partial \tau} \psi \right|^2 + K_3 |\nabla \psi|^2 + c_2 |\psi|^2 + c_4 |\psi|^4 \right\} \quad (2.28)$$

where the constant term  $\mathcal{E}_0$  is the total contribution of all single-site energy terms, i.e. the mean-field contribution for the disordered phase:

$$\mathcal{E}_0 = V \left[ -(\mu - \varepsilon)n + \frac{U}{2}n(n-1) \right] \quad (2.29)$$

as defined in Section 1.3.1. Such a term in fact describes the “Local Limit”, i.e. the “pure” Mott insulating phase, seen in the Chapter 1, where the order parameter  $\psi$  vanishes. The phase transition involves the “switch” in sign of the coefficient of the quadratic term,  $c_2$ . We now expand  $\psi$  as:

$$\psi(\vec{r}, \tau) = \psi_0 + \chi(\vec{r}, \tau) \quad (2.30)$$

where  $\psi_0$  is the mean-field contribution and  $\chi$  is the fluctuation field. As in the previous Section we minimize the mean-field contribution of the action by minimizing the effective potential:

$$V_{eff} = c_2 |\psi_0|^2 + c_4 |\psi_0|^4 \quad (2.31)$$

which gives:

$$|\psi_0| = \begin{cases} 0 & \text{if } c_2 > 0 \\ \sqrt{\frac{-c_2}{2c_4}} & \text{if } c_2 < 0 \end{cases} \quad (2.32)$$

The first case corresponds to the Mott phase, characterized by a mean value of order parameter equal to zero. Note that for the superfluid phase, the mean-field value of the order parameter is non-vanishing and therefore we have a spontaneous symmetry breaking. For both the Mott and superfluid phases we choose the real-valued vacuum, let us call it  $\psi_0$ . We now write the action expanded up to the second order in the fluctuations<sup>4</sup>, maintaining for generality the value of  $\psi_0$  implicit. We obtain:

$$S[\chi, \chi^*] = \beta(\mathcal{E}_0 + Vc_2\psi_0^2 + Vc_4\psi_0^4) + \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ \frac{K_1}{2} \left( \chi^* \frac{\partial}{\partial \tau} \chi - \chi \frac{\partial}{\partial \tau} \chi^* \right) + K_2 \left| \frac{\partial}{\partial \tau} \chi \right|^2 + K_3 |\nabla \chi|^2 + c_2 |\chi|^2 + c_4 \psi_0^2 (\chi \chi + \chi^* \chi^* + 4|\chi|^2) \right\} \quad (2.33)$$

The constant term:

$$S^{(MF)} = \beta \mathcal{E}_0 + V\beta(c_2\psi_0^2 + c_4\psi_0^4) \quad (2.34)$$

gives a contribution to the grand canonical potential density:

$$\Omega^{(MF)} = \mathcal{E}_0 + V(c_2\psi_0^2 + c_4\psi_0^4) \quad (2.35)$$

whereas the second-order correction of the action can be written in a matrix form:

$$S^{(G)}[\chi, \chi^*] = \frac{1}{2} \sum_{n, \vec{q}} \begin{bmatrix} \chi_{n, \vec{q}}^* & \chi_{-n, -\vec{q}} \end{bmatrix} M \begin{bmatrix} \chi_{n, \vec{q}} \\ \chi_{-n, -\vec{q}}^* \end{bmatrix} \quad (2.36)$$

where  $M$  is the matrix given by:

$$M = \begin{bmatrix} K_2 \omega_n^2 + i\omega_n K_1 + K_3 q^2 + c_2 + 4c_4 \psi_0^2 & 2c_4 \psi_0^2 \\ 2c_4 \psi_0^2 & K_2 \omega_n^2 - i\omega_n K_1 + K_3 q^2 + c_2 + 4c_4 \psi_0^2 \end{bmatrix} \quad (2.37)$$

<sup>3</sup>We are working at  $T=0$  and with units  $l = 1$ ,  $J = 1$ ,  $\hbar = 1$ . In these units the total number of sites,  $M$ , is equal to the volume of the system,  $V$

<sup>4</sup>The linear terms in the fluctuations cancel out. The linear terms in the time derivatives do not contribute to the equation of motion

The second order contribution to the grand canonical potential at zero temperature<sup>5</sup> then results:

$$\Omega^{(G)} = \frac{1}{2\beta} \sum_{n, \vec{q}} \ln(\det M) = \frac{1}{2\beta} \sum_{n, \vec{q}} \sum_{j=\pm} \ln[K_2 \omega_n^2 + K_2 (E_{j, \vec{q}}^{(G)})^2] \quad (2.38)$$

where  $E_{\pm, \vec{q}}^{(G)}$  is given by:

$$E_{\pm, \vec{q}}^{(G)} = \frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} + \frac{c_2 + 4c_4 \psi_0^2}{K_2} \right) \pm \sqrt{\frac{K_1^2 K_3}{K_2^2 K_2} q^2 + \frac{K_1^4}{4K_2^4} + \frac{K_1^2 c_2 + 4c_4 \psi_0^2}{K_2} + 4 \frac{c_4^2 \psi_0^4}{K_2^2}} \quad (2.39)$$

Summing over the Matsubara Frequencies:

$$\Omega^{(G)} = \sum_{\vec{q}, j} \left\{ \frac{E_{\vec{q}, j}^{(G)}}{2} \right\} \quad (2.40)$$

Putting all terms of the grand canonical potential density we obtain:

$$\Omega = \Omega^{(MF)} + \Omega^{(G)} \quad (2.41)$$

where  $\Omega^{(G)}$ , the zero-point Gaussian grand canonical potential:

$$\Omega^{(G)} = \sum_{\vec{q}, j} \frac{E_{\vec{q}, j}^{(G)}}{2} \quad (2.42)$$

Finally we give the equations of motion for  $\psi$  and  $\psi^*$ :

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi + K_3 \nabla^2 \chi - K_1 \frac{\partial}{\partial \tau} \chi - c_2 \chi - 2c_4 \psi_0^2 (2\chi + \chi^*) = 0 \quad (2.43)$$

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi^* + K_3 \nabla^2 \chi^* - K_1 \frac{\partial}{\partial \tau} \chi^* - c_2 \chi^* - 2c_4 \psi_0^2 (2\chi^* + \chi) = 0 \quad (2.44)$$

Until now we have left implicit the value of  $\psi_0$ . This means that the results found are fully general and can be used for both the superfluid phase and the Mott phase. In order to find the results for each phase we have to substitute the appropriate values of  $\psi_0$ .

**Superfluid phase** We consider now the superfluid phase, i.e. when  $c_2 < 0$  and  $\psi_0 = \sqrt{\frac{-c_2}{2c_4}}$ . In this case the spectrum becomes:

$$E_{\pm, \vec{q}}^{(G, SF)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)} \pm \sqrt{\frac{K_1^2 K_3}{K_2^2 K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)^2} \quad (2.45)$$

and analogously the equations of motion are:

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi + K_3 \nabla^2 \chi - K_1 \frac{\partial}{\partial \tau} \chi + c_2 (\chi + \chi^*) = 0 \quad (2.46)$$

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi^* + K_3 \nabla^2 \chi^* - K_1 \frac{\partial}{\partial \tau} \chi^* + c_2 (\chi^* + \chi) = 0 \quad (2.47)$$

Finally to find the expression of the grand canonical potential we have to use the above spectrum.

<sup>5</sup>Note that both the effective theories introduced in Section 1.4 are valid at zero temperature

**Mott phase** For the Mott phase, i.e. when  $c_2 > 0$  and  $\psi_0 = 0$ . The excitation spectrum becomes:

$$E_{\pm, \vec{q}}^{(G,M)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)} \pm \frac{|K_1|}{2K_2} \quad (2.48)$$

and the equation of motion are given by:

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi + K_3 \nabla^2 \chi - K_1 \frac{\partial}{\partial \tau} \chi - c_2 \chi = 0 \quad (2.49)$$

$$K_2 \frac{\partial^2}{\partial \tau^2} \chi^* + K_3 \nabla^2 \chi^* - K_1 \frac{\partial}{\partial \tau} \chi^* - c_2 \chi^* = 0 \quad (2.50)$$

It is also interesting to note what happens to the spectrum for  $\vec{q} = \vec{0}$ :

$$E_{\pm, \vec{q}=\vec{0}}^{(G,M)} = \sqrt{\frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2}} \pm \frac{|K_1|}{2K_2} \quad (2.51)$$

therefore we have two gapped modes, whereas in the superfluid phase there is only a gapped mode.

Indeed, as expected from the spontaneous symmetry breaking we have two gapped modes for the disordered phase and one gapless (Goldstone) mode and a gapped (Higgs) mode in the ordered phase[19, 34]. In this case, at multicritical points (the tips of the lobes), where  $K_1 = c_2 = 0$ , we have the softening of the gaps. Again to find the expression of the grand canonical potential density it is sufficient to use the form of the elementary excitation found above.

### 2.2.1 Transition far from the tips of Mott lobes

An interesting approximation can be done when we are studying the regime far from the tips of Mott lobes. In that regions, for small momenta and near the transition line, as we will show in Section 2.4, the second-order time derivative term can be neglected. The action reduces to:

$$S = \beta \mathcal{E}_0 + \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ K_1 \psi^* \frac{\partial}{\partial \tau} \psi + K_3 |\nabla \psi|^2 + c_2 |\psi|^2 + c_4 |\psi|^4 \right\} \quad (2.52)$$

We note that we have a first-order time derivative and a second-order spatial derivative terms as in the Coherent States Approximation studied in Section 2.1. In particular if we follow the same procedure used in previous calculations we find the following expression of the grand canonical potential:

$$\Omega = \Omega^{(MF)} + \Omega^{(G)} \quad (2.53)$$

where the first term is the contribution due to mean field theory, given by Equation (2.35), and the second one is the contribution due to Gaussian fluctuations at zero temperature:

$$\Omega^{(G)} = \sum_{\vec{q}} \frac{E_{\vec{q}}^{(G)}}{2} \quad (2.54)$$

Here as in the Coherent State Approximation we have only one mode which is given by:

$$E_{\vec{q}}^{(G)} = \frac{1}{|K_1|} \sqrt{K_3^2 q^4 + 2K_3 q^2 (c_2 + 4c_4 \psi_0) + c_2^2 + 8c_4 c_2 \psi_0^2 + 12c_4^2 \psi_0^4} \quad (2.55)$$

where  $\psi_0$  as before is the value of the minimum of the order parameter. Therefore for the Mott phase, where  $\psi_0 = 0$  we have:

$$E_{\vec{q}}^{(G,M)} = \frac{\sqrt{K_3}}{|K_1|} q + \frac{c_2}{|K_1|} \quad (2.56)$$

whereas for the superfluid phase where  $\psi_0 = \sqrt{\frac{-c_2}{2c_4}}$  we find a Bogoliubov-like spectrum, given by:

$$E_{\vec{q}}^{(G,SF)} = \sqrt{\frac{K_3}{|K_1|} q^2 \left( \frac{K_3}{|K_1|} q^2 - 2 \frac{c_2}{|K_1|} \right)} \quad (2.57)$$

These expressions for the elementary excitations are similar to what we found for the Coherent State in Section 2.1 and for the non-relativistic gas in Section B.1. In fact we can see that if we make the following identifications:

$$\begin{aligned}\frac{K_3}{|K_1|} &\leftrightarrow \frac{\hbar^2}{2m} \\ \frac{|c_2|}{|K_1|} &\leftrightarrow |\mu|\end{aligned}$$

we find exactly the expression of the spectra for the normal and superfluid phase of an ideal weakly interacting boson gas, respectively (B.31) and (B.32) (which is the Bogoliubov spectrum).

## 2.3 Comparison of the elementary excitation in the superfluid region

As we saw above we have found two different excitation spectra for the superfluid phase: one relative to the Coherent State Approximation and the other relative near the transition. We now shall make a comparison between the two. In the first case we have seen that we arrive to a Bogoliubov-like spectrum, more precisely:

$$E_{\vec{q}}^{(CS)} = \sqrt{q^2(q^2 + 2(\mu - \varepsilon + 2D))} \quad (2.58)$$

which is the typical elementary excitation of a superfluid. The two most important characteristics of this spectrum are the limits to low and high momentum (which in these units correspond to the wavenumber):

$$E_{\vec{q}}^{(CS)} \simeq \sqrt{2(\mu - \varepsilon + 2D)}q \quad \text{if } q^2 \ll \mu - \varepsilon + 2D \quad (2.59)$$

$$E_{\vec{q}}^{(CS)} \simeq q^2 \quad \text{if } q^2 \gg \mu - \varepsilon + 2D \quad (2.60)$$

we see that in the first case we have a linear dependence on  $q$  and we can see that the mode is gapless, i.e. it is vanishing when  $q = 0$ . On the other hand at great momenta the energy is proportional to the squared momenta as in the case of a free particle. This is in accord with the fact that the influence of the interactions at very high energies in a superfluid is negligible. It should however be stressed that for this particular superfluid as we saw in Section 1.2, it is the “effective chemical potential”,  $(\mu - \varepsilon + 2D)$  and not the real chemical potential,  $\mu$  that must be positive. Near the transition line we get a quite different spectrum:

$$E_{\pm, \vec{q}}^{(G, SF)} = \sqrt{\frac{K_3}{K_2}q^2 + \left(\frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2}\right) \pm \sqrt{\frac{K_1^2}{K_2^2} \frac{K_3}{K_2}q^2 + \left(\frac{K_1^2}{2K_2} - \frac{c_2}{K_2}\right)^2}} \quad (2.61)$$

there are two modes and we will now see that at small momenta one is gapped (and hence is called often the Higgs mode) and the other is gapless:

$$E_{+, \vec{q}}^{(G, SF)} = \sqrt{2\left(\frac{1}{2}\frac{K_1^2}{K_2^2} - \frac{c_2}{K_2}\right) + \frac{\frac{K_3}{K_2}\left(\frac{K_1^2}{K_2^2} - \frac{c_2}{K_2}\right)}{2\sqrt{2}\left(\frac{1}{2}\frac{K_1^2}{K_2^2} - \frac{c_2}{K_2}\right)^{3/2}}}q^2 \quad (2.62)$$

$$E_{-, \vec{q}}^{(G, SF)} = \sqrt{\frac{-\frac{1}{2}\frac{K_3}{K_2}\frac{c_2}{K_2}}{\frac{1}{2}\frac{K_1^2}{K_2^2} - \frac{c_2}{K_2}}}q \quad (2.63)$$

we can see from the results above that the second mode, the gapless one, is linear in the momenta exactly like the Bogoliubov-like spectrum found from the Coherent State Approximation. For now, in general, in the regime near the transition we have obtained the form of the Bogliubov spectrum. However, in Section 2.4, we will see that using an approximation valid near the transition line when  $K_1 \neq 0$ , we recover a Bogoliubov-like spectrum from the gapless mode, for small momenta.

## 2.4 Elementary excitation near the phase transition

For  $c_2 \ll \frac{K_1^2}{K_2}$  we obtain for the superfluid phase:

$$E_{\pm, \vec{q}}^{(G, SF)} = \sqrt{\frac{K_3}{K_2}q^2 + \left(\frac{K_1^2}{4K_2^2} - \frac{c_2}{K_2}\right) \pm \frac{|K_1|}{2K_2}} \quad (2.64)$$

whereas for the Mott phase we have:

$$E_{\pm, \vec{q}}^{(G,M)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)} \pm \frac{|K_1|}{2K_2} \quad (2.65)$$

At the phase transition therefore the spectra become equal. The total gap at the transition line is given by:

$$E_{+, \vec{q}}^{(G,M)}(q=0) + E_{-, \vec{q}}^{(G,M)}(q=0) = E_{+}^{(G,SF)}(q=0) + E_{-}^{(G,SF)}(q=0) = 2\sqrt{\frac{K_1^2}{4K_2^2}} = \frac{|K_1|}{K_2} \quad (2.66)$$

and at the tips of the Mott lobes, where  $K_1 = 0$ , we have that the gaps vanish. Another interesting feature occurs when the momenta are small. Let us now consider the gapless spectrum of the superfluid phase:

$$E_{-, \vec{q}}^{(G,SF)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right) - \sqrt{\frac{K_1^2}{K_2^2} \frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)^2}} \quad (2.67)$$

We can, for small momenta use the Taylor expansion:

$$\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 \quad (2.68)$$

valid for  $x \rightarrow 0$ . From this we obtain:

$$E_{-, \vec{q}}^{(G,SF)} = \sqrt{\frac{K_3}{K_2} q^2 - \frac{K_1^2}{2K_2^2} \frac{K_3}{K_2} q^2 + \frac{K_1^4}{K_2^4} \frac{K_3^2}{K_2^2} q^4 - \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} + \frac{K_1^4}{8 \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)^3}} \quad (2.69)$$

which in turn gives:

$$E_{-, \vec{q}}^{(G,SF)} = \sqrt{\frac{\frac{K_3}{K_2} q^2}{2 \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)} \left[ \frac{\frac{K_1^4}{K_2^4} \frac{K_3}{K_2} q^2}{4 \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)^2} - \frac{2c_2}{K_2} \right]} \quad (2.70)$$

This spectrum already seems familiar to the Bogoliubov spectrum: we have in the squared root a quartic term and a quadratic term in the momenta. But interestingly if we use again the approximation  $c_2 \ll \frac{K_1^2}{K_2}$ , valid in the proximity of transition line, we find:

$$E_{-, \vec{q}}^{(G,SF)} = \sqrt{\frac{K_3}{|K_1|} q^2 \left( \frac{K_3}{|K_1|} q^2 - 2 \frac{c_2}{|K_1|} \right)} \quad (2.71)$$

Clearly we get the Bogoliubov spectrum if we do the following identifications:

$$\begin{aligned} \frac{K_3}{|K_1|} &\leftrightarrow \frac{\hbar^2}{2m} \\ \frac{|c_2|}{|K_1|} &\leftrightarrow |\mu| \end{aligned}$$

In fact, we can see it as a low-momenta limit approximation of the general formula, exactly like we show in Appendix B.3 that for low energies we recover exactly the formula of Bogoliubov from the gapless relativistic mode of the weakly interacting bosonic gas in its superfluid phase. Let us now see if the same is true for the Mott phase. Here we do not have a gapless spectrum, but if we consider the mode that has the smaller gap, i.e.:

$$E_{-, \vec{q}}^{(G,M)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right) - \frac{|K_1|}{2K_2}} \quad (2.72)$$

If we perform the same Taylor expansion performed previously in the momenta we find:

$$E_{-, \vec{q}}^{(G,M)} = \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)^{\frac{1}{2}} + \frac{\frac{K_3}{2K_2} q^2}{\left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)^{\frac{1}{2}}} - \frac{|K_1|}{2K_2} \quad (2.73)$$

Now, using the fact that we are near the transition line, as in the superfluid phase, we get:

$$E_{-, \vec{q}}^{(G,M)} = \frac{c_2}{|K_1|} + \frac{K_3}{|K_1|} q^2 \quad (2.74)$$

which has exactly the same form of the spectrum in the case of the normal phase of the weakly interacting gas and we recover the same expression if we perform the substitutions mentioned for the superfluid phase. On the other hand the gap of the gapped mode in the superfluid phase is given by:

$$E_{+, \vec{q}}^{(G,SF)} = \sqrt{2 \left( \frac{K_1^2}{4K_2^2} - \frac{c_2}{K_2} \right)} \quad (2.75)$$

if we compare this gap of the superfluid phase of the relativistic gas, i.e.:

$$E_{+, \vec{q}} = \sqrt{2 \left( \frac{3\mu_r^2}{mc^2} - mc^2 \right)} \quad (2.76)$$

we have to use the same identifications used in Section 1.4. The same is true for the Mott phase. If we use the approximation  $|c_2| \ll K_1^2/K_2$  we obtain:

$$E_{+, q}^{(G,SF)} = \frac{|K_1|}{K_2} - \frac{c_2}{|K_1|} \quad (2.77)$$

if we now use the identifications used in Section 1.4 for the first term and those used in this Section for the second we obtain:

$$\frac{|K_1|}{K_2} - \frac{c_2}{|K_1|} \leftrightarrow \frac{1}{\hbar} (2mc^2 + \mu) \quad (2.78)$$

which is the same result obtained for the non-relativistic limit of the relativistic gapped mode in the superfluid phase apart from a  $\hbar$  factor. The same, again, holds for the Mott phase and the normal phase. We stress that the small momenta approximation works better for sufficiently high values of  $K_1$ , because the approximation of small momenta reads:

$$K_3 q^2 \ll \frac{K_1^2}{K_2}$$

In particular, we cannot neglect the presence of the gapped mode. Note that, in Appendix B.3, the equivalent approximation for the relativistic gas is assume that the kinetic energy is negligible with the respect to the mass. Also, we note that in order to recover the Bogoliubov spectrum for that system we needed to use the assumption  $\mu \ll mc^2$ , which corresponds to, in our case,  $|c_2| \ll K_1^2/K_2$ . When  $K_1 = 0$ , which is true for  $\frac{(\mu-\epsilon)}{U} = \frac{(\mu-\epsilon)^c}{U^c}$ , the spectra assume the form:

$$E_{\pm, \vec{q}}^{(M,G)} = \sqrt{\frac{K_3}{K_2} q^2 + \frac{c_2}{K_2}} \quad (2.79)$$

$$E_{\pm, \vec{q}}^{(SF,G)} = \sqrt{\frac{K_3}{K_2} q^2 - \frac{c_2}{K_2} \mp \frac{c_2}{K_2}} \quad (2.80)$$

We note that for the Mott phase we have that the two excitation modes have exactly the same gap. Note that in this case the action (2.28) has the same form as the Klein-Gordon action [20, 21]: it has both quadratic spatial and temporal derivatives.

## 2.5 Comparison between the two models for the regime near the transition

Until now, all results we have found were model-independent. In fact, as we will see in the next section the results can be extended to a more general class of theory, of which the Bose-Hubbard is a particular case. Nevertheless we have not discuss the compatibility with experimental data, yet. Experimentally, the transitions are performed by varying the shifted chemical potential  $(\mu - \epsilon)$  when we are not at the tips of the Mott lobes. At the tips, which are multicritical points, the density is constant at the transition and we perform it by varying the ratio  $J/U$ . Let us compare the gaps of the spectra predicted by our theories

at critical transitions. In particular we will compare the predictions of our theories with the experimental results for  $n = 1$  at  $D = 2$  in [16] for a bosonic atomic gas trapped in an optical lattice. In that work, they performed the quantum phase transition by varying  $J$ , and therefore we will reintroduce it.  $U$  is fixed at an arbitrary value. The expressions of the gaps is given by:

$$\Delta = \begin{cases} 2 \frac{c_2^{\frac{1}{2}}}{K_2^{\frac{3}{2}}} & \text{if } c_2 > 0 \\ \sqrt{2} \frac{|c_2|^{\frac{1}{2}}}{K_2^{\frac{3}{2}}} & \text{if } c_2 < 0 \end{cases} \quad (2.81)$$

$$\tilde{\Delta} = \begin{cases} 2 \frac{\tilde{c}_2^{\frac{1}{2}}}{\tilde{K}_2^{\frac{3}{2}}} & \text{if } c_2 > 0 \\ \sqrt{2} \frac{|\tilde{c}_2|^{\frac{1}{2}}}{\tilde{K}_2^{\frac{3}{2}}} & \text{if } c_2 < 0 \end{cases} \quad (2.82)$$

where we have indicated with  $\Delta$  and  $\tilde{\Delta}$  the gaps predicted by the two effective theories. Writing explicitly  $J$  in the expressions above we have:

$$\Delta = \begin{cases} 2 \sqrt{\frac{[(\mu-\varepsilon)+U](\mu-\varepsilon)^3[U-(\mu-\varepsilon)]^3}{(\mu-\varepsilon)[U-(\mu-\varepsilon)]\{(\mu-\varepsilon)^3+[U-(\mu-\varepsilon)]^3\}}} \frac{J_c}{J} (1 - \frac{J}{J_c}) & \text{if } \frac{J}{J_c} < 1 \\ \sqrt{2} \sqrt{\frac{[(\mu-\varepsilon)+U](\mu-\varepsilon)^3[U-(\mu-\varepsilon)]^3}{(\mu-\varepsilon)[U-(\mu-\varepsilon)]\{(\mu-\varepsilon)^3+[U-(\mu-\varepsilon)]^3\}}} \frac{J_c}{J} (\frac{J}{J_c} - 1) & \text{if } \frac{J}{J_c} > 1 \end{cases} \quad (2.83)$$

$$\tilde{\Delta} = \begin{cases} 2 \sqrt{2} \sqrt{\frac{[(\mu-\varepsilon)+U]^3}{U^2}} J_c (1 - \frac{J}{J_c}) & \text{if } \frac{J}{J_c} < 1 \\ 2 \sqrt{\frac{[(\mu-\varepsilon)+U]^3}{U^2}} J_c (\frac{J}{J_c} - 1) & \text{if } \frac{J}{J_c} > 1 \end{cases} \quad (2.84)$$

where  $J_c$  is the critical value of  $J$  at which the transition occurs, predicted by both models to be equal to:

$$J_c = \frac{(\mu - \varepsilon)[U - (\mu - \varepsilon)]}{4[U + (\mu - \varepsilon)]} \quad (2.85)$$

where  $U$  is arbitrary and  $(\mu - \varepsilon)$  is the shifted chemical potential of the multicritical point. The value of  $J_c$  in units of  $U$  for our theory is equal to:

$$\frac{J_c}{U} \simeq 0.04 \quad (2.86)$$

Unfortunately, our theories do not predict the exact value for  $J_c/U$ , hence in our comparison we have substituted it with the one predicted by the Monte Carlo Simulations which is equal to [16]:

$$\frac{J_c}{U} \simeq 0.06 \quad (2.87)$$

Once this is done we obtained the results in Figure 2.1. In order to avoid confusion let us, for convention, call “old” the theory obtained in Section 1.4 by a single Hubbard-Stratonovich transformation, whereas “new” the theory obtained with the second. We will follow this convention also in the Chapter 3. In Figure 2.1 we plotted the behavior of the gaps normalized to the quartic coefficient  $U$  and the experimental data. We can see that near the critical point, the two theories are very close to each other and to the experimental data. In the Mott phase, the “new” theory is very close to the experimental results, while the “old” one, instead, fails to reproduce the correct result. Far from the transition in the superfluid phase the behavior of the “new” theory is much closer to the experimental points than the “old” but in this case at a certain point even the “new” theory fails to fit the experimental data (this begins to be more evident after  $J/J_c \simeq 1.5$ ). Anyway, at least near the transition we can conclude that both theory are close to what is found experimentally (after shifting appropriately the value of  $J_c/U$ ) and the better agreement found for the “new” effective theory can be explained by the fact that in this theory the field has the same meaning of the order parameter of the initial theory, whereas the field used for the other theory had no direct physical meaning, as explained in [26].

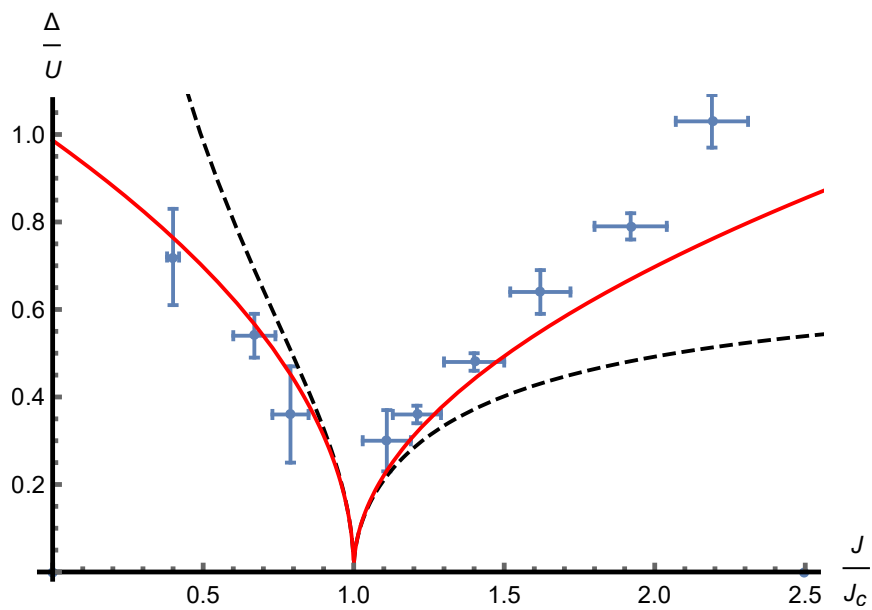


Figure 2.1: In this plot, the blue dots are the experimental points, the black dashed line is the prediction of the “old” theory, while the red one is the prediction of the “new” (see text for more information). In particular we note that very close to the critical point, both theories are in good agreement with the experiment. Once we get away from the critical point the “old” theory quickly fails to reproduce the data. On the other hand, much better agreement is obtained by using the “new” theory, especially for the Mott phase (in fact, sufficiently far from the transition this theory too fails in the superfluid phase).





## Chapter 3

# Effective field theory for superfluid quantum phase transitions

Until now we have worked with the Bose-Hubbard model. However, the results we have found can be easily extended for a D-dimensional system to a more general theory at volume  $V$  equal to:

$$V = L^D \quad (3.1)$$

where  $L$  is the maximal length, and temperature  $T$ , which has a quantum phase transition described by the action:

$$S[\psi, \psi^*] = \beta \mathcal{E}_0 + \int_0^\beta d\tau \int_V d^D \vec{r} \left\{ K_1 \psi^* \frac{\partial}{\partial \tau} \psi + K_2 \left| \frac{\partial}{\partial \tau} \psi \right|^2 + K_3 |\vec{\nabla} \psi|^2 + c_2 |\psi|^2 + c_4 |\psi|^4 \right\} \quad (3.2)$$

where  $\beta$  is given by:

$$\beta = \frac{1}{T} \quad (3.3)$$

$\psi(\vec{r}, \tau)$  is the order parameter,  $\mathcal{E}_0$  is the mean-field value of the energy of the disordered phase. The transition occurs if, by varying the value of a control parameter, let us call it  $\lambda$ , the coefficient of the quadratic term  $c_2$  changes sign. Near the transition we take  $c_2$  to be of the form:

$$c_2 = A(\lambda - \lambda_c) \quad (3.4)$$

where  $\lambda_c$  is the critical value of the parameter and  $A$  is a positive constant. For  $\lambda > \lambda_c$  ( $\lambda < \lambda_c$ ) we are in the disordered (ordered) phase. This action can be considered a generalization of the Ginzburg-Landau energy functional, because it includes both quadratic and linear temporal derivatives in addition to the quadratic spatial derivative already present there. In Appendix E, there is a brief comparison between classical and quantum theories. We assume that  $K_2$ ,  $K_3$  and  $c_4$  are smooth function in  $\lambda$  and that they are always positive, whereas  $K_1$  is also a smooth function and does not change sign during the transition. This allows us to approximate the couplings to their value at the transition. If we write the order parameter as:

$$\psi(\vec{r}, \tau) = \psi_0 + \chi(\vec{r}, \tau) \quad (3.5)$$

where  $\psi_0$  is its mean-field (independent of space and time) value and  $\chi$  is the fluctuation field. If we expand to the second-order in the fluctuations and we follow the same procedure as in Chapter 2 we obtain the following expression for the grand-canonical potential:

$$\Omega = \Omega^{(MF)} + \Omega^{(G)} \quad (3.6)$$

where  $\Omega^{(MF)}$  is the mean-field contribution to the grand canonical potential, given by:

$$\Omega^{(MF)} = \mathcal{E}_0 + V(c_2 |\psi_0|^2 + c_4 |\psi_0|^4) \quad (3.7)$$

whereas  $\Omega^{(G)}$  is the contribution due to the Gaussian fluctuations at zero temperature reads:

$$\Omega^{(G)} = \frac{1}{2} \sum_{\vec{q}} \sum_{j=0,1} E_{j,\vec{q}}^{(G)} \quad (3.8)$$

where  $E_{j,\vec{q}}^{(G)}$  is the oscillation spectrum given by:

$$E_{j,\vec{q}}^{(G)} = \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} + \frac{c_2 + 4c_4|\psi_0|^2}{K_2} \right)} + (-1)^j \sqrt{\frac{K_1^2 K_3}{K_2^2 K_2} q^2 + \frac{K_1^4}{4K_2^4} + \frac{K_1^2 c_2 + 4c_4|\psi_0|^2}{K_2^2} + 4 \frac{c_4^2 |\psi_0|^4}{K_2^2}} \quad (3.9)$$

We assume that  $\psi_0$  is obtained by minimizing  $\Omega^{(MF)}$ , namely:

$$\frac{\partial}{\partial \psi_0} \Omega^{(MF)} = 0 \quad (3.10)$$

The minimum is given by:

$$|\psi_0| = \begin{cases} 0 & \text{if } \lambda \geq \lambda_c \\ \sqrt{\frac{-c_2}{2c_4}} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.11)$$

We note that for  $\lambda < \lambda_c$  the mean-field value of the order parameter is non-zero and therefore we are in the ordered phase. The mean-field contribution to the grand-canonical potential can be written as:

$$\Omega^{(MF)} = \begin{cases} \mathcal{E}_0 & \text{if } \lambda \geq \lambda_c \\ \mathcal{E}_0 - V \frac{c_2^2}{4c_4} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.12)$$

whereas the excitation spectra can be written as:

$$E_{j,\vec{q}}^{(G)} = \begin{cases} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)} + (-1)^j \frac{|K_1|}{2K_2} & \text{if } \lambda \geq \lambda_c \\ \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)} + (-1)^j \sqrt{\frac{K_1^2 K_3}{K_2^2 K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)^2} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.13)$$

as expected by the Goldstone theorem, in the ordered phase we get both a gapless (Goldstone) and gapped (Higgs) mode. Note that similar results can be found for the weakly interacting relativistic gas, as is reported in Appendix B.2, which also has both quadratic and linear terms in the time derivatives. In what follows we are interested in studying the properties of the pressure (i.e. the equation of state), which is simply given by for a homogenous system:

$$P = -\frac{\Omega}{V} = -\frac{1}{V} (\Omega^{(MF)} + \Omega^{(G)}) \quad (3.14)$$

which suggests that we can define also the mean-field contribution to the pressure,  $P^{(MF)}$ , and the contribution due to the fluctuations  $P^{(G)}$ :

$$P^{(MF)} = -\frac{\Omega^{(MF)}}{V} \quad (3.15)$$

$$P^{(G)} = -\frac{\Omega^{(G)}}{V} \quad (3.16)$$

For the mean-field contribution the study of the equation of state is straightforward and independent from dimensionality. The mean-field contribution is given by:

$$P^{(MF)} = \begin{cases} -\frac{\mathcal{E}_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.17)$$

or in terms of  $\lambda$ :

$$P^{(MF)} = \begin{cases} -\frac{\mathcal{E}_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c - \lambda)^2}{4c_4} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.18)$$

this expression is continuous at the transition line. The first derivative with the respect to  $\lambda$  is given by:

$$\frac{\partial}{\partial \lambda} P^{(MF)} = \begin{cases} 0 & \text{if } \lambda \geq \lambda_c \\ A \frac{c_2}{2c_4} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.19)$$

since  $c_2$  vanishes at the transition line the first derivative, like the pressure, is continuous. For the second order derivative we have:

$$\frac{\partial^2}{\partial \lambda^2} P^{(MF)} = \begin{cases} 0 & \text{if } \lambda \geq \lambda_c \\ A^2 \frac{1}{2c_4} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.20)$$

The second derivative, instead, has a jump discontinuity at the transition line: the expression for the ordered phase does not vanish for  $\lambda = \lambda_c$ . Since the second derivative is discontinuous, the transition is of the second-order. This is true for all dimensions. Note that, strictly speaking, to determine the order of the transition we should study  $\Omega$  and its derivatives because  $\Omega$  is an extensive quantity whereas  $P$  is intensive. In the general case, the pressure is equal to:

$$P = -\frac{\partial}{\partial V} \Omega \quad (3.21)$$

Yet, in our case we assume that the system is homogeneous and therefore, the pressure is given by Equation (3.14). Since in our case, the pressure is proportional to the grand canonical potential, they have the same properties. In the following sections we will treat the contribution due to the fluctuations. Finally in Appendix E, we will compare the properties the predictions of classical statistical mechanics for the specific heat and its analogue for our theory, i.e. the second-order derivative of the pressure with the respect to  $\lambda$ .

For the correction to the pressure due to the quantum fluctuations, we will make a continuum approximation and then we will use the dimensional regularization technique to cure the divergences. When, after regularization divergences still remain we will use renormalization. In particular the renormalized parameter that will be used is the coefficient of the quartic interaction,  $c_4$ . The renormalization procedure is described in Appendix D.

### 3.1 Study of the equation of state for $K_1 \neq 0$ and $K_2 \neq 0$

The contribution to the fluctuations to the pressure in the general case is given by:

$$P^{(G)} = \begin{cases} -\frac{1}{V} \sum_{\vec{q}} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)} & \text{if } \lambda \geq \lambda_c \\ -\frac{1}{2V} \sum_{\vec{q}} \sum_{j=0,1} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{2K_2^2} - \frac{c_2}{K_2} \right)} + (-1)^j \sqrt{\frac{K_1^2 K_3}{K_2^2} q^2 + \left( \frac{K_1^2}{4K_2^2} - \frac{c_2}{K_2} \right)^2} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.22)$$

In order to compute the contribution we need to make a continuum approximation which leads to:

$$P^{(G)} = \begin{cases} -\frac{1}{(2\pi)^D} \int d^D \vec{q} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{c_2}{K_2} \right)} & \text{if } \lambda \geq \lambda_c \\ -\frac{1}{2(2\pi)^D} \sum_{j=0,1} \int d^D \vec{q} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} - \frac{c_2}{K_2} \right)} + (-1)^j \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} - \frac{c_2}{K_2} \right)^2} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.23)$$

While the first integral can be analytically computed, the second integral, as it stands is impossible to compute. We need to perform an approximation, namely:

$$|c_2| \ll \frac{K_1^2}{4K_2} \quad (3.24)$$

or in terms of the control parameter:

$$|\lambda - \lambda_c| \ll \frac{K_1^2}{4K_2 A} \quad (3.25)$$

which is satisfied near the transition line, where  $c_2$  vanishes and the other parameters are nonzero. With this approximation, for both phases we have the expression:

$$P^{(G)} = -\frac{1}{(2\pi)^D} \int d^D \vec{q} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{|c_2|}{K_2} \right)} \quad (3.26)$$

We can now work with polar coordinates, obtaining:

$$P^{(G)} = \frac{S_D}{(2\pi)^D} \int_0^\infty dq q^{D-1} \sqrt{\frac{K_3}{K_2} q^2 + \left( \frac{K_1^2}{4K_2^2} + \frac{|c_2|}{K_2} \right)} \quad (3.27)$$

where  $S_D$  is the factor related to the solid angle contribution:

$$S_D = \frac{2\pi^{\frac{D}{2}}}{\Gamma(\frac{D}{2})} \quad (3.28)$$

where  $\Gamma$  is the Gamma Euler function. If we perform the substitution in the integral:

$$\tilde{q} = \frac{q}{q_{ph}} \quad (3.29)$$

where:

$$q_{ph} = \sqrt{\frac{K_1^2}{4K_2K_3} + \frac{|c_2|}{K_3}} \quad (3.30)$$

is a physical scale in the momenta, we obtain:

$$P^{(G)} = -\frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^{D-1} \pi^{\frac{D}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{D}{2})} \int_0^\infty d\tilde{q} \tilde{q}^{D-1} \sqrt{1+\tilde{q}^2} \quad (3.31)$$

We can make, now, a second substitution:

$$Q = \tilde{q}^2 \quad (3.32)$$

obtaining:

$$P^{(G)} = -\frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^D \pi^{\frac{D}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{D}{2}-1} (1+Q)^{\frac{1}{2}} \quad (3.33)$$

Now, we need to use the dimensional regularization technique, in order to regularize the integral. First of all, we introduce shift the dimensionality  $D$  in the following way:

$$D \rightarrow \mathfrak{D} = D - \epsilon \quad (3.34)$$

where  $\epsilon$  is a small, complex parameter. The correction becomes:

$$P^{(G)} = -\frac{q_{ph}^{\mathfrak{D}+1} K_3^{\frac{1}{2}} \kappa^\epsilon}{2^{\mathfrak{D}} \pi^{\frac{\mathfrak{D}}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{\mathfrak{D}}{2})} \int_0^\infty dQ Q^{\frac{\mathfrak{D}}{2}-1} (1+Q)^{\frac{1}{2}} \quad (3.35)$$

where  $\kappa$  is an unspecified scale in the momenta. Now the integral can be computed as:

$$\int dQ Q^{\frac{\mathfrak{D}}{2}-1} (1+Q)^{\frac{1}{2}} = B\left(\frac{\mathfrak{D}}{2}, -\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) = \frac{\Gamma(\frac{\mathfrak{D}}{2})\Gamma(-\frac{\mathfrak{D}}{2} - \frac{1}{2})}{\Gamma(-\frac{1}{2})} \quad (3.36)$$

where  $B(x, y)$  is the analytic continuation of the Beta Euler function. Hence the correction to the pressure is given by:

$$P^{(G)} = \frac{q_{ph}^{\mathfrak{D}+1} K_3^{\frac{1}{2}} \kappa^\epsilon}{2^{\mathfrak{D}+1} \pi^{\frac{\mathfrak{D}}{2} + \frac{1}{2}} K_2^{\frac{1}{2}}} \Gamma\left(-\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) \quad (3.37)$$

where we have used:

$$\Gamma\left(-\frac{1}{2}\right) = -2\sqrt{\pi} \quad (3.38)$$

This result holds for all dimensions. However, for practical applications we are interested in the cases  $D = 1, 2, 3$ . Since the Gamma function has poles for every negative integer, the result is finite only for  $D = 2$ , whereas for odd dimensions we need to treat the divergences.

**2D case** We have for  $D = 2$ :

$$P^{(G)} = \frac{q_{ph}^3 K_3^{\frac{1}{2}}}{6\pi K_2^{\frac{1}{2}}} \quad (3.39)$$

Hence for the 2D system, the total pressure has the form:

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^3 K_3^{\frac{1}{2}}}{6\pi K_2^{\frac{1}{2}}} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} + \frac{q_{ph}^3 K_3^{\frac{1}{2}}}{6\pi K_2^{\frac{1}{2}}} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.40)$$

which can be written as in terms of  $\lambda$ :

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} + \frac{\left[\frac{K_1^2}{4K_2} + A(\lambda - \lambda_c)\right]^{\frac{3}{2}}}{6\pi K_2^{\frac{1}{2}} K_3} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c - \lambda)^2}{4c_4} + \frac{\left[\frac{K_1^2}{4K_2} + A(\lambda_c - \lambda)\right]^{\frac{3}{2}} K_3}{6\pi K_2^{\frac{1}{2}} K_3} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.41)$$

As for the mean-field, we now have a continuous function. The derivative of the correction, however, is given by:

$$\frac{\partial}{\partial \lambda} P^{(G)} = A \frac{\left[\frac{K_1^2}{4K_2} + A|\lambda_c - \lambda|\right]^{\frac{1}{2}}}{4\pi K_2^{\frac{1}{2}} K_3} \text{sign}(\lambda - \lambda_c) \quad (3.42)$$

At  $\lambda = \lambda_c$ , in general we have a jump discontinuity if the derivative of  $c_2$  does not vanish. Hence the inclusion of the fluctuations produce a jump discontinuity in the first derivative. So, in conclusion, the inclusion of fluctuations causes a jump discontinuity in the first derivative of the pressure. Hence, it is similar to a first-order phase transition in the classical phase. Note that in the mean-field the transition was of the second-order.

### 3.1.1 Results for odd dimensions

As anticipated, for odd dimensions we will find the full result only for the ordered phase by a renormalization procedure. We will now only present the main results, the full computation can be found at Appendix D. We need to write we need to expand the Gamma function as:

$$\Gamma\left(-\frac{D+1}{2} + \frac{\epsilon}{2}\right) = \frac{(-1)^{\frac{D+1}{2}}}{\frac{D+1}{2}!} \left[\frac{2}{\epsilon} + \theta\left(\frac{D+1}{2} + 1\right)\right] \quad (3.43)$$

where  $\theta(z) = \Gamma(z)'/\Gamma(z)$  is the Digamma Euler function. In particular, for  $z = 1$  we have:

$$\theta(1) = \frac{1}{2}(\gamma - 1) \quad (3.44)$$

where  $\gamma = 0.577$  is the constant of Euler Mascheroni. The  $\frac{1}{\epsilon}$  divergences lead to a logarithmic correction, as explained in Appendix D. For the 1D system we find:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^2 K_3^{\frac{1}{2}}}{2\pi} \ln \frac{q_{ph}}{q_0} + \frac{q_{ph}^2 K_3^{\frac{1}{2}}}{4\pi} (\gamma - 1) \quad (3.45)$$

Here  $q_0$  is an infrared cut-off, related to the maximal length of the system,  $L$ . The theory has asymptotic freedom for  $D = 1$ . If we write explicitly  $q_{ph}$  the pressure for the ordered phase reads:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{\left(\frac{K_1^2}{4K_2} + A(\lambda_c - \lambda)\right)}{2\pi K_2^{\frac{1}{2}} K_3^{\frac{1}{2}}} \left[ \ln \frac{\left(\frac{K_1^2}{4K_2 K_3} + \frac{A(\lambda_c - \lambda)}{K_3}\right)^{\frac{1}{2}}}{q_0} + \frac{1}{2}(\gamma - 1) \right] \quad (3.46)$$

For 3D system we obtain:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^4 K_3^{\frac{1}{2}}}{16\pi^2 K_2^{\frac{1}{2}}} \left[ \ln \frac{q_0}{q_{ph}} + \frac{3}{4} - \frac{\gamma}{2} \right] \quad (3.47)$$

or in terms of  $\lambda$ :

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{\left( \frac{K_1^2}{4K_2} + A(\lambda_c - \lambda) \right)^2}{16\pi^2 K_2^{\frac{1}{2}} K_3^{\frac{3}{2}}} \left[ \ln \frac{q_0}{\left( \frac{K_1^2}{4K_2 K_3^{\frac{1}{2}}} + \frac{A(\lambda_c - \lambda)}{K_3^{\frac{1}{2}}} \right)^{\frac{1}{2}}} + \frac{3}{4} - \frac{\gamma}{2} \right] \quad (3.48)$$

Here  $q_0$  is, in contrast, a Landau Pole, i.e. a ultraviolet cut-off inversely related to the microscopic length of the system,  $l$ .

### 3.2 Study of the equation of state for $K_1 = 0$ and $K_2 \neq 0$

The calculations for  $K_1 = 0$  are similar to the previous section, hence we will not write all the computations. For  $K_1 = 0$ , the spectrum simplifies to:

$$\frac{1}{2} E_{j,\vec{q}}^{(G)} = \begin{cases} \frac{1}{K_2^{\frac{1}{2}}} \sqrt{K_3 q^2 + |c_2|} & \text{if } \lambda \geq \lambda_c \\ \frac{1}{K_2^{\frac{1}{2}}} \sqrt{K_3 q^2 + |c_2| + (-1)^j |c_2|} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.49)$$

Hence by performing a continuum approximation we obtain the following expression for the correction to pressure:

$$P^{(G)} = \begin{cases} -\frac{1}{K_2^{\frac{1}{2}}} \frac{1}{(2\pi)^D} \int d^D q \sqrt{K_3 q^2 + |c_2|} & \text{if } \lambda \geq \lambda_c \\ -\frac{1}{K_2^{\frac{1}{2}}} \frac{1}{2(2\pi)^D} \sum_{j=0,1} \int d^D q \sqrt{K_3 q^2 + |c_2| + (-1)^j |c_2|} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.50)$$

where we have already performed the sum in the first term. We can neglect the  $j = 1$  mode in the disordered phase because in the dimensional regularization framework, which we use to tame the divergences, the t'Hooft-Veltman conjecture (Equation (D.23)) is valid. Hence, we have:

$$P^{(G)} = \begin{cases} -\frac{1}{K_2^{\frac{1}{2}}} \frac{1}{(2\pi)^D} \int d^D q \sqrt{K_3 q^2 + |c_2|} & \text{if } \lambda \geq \lambda_c \\ -\frac{1}{K_2^{\frac{1}{2}}} \frac{1}{2(2\pi)^D} \int d^D q \sqrt{K_3 q^2 + 2|c_2|} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.51)$$

There is a slight difference in form in the two integrals above. In what follows we will compute the expression of the correction for the disordered phase in dimensional regularization framework. The result for the ordered phase will be obtained by making the appropriate modifications. For the ordered phase we can write the integral in the polar coordinates, obtaining:

$$P^{(G,DO)} = -\frac{1}{K_2^{\frac{1}{2}}} \frac{1}{2^{D-1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dq q^{D-1} \sqrt{K_3 q^2 + |c_2|} \quad (3.52)$$

By making the substitution:

$$Q = \frac{q^2}{q_{ph}^2} \quad (3.53)$$

where  $q_{ph}$  is a physical scale in the momenta and is given by:

$$q_{ph} = \sqrt{\frac{|c_2|}{K_3}} \quad (3.54)$$

we have:

$$P^{(G,DO)} = -\frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^D \pi^{\frac{D}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{D}{2}-1} \sqrt{1+Q} \quad (3.55)$$

which can be written as, by using the shift in dimensionality as in Equation (3.34):

$$P^{(G,DO)} = \frac{q_{ph}^{\mathfrak{D}+1} K_3^{\frac{1}{2}} \kappa^\epsilon}{2^{\mathfrak{D}+1} \pi^{\frac{\mathfrak{D}}{2} + \frac{1}{2}} K_2^{\frac{1}{2}}} \Gamma\left(-\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) \quad (3.56)$$

The expression for the ordered state can be obtained in a similar way:

$$P^{(G,O)} = \frac{q_{ph}^{\mathfrak{D}+1} K_3^{\frac{1}{2}} \kappa^\epsilon}{2^{\frac{\mathfrak{D}}{2} + \frac{3}{2}} \pi^{\frac{\mathfrak{D}}{2} + \frac{1}{2}} K_2^{\frac{1}{2}}} \Gamma\left(-\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) \quad (3.57)$$

Just as the previous Section we see that a finite result will be obtained for the 2D system and a divergent result will be the case for odd dimensions. For  $D = 2$  we have:

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^3 K_3^{\frac{1}{2}}}{3\pi K_2^{\frac{1}{2}}} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} + \frac{q_{ph}^3 K_3^{\frac{1}{2}}}{3\sqrt{2}\pi K_2^{\frac{1}{2}}} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.58)$$

or in terms of  $\lambda$ :

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} + \frac{A^{\frac{3}{2}}(\lambda - \lambda_c)^{\frac{3}{2}}}{3\pi K_2^{\frac{1}{2}} K_3} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c - \lambda)^2}{4c_4} + \frac{A^{\frac{3}{2}}(\lambda_c - \lambda)^{\frac{3}{2}}}{3\sqrt{2}\pi K_2^{\frac{1}{2}} K_3} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.59)$$

With the inclusion of the fluctuations the pressure is still continuous: for both phases we have an additional finite term. For the second derivative, however, we get:

$$\frac{\partial^2}{\partial \lambda^2} P = \begin{cases} -\frac{\mathcal{E}_0}{V} + \frac{A^{\frac{3}{2}}}{4\pi K_2^{\frac{1}{2}} K_3 (\lambda - \lambda_c)^{\frac{1}{2}}} & \text{if } \lambda > \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{A^2}{2c_4} + \frac{A^{\frac{3}{2}}}{4\sqrt{2}\pi K_2^{\frac{1}{2}} K_3 (\lambda_c - \lambda)^{\frac{1}{2}}} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.60)$$

The inclusion of the fluctuations produced a divergent discontinuity for  $\lambda = \lambda_c$ , in contrast to the jump discontinuity of the mean-field. Also, for  $K_1 \neq 0$  and  $K_2 \neq 0$  we found that the first derivative had a jump discontinuity due to the inclusion of the fluctuations. In this case, however, such a discontinuity is not present. It should be noted that this divergent result is similar to what is found for the specific heat in statistical mechanics for  $D = 3$ . Also, like in that case, which is a second-order phase transition, here it is the second derivative of the pressure that is divergent. For more information see Appendix E. For odd dimensions, only the result for the ordered phase will be possible to compute.

### 3.2.1 Results for odd dimensions

For odd dimensions, the results are divergent, since the correction includes a Gamma function with a negative integer as the argument. Hence, we need to use the renormalization technique. It can be shown that following the same procedure as in Appendix D, we obtain for the 1D system:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^2 K_3^{\frac{1}{2}}}{2\pi K_2^{\frac{1}{2}}} \left[ \ln \frac{q}{q_0} + \frac{1}{2}(\gamma - 1) \right] = -\frac{\mathcal{E}_0}{V} + \frac{A(\lambda_c - \lambda)}{2\pi K_2^{\frac{1}{2}} K_3^{\frac{1}{2}}} \left[ \ln \frac{A^{\frac{1}{2}}(\lambda_c - \lambda)^{\frac{1}{2}}}{q_0 K_3^{\frac{1}{2}}} + \frac{1}{2}(\gamma - 1) \right] \quad (3.61)$$

Here  $q_0$  is an infrared cut-off. For the 3D case we have:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^4 K_3^{\frac{1}{2}}}{16\pi^2 K_2^{\frac{1}{2}}} \left[ \ln \frac{q_0}{q_{ph}} + \frac{3}{4} - \frac{\gamma}{2} \right] = -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c - \lambda)^2}{16\pi^2 K_2^{\frac{1}{2}} K_3^{\frac{3}{2}}} \left[ \ln \frac{q_0 K_3^{\frac{1}{2}}}{A^{\frac{1}{2}}(\lambda - \lambda_c)^{\frac{1}{2}}} + \frac{3}{4} - \frac{\gamma}{2} \right] \quad (3.62)$$

now  $q_0$  is an ultraviolet cut-off.



### 3.3 Study of the equation of state for $K_1 \neq 0$ and $K_2 = 0$

If we can neglect the second-derivative term, which is equivalent to assume  $K_2 = 0$ , the spectrum becomes:

$$E_{\vec{q}}^{(G)} = \begin{cases} \frac{1}{|K_1|}(K_3 q^2 + |c_2|) & \text{if } \lambda > \lambda_c \\ \frac{1}{|K_1|} \sqrt{K_3 q^2 (K_3 q^2 + 2|c_2|)} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.63)$$

In this case the correction to grand-canonical potential<sup>1</sup> due to the fluctuations is given by:

$$\Omega^{(G)} = \frac{1}{2} \sum_{\vec{q}} E_{\vec{q}}^{(G)} \quad (3.64)$$

by doing a continuum approximation, the correction to the pressure can be written as:

$$P^{(G)} = - \begin{cases} \frac{1}{|K_1|} \frac{1}{2(2\pi)^D} \int d^D q \{K_3 q^2 + |c_2|\} & \text{if } \lambda > \lambda_c \\ \frac{1}{|K_1|} \frac{1}{2(2\pi)^D} \int d^D q \sqrt{K_3 q^2 (K_3 q^2 + 2|c_2|)} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.65)$$

Note that we can neglect the contribution of the fluctuations in the disordered phases, because in treating the divergences we employ dimensional regularization, where the t'Hooft-Veltman conjecture (Equation (D.23)) is valid. We, therefore, need only to study what happens for the ordered phase. We write the expression in the polar coordinates:

$$P^{(G,O)} = - \frac{1}{2^D \pi^{\frac{D}{2}} |K_1| \Gamma(\frac{D}{2})} \int_0^\infty dq q^{D-1} \sqrt{K_3 q^2 (K_3 q^2 + 2|c_2|)} \quad (3.66)$$

if we perform the substitution:

$$Q = \frac{q^2}{2q_{ph}^2} \quad (3.67)$$

where  $q_{ph}$  is the physical scale in the momentum, which is the same as Equation (3.54), the correction becomes:

$$P^{(G,O)} = - \frac{q_{ph}^{D+2} K_3^{\frac{1}{2}}}{2^{\frac{D}{2}} \pi^{\frac{D}{2}} |K_1| \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{D}{2}-\frac{1}{2}} \sqrt{1+Q} \quad (3.68)$$

which is equal to in the Dimensional regularization framework:

$$P^{(G,O)} = - \frac{q_{ph}^{D+2} K_3^{\frac{1}{2}} \kappa^\epsilon}{2^{\frac{D}{2}+1} \pi^{\frac{D}{2}+\frac{1}{2}} |K_1|} \frac{\Gamma(\frac{D}{2} + \frac{1}{2}) \Gamma(-\frac{D}{2} - 1)}{\Gamma(\frac{D}{2}) \Gamma(-\frac{1}{2})} \quad (3.69)$$

this time we have a finite expression for odd dimensions and divergent for the bidimensional system.

**1D system** In particular for  $D = 1$  we have:

$$P^{(G,O)} = \frac{\sqrt{2} q_{ph}^3 K_3^{\frac{1}{2}}}{3\pi |K_1|} \quad (3.70)$$

therefore the expression of the pressure reads:

$$P = \begin{cases} -\frac{\varepsilon_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\varepsilon_0}{V} + \frac{c_2^2}{4c_4} + \frac{\sqrt{2} q_{ph}^3 K_3^{\frac{1}{2}}}{3\pi |K_1|} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.71)$$

and if we write it in terms of  $\lambda$  we get:

$$P = \begin{cases} -\frac{\varepsilon_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\varepsilon_0}{V} + \frac{A^2 (\lambda_c - \lambda)^2}{4c_4} + \frac{\sqrt{2} A^{\frac{3}{2}} (\lambda_c - \lambda)^{\frac{3}{2}}}{3\pi |K_1| K_3} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.72)$$

<sup>1</sup>For more details see Section 2.2.1 for the case of the Bose-Hubbard.

The second derivative of the pressure is equal to:

$$\frac{\partial^2}{\partial \lambda^2} P = \begin{cases} 0 & \text{if } \lambda \geq \lambda_c \\ \frac{A^2}{2c_4} + \frac{A^{\frac{3}{2}}}{2\sqrt{2}\pi|K_1|K_3A^{\frac{1}{2}}(\lambda_c-\lambda)^{\frac{1}{2}}} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.73)$$

we note that, as we have seen for the 2D system for  $K_1 = 0$ , we have the jump discontinuity for the mean-field and the divergence when fluctuations are included, like second-order phase transitions, but, in this case, there is no correction for the ordered phase. In Appendix E we will compare this result with the analogue of classical physics, the specific heat.

**3D system** For  $D = 3$  instead we have:

$$P^{(G,O)} = -\frac{\sqrt{2}q_{ph}^5 K_3^{\frac{1}{2}}}{15\pi^2|K_1|} \quad (3.74)$$

which, this time, interestingly is a negative correction. Therefore the expression of the pressure reads:

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} - \frac{\sqrt{2}q_{ph}^5 K_3^{\frac{1}{2}}}{15\pi^2|K_1|} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.75)$$

and if we write explicitly its dependence on  $\lambda$  we find:

$$P = \begin{cases} -\frac{\mathcal{E}_0}{V} & \text{if } \lambda \geq \lambda_c \\ -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c-\lambda)^2}{4c_4} - \frac{\sqrt{2}A^{\frac{5}{2}}(\lambda_c-\lambda)^{\frac{5}{2}}}{15\pi^2|K_1|K_3^2} & \text{if } \lambda < \lambda_c \end{cases} \quad (3.76)$$

Since the correction now is proportional to  $(\lambda - \lambda_c)^{\frac{5}{2}}$ , divergences appear only at the third order derivative. However, it is still a second order phase transition because, as in the mean-field, the second order derivative has a jump discontinuity.

### 3.3.1 Results for the 2D system

For  $D = 2$  we have still a divergent result and therefore we need to use renormalization. Following the same procedure as in Appendix D we obtain for the ordered phase:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{q_{ph}^4 K_3^{\frac{1}{2}}}{16\pi|K_1|} \left[ \ln \frac{q_0}{q_{ph}} + \frac{3}{4} - \frac{\gamma}{2} \right] \quad (3.77)$$

by writing explicitly  $q_{ph}$  we find:

$$P^{(G,O)} = -\frac{\mathcal{E}_0}{V} + \frac{A^2(\lambda_c - \lambda)^2}{16\pi|K_1|K_3^{\frac{3}{2}}} \left[ \ln \frac{q_0 K_3^{\frac{1}{2}}}{A^{\frac{1}{2}}(\lambda_c - \lambda)} + \frac{3}{4} - \frac{\gamma}{2} \right] \quad (3.78)$$

where  $q_0$  is an ultraviolet cut-off.

## 3.4 Application: The Bose-Hubbard model - Regime near the transition

Until now the results found in this Chapter were completely general. In fact, the only requirement we made on the parameters were the smoothness at the transition and that the quartic parameter,  $c_2$  had to have the form as in Equation (3.4). This approximation is compatible for what we have found for the Bose-Hubbard model. Indeed it can be shown all parameters are smooth functions at the transition. Here we show that  $c_2$  is of the required form. In fact for the transition with constant density, where we have  $K_1 = 0$  and  $\tilde{K}_1 = 0$  we have that:

$$\lambda = U \quad (3.79)$$

For example, for  $n = 1$  the expression of  $c_2$  and  $\tilde{c}_2$  is given by:

$$c_2 = A(U)(U - U_c) \quad (3.80)$$

$$\tilde{c}_2 = \tilde{A}(U)(U - U_c) \quad (3.81)$$

where:

$$U_c = \frac{(\mu - \varepsilon)[(\mu - \varepsilon) + 2D]}{(\mu - \varepsilon) - 2D} \quad (3.82)$$

$$A(U) = \frac{2D[(\mu - \varepsilon) - 2D]}{(\mu - \varepsilon)[U - (\mu - \varepsilon)]} \quad (3.83)$$

$$\tilde{A}(U) = \frac{(\mu - \varepsilon) - 2D}{(\mu - \varepsilon) + U} \quad (3.84)$$

$A(U)$  and  $\tilde{A}(U)$  are continuous functions in  $U$  and during the transition we can take their value at  $U = U_c$ . For a generic  $n$  the form of the parameters is more complicated. It can be shown, however, that the form of  $c_2$  and, in particular, the critical value  $U_c$  is given by:

$$U_c = 2D[(2n + 1) + \sqrt{(2n + 1)^2 - 1}] \quad (3.85)$$

Also we have that  $A(U)$  and  $\tilde{A}(U)$  are still smooth functions. Note that if we fix  $U$  instead of  $J$ , we have instead that the control parameter is equal to:

$$\lambda = -J \quad (3.86)$$

The same reasoning is valid for transitions with non-constant density, where  $K_1 \neq 0$  and  $\tilde{K}_1 \neq 0$ . In this case we have, for all  $n$ , two possible transitions: we have the transition from the superfluid to the Mott phase in one case by increasing  $(\mu - \varepsilon)$  and in another case by decreasing  $(\mu - \varepsilon)$ . In the first case we have:

$$\lambda = (\mu - \varepsilon) \quad (3.87)$$

$$\lambda_c = (\mu - \varepsilon)_c = \left( \frac{U(2n - 1) - 2D}{2} - 2 \right) + \sqrt{\left( \frac{U(2n - 1) - 2D}{2} - 2 \right)^2 - 2DU - U^2n(n - 1)} \quad (3.88)$$

whereas in the second case we have:

$$\lambda = -(\mu - \varepsilon) \quad (3.89)$$

$$\lambda_c = -(\mu - \varepsilon)_c = - \left( \frac{U(2n - 1) - 2D}{2} - 2 \right) + \sqrt{\left( \frac{U(2n - 1) - 2D}{2} - 2 \right)^2 - 2DU - U^2n(n - 1)} \quad (3.90)$$

We will now show the results obtained for the Bose-Hubbard model for  $n = 1$  with both theories for the cases where we obtained a finite non-logarithmic correction. All results in this Section will be given in units of  $J$ .

### 3.4.1 Regime near the transition in $D=2$ , $K_1 \neq 0$ , $K_2 \neq 0$

The transition occurs by varying the shifted chemical potential  $(\mu - \varepsilon)$ . We have chosen to work at  $U = 25J$ , which is close to the multicritical point. We have chosen such a value, because here  $K_1$  is small and therefore we cannot neglect the quadratic term in the temporal derivatives.

## Results obtained with the “old” theory

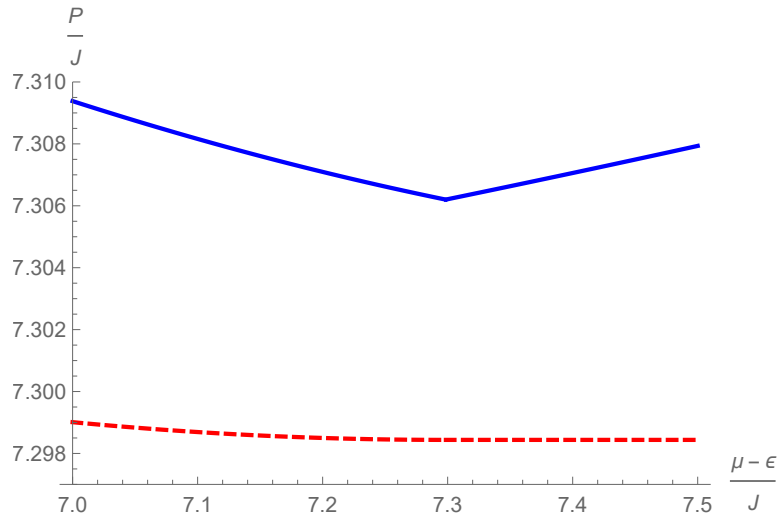


Figure 3.1: Plot of the pressure for  $D = 2$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

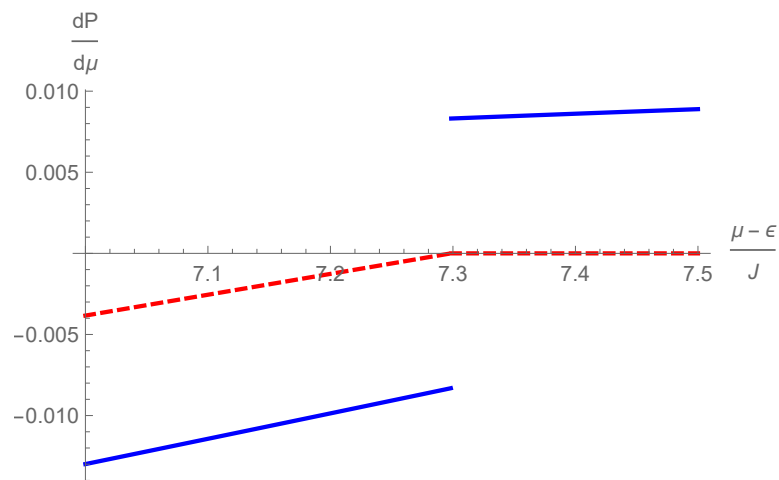


Figure 3.2: Plot of the first derivative of the pressure for  $D = 2$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note the presence of a jump discontinuity in the first derivative due to the fluctuations. Note that the plot is in units of  $J$ .

## Results obtained with the “new” theory

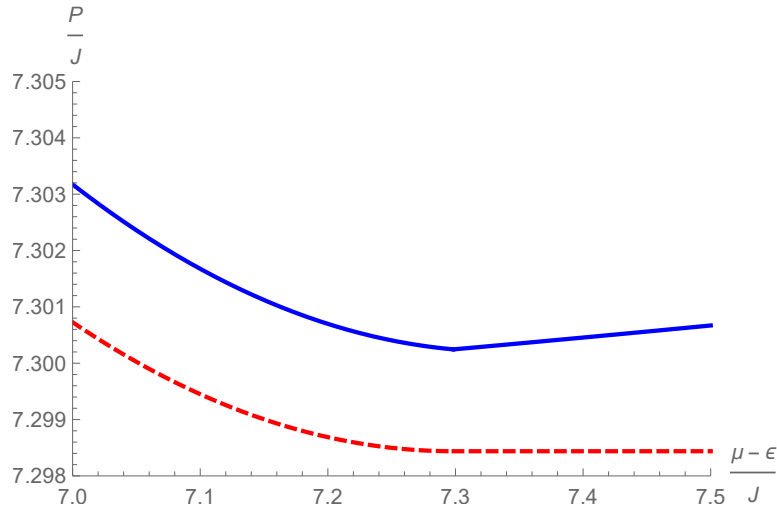


Figure 3.3: Plot of the pressure for  $D = 2$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

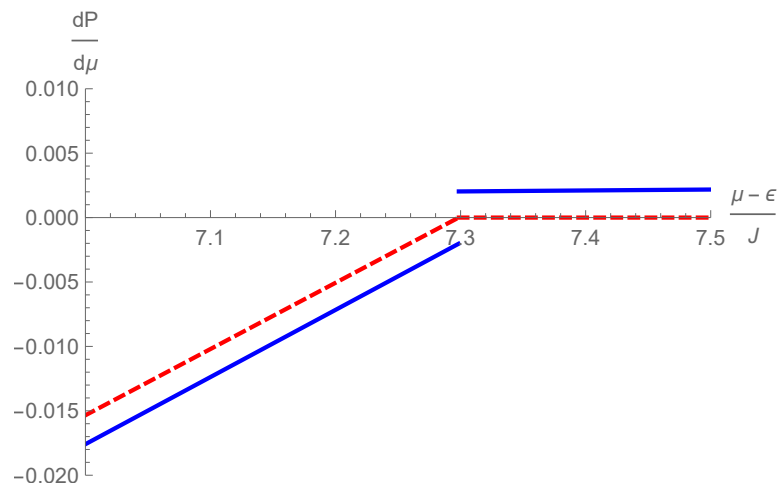


Figure 3.4: Plot of the first derivative of the pressure for  $D = 2$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note the presence of a jump discontinuity in the first derivative due to the fluctuations. Note that the plot is in units of  $J$ .

**Comment** Figures 3.1 and 3.3 are the predictions of, respectively, the “old” and the “new” theories for the pressure at varying values of the shifted chemical potential around the transition point, at  $U = 25J$  (which is near the multicritical point). We can see that the two theories are in agreement to the second significant digit. Also, we notice that the contribution of the fluctuations is more evident for the “old” theory. As we can see in Figures 3.2 and 3.4, the first derivative acquires a jump discontinuity for both models. It should be noted that the inclusion of the fluctuations produces a more evident effect on the results given by the “old” theory.

### 3.4.2 Regime near the transition in $D=2$ , $K_1 = 0$ , $K_2 \neq 0$

We will now show the results obtained for the transition at the multicritical point (the tip of the Mott lobe), which occurs by varying the coupling  $U$ . The shifted chemical potential is fixed at  $(\mu - \varepsilon)_c \simeq 9.35J$ . As seen in Section 1.3, the density for these transitions remains constant.

## Results obtained with the “old” theory

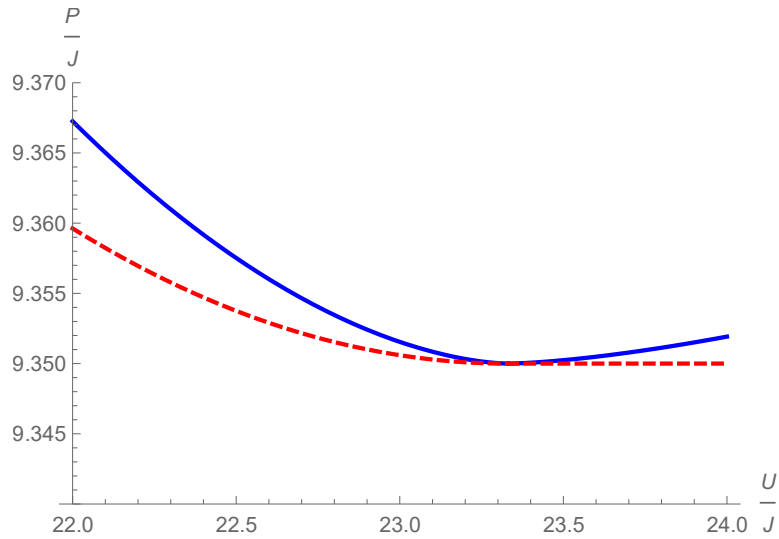


Figure 3.5: Plot of the pressure for  $D = 2$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the coupling of the quartic interaction,  $U$ . Note that the plot is in units of  $J$ .

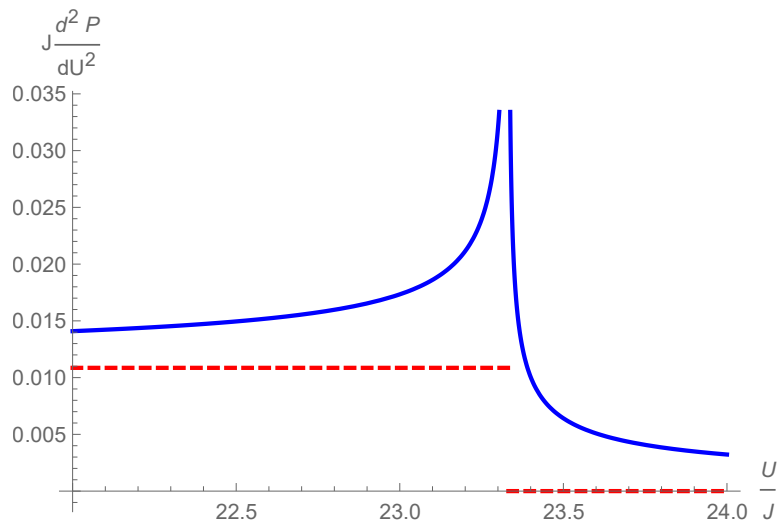


Figure 3.6: Plot of the second derivative of the pressure for  $D = 2$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the coupling of the quartic interaction,  $U$ . Note that the inclusion of the fluctuations led to a divergence at the transition. Note that the plot is in units of  $J$ .

## Results obtained with the “new” theory

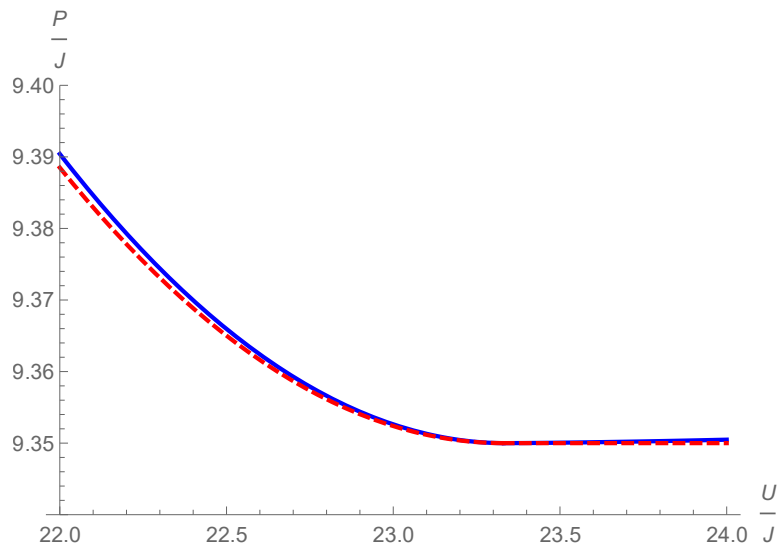


Figure 3.7: Plot of the pressure for  $D = 2$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the coupling of the quartic interaction,  $U$ . Note that the plot is in units of  $J$ .

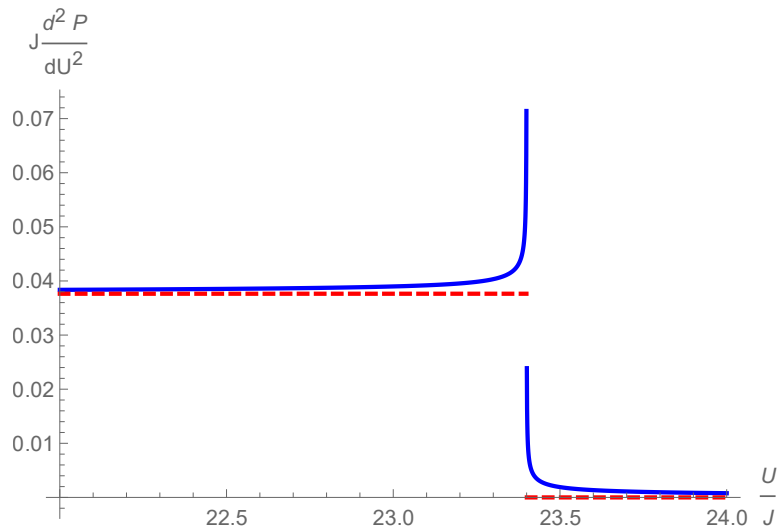


Figure 3.8: Plot of the second derivative of the pressure for  $D = 2$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the coupling of the quartic interaction,  $U$ . Note that the inclusion of the fluctuations led to a divergence at the transition. Note that the plot is in units of  $J$ .

**Comment** As we have seen before, the value of the pressure predicted by the models is similar (see Figures 3.5 and 3.7, respectively for the “old” and “new” theories): their value differ only at the second significant digit. Note that, although there is more difference between the predictions, the plot of the second derivative shows a divergence in both cases. Anyway, from what we have seen in Section 2.5, we expect better results from the “new” theory, especially for the Mott phase. As in the previous case, the effect of the fluctuations is more evident in the predictions of the “old” and this might be a suggestion, together with the comparison with experimental data in Section 2.5, that even near the critical point the theory is less reliable. On the other hand, while the difference in the behavior of the pressure is evident (especially when the derivatives are taken into account) we emphasize again that the numerical values are, however, very similar.

### 3.4.3 Regime near the transition in $D=1$ , $K_1 \neq 0$ , $K_2 = 0$

Sufficiently far from the multicritical point, where the approximation:

$$K_3 q^2 \ll \frac{K_1^2}{4K_2} \quad (3.91)$$

we can neglect the quadratic term in the temporal derivatives. We have chosen the transition at  $U = 50J$ .

#### Results obtained with the “old” theory

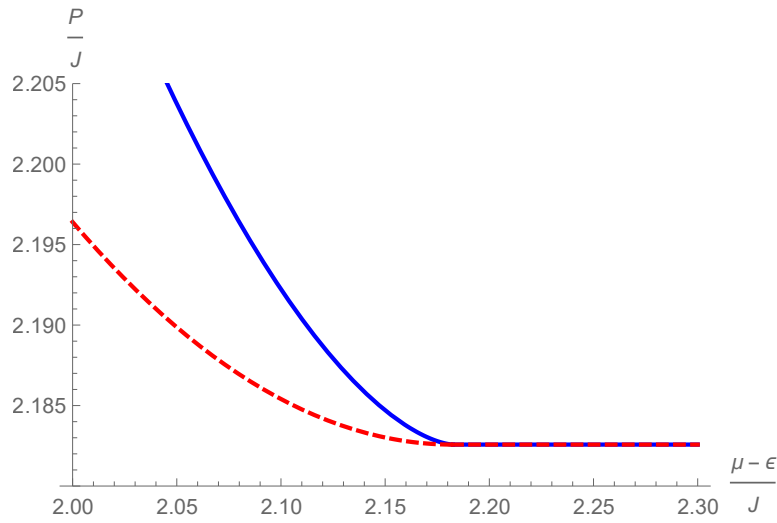


Figure 3.9: Plot of the pressure for  $D = 1$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

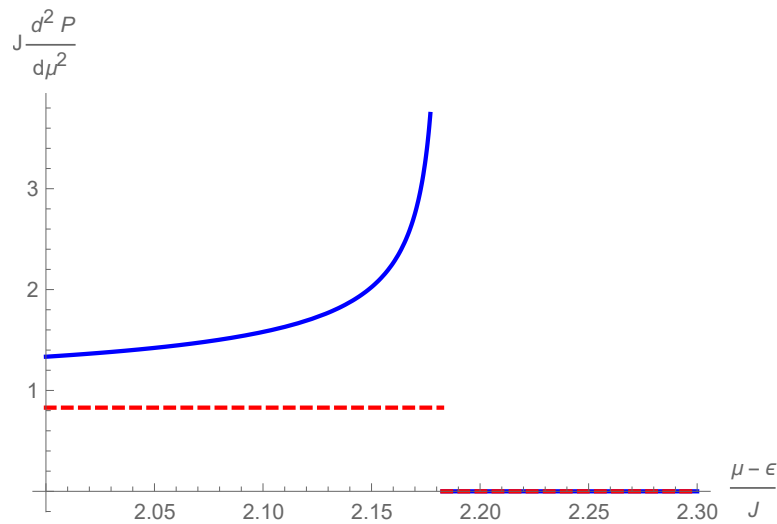


Figure 3.10: Plot of the second derivative of the pressure for  $D = 1$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . The inclusion of the fluctuations led to the appearance of a divergence. Note that the plot is in units of  $J$ .



## Results obtained with the “new” theory

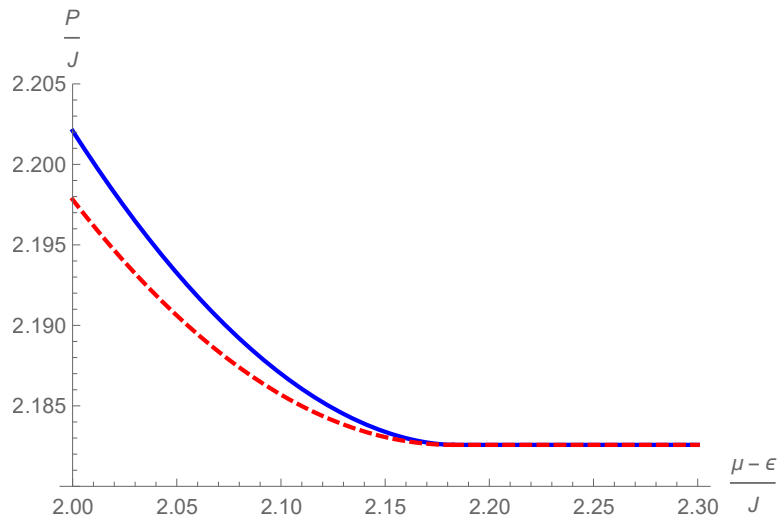


Figure 3.11: Plot of the pressure for  $D = 1$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

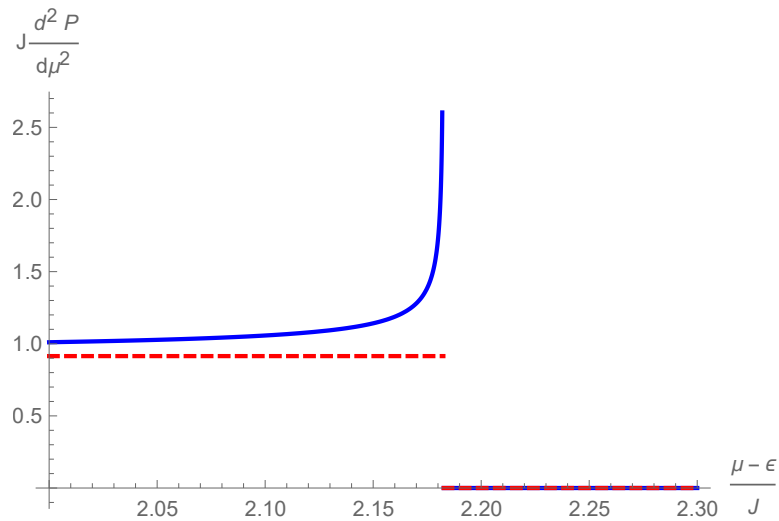


Figure 3.12: Plot of the second derivative of the pressure for  $D = 1$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . The inclusion of the fluctuations led to the appearance of a divergence. Note that the plot is in units of  $J$ .

**Comment** We note again the substantial agreement in the numerical values predicted for the pressure in the two cases and the fact that for the “old” theory the fluctuations appear to be more relevant. Notice, however, that the mean-field result is very similar for both theories in contrast to the somewhat greater difference seen for  $D = 2$  near the tip of the lobes.

### 3.4.4 Regime near the transition in $D=3$ , $K_1 \neq 0$ , $K_2 = 0$

As for  $D = 1$  we fixed  $U = 50J$ .

## Results obtained with the “old” theory

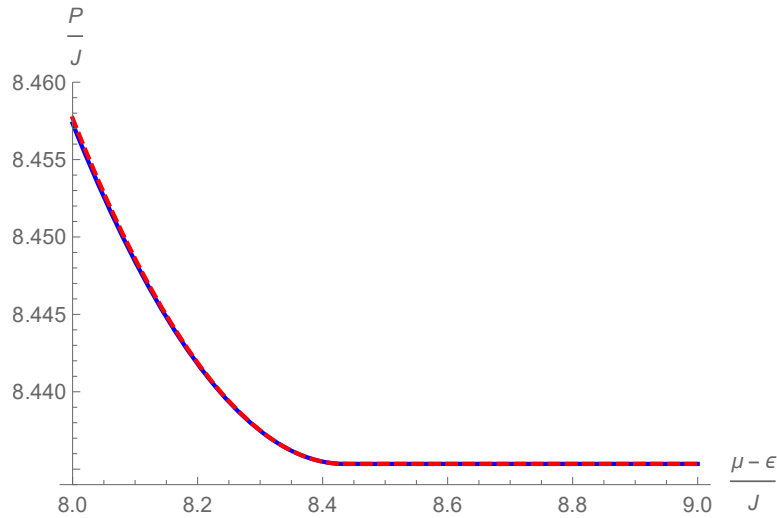


Figure 3.13: Plot of the pressure for  $D = 3$ , obtained by using the “old” theory. The orange line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

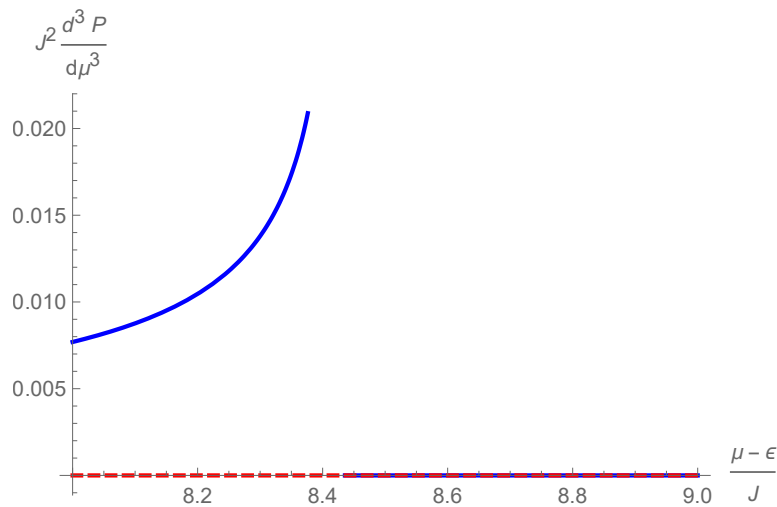


Figure 3.14: Plot of the third derivative of the pressure for  $D = 3$ , obtained by using the “old” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . The inclusion of the fluctuations led to the appearance of a divergence. Note that the plot is in units of  $J$ .

## Results obtained with the “new” theory

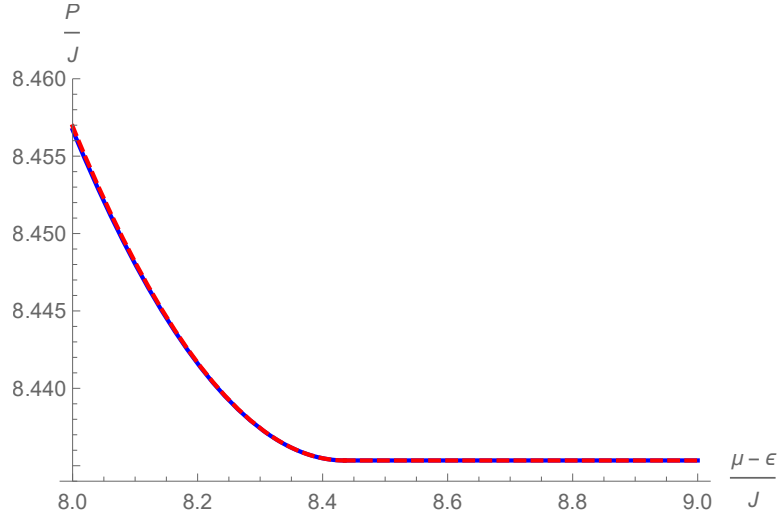


Figure 3.15: Plot of the pressure for  $D = 3$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . Note that the plot is in units of  $J$ .

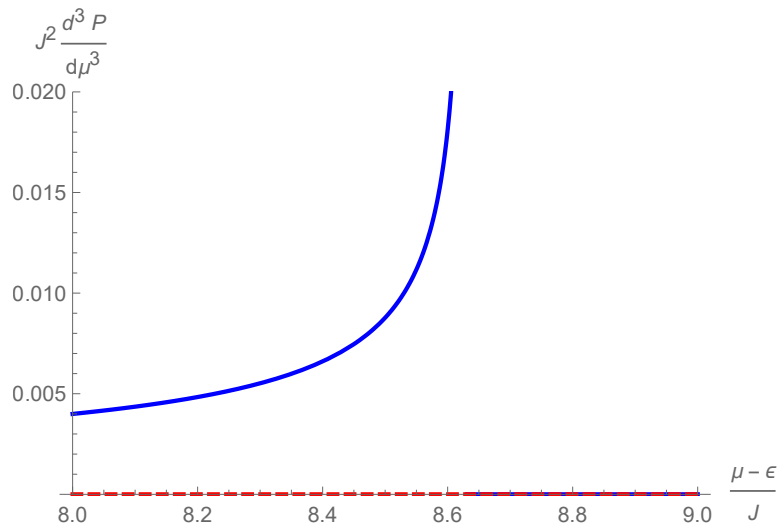


Figure 3.16: Plot of the third derivative of the pressure for  $D = 3$ , obtained by using the “new” theory. The red dashed line refers to the mean-field result, whereas the blue line refers to the result obtained including the fluctuations. On the x-axis we have the shifted chemical potential,  $\mu - \varepsilon$ . The inclusion of the fluctuations led to the appearance of a divergence. Note that the plot is in units of  $J$ .

**Comment** Analogously as for the  $D = 1$  case, the results between the two model are very similar for the mean-field. We notice that this is even true when the fluctuations are considered: in both cases their influence does not vary substantially the behavior of the pressure, which might suggest that for this dimensionality the mean-field is a good approximation. Also, as expected, the divergent appears only at the third derivative.

### 3.5 Application: The Bose-Hubbard model - Fully superfluid regime

Using a similar procedure we can also find the form of the equation of state in the fully superfluid region of the phase space, using the Coherent State Approximation. We found that the gas behaves like a weakly interacting non-relativistic gas in the superfluid phase, assuming that we can make the following substitution:

$$\mu \Rightarrow \mu - \varepsilon + 2D$$

and in fact we obtained a Bogoliubov-like spectrum:

$$E_{\vec{q}}^{(CS)} = \sqrt{q^2(q^2 + 2(\mu - \varepsilon + 2D))} \quad (3.92)$$

We also saw in Section 2.1 that in this regime the correction to the grand canonical potential density due to Gaussian quantum fluctuation is given by:

$$\frac{\Omega_0^{(G,CS)}}{V} = \frac{1}{V} \sum_{\vec{q}} \frac{E_{\vec{q}}}{2} = \int \frac{d^D q}{2(2\pi)^D} E_{\vec{q}}^{(CS)} \quad (3.93)$$

where in the last passage we performed a continuum approximation. If we use the explicit form of the spectrum we obtain:

$$\frac{\Omega_0^{(G,CS)}}{V} = \int \frac{d^D q}{2(2\pi)^D} \sqrt{q^2(q^2 + 2(\mu - \varepsilon + 2D))} = \frac{2\pi^{\frac{D}{2}}}{\Gamma(\frac{D}{2})} \int_0^\infty \frac{dq}{2(2\pi)^D} q^D \sqrt{q^2 + 2(\mu - \varepsilon + 2D)} \quad (3.94)$$

If we now define a new variable of integration, namely:

$$\tilde{q} = \sqrt{\frac{1}{\mu - \varepsilon + 2D}} q \quad (3.95)$$

we have:

$$\frac{\Omega_0^{(G,CS)}}{V} = \frac{2[2(\mu - \varepsilon + 2D)]^{\frac{D}{2}+1}}{2(4\pi)^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dk k^D (1 + k^2)^{\frac{1}{2}} \quad (3.96)$$

using another substitution, namely:

$$Q = k^2 \quad (3.97)$$

and we obtain:

$$\frac{\Omega_0^{(G,CS)}}{V} = \frac{2[2(\mu - \varepsilon + 2D)]^{\frac{D}{2}+1}}{4(4\pi)^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{D-1}{2}} (1 + Q)^{\frac{1}{2}} \quad (3.98)$$

which in turn leads to the following expression for the correction to the pressure due to quantum fluctuations in the dimensional regularization framework<sup>2</sup>:

$$P_0^{(G,CS)} = -\frac{2[2(\mu - \varepsilon + 2\mathfrak{D})\kappa^\varepsilon]^{\frac{\mathfrak{D}}{2}+1}}{4(4\pi)^{\frac{\mathfrak{D}}{2}} \Gamma(\frac{\mathfrak{D}}{2})} \beta \left( \frac{\mathfrak{D} + 1}{2}, -\frac{\mathfrak{D}}{2} - 1 \right) = -\frac{2[2(\mu - \varepsilon + 2\mathfrak{D})\kappa^\varepsilon]^{\frac{\mathfrak{D}}{2}+1}}{4(4\pi)^{\frac{\mathfrak{D}}{2}}} \frac{\Gamma(\frac{\mathfrak{D}+1}{2})\Gamma(-\frac{\mathfrak{D}}{2} - 1)}{\Gamma(\frac{\mathfrak{D}}{2})\Gamma(-\frac{1}{2})} \quad (3.99)$$

For the cases  $D = 1$  and  $D = 3$  the result is now finite. Unfortunately for  $D = 2$  we have a divergence since the Euler Gamma function diverges for negative integers.

**D=1** For  $D = 1$ , there are no divergences, so we can write directly:

$$P_0^{(G,CS)} = -\frac{2[2(\mu - \varepsilon + 2)]^{\frac{3}{2}}}{4\sqrt{4\pi}} \frac{\Gamma(-\frac{3}{2})}{\Gamma(-\frac{1}{2})\Gamma(\frac{1}{2})} \quad (3.100)$$

which leads to the following result for the total pressure:

$$P^{(CS)} = \frac{(\mu - \varepsilon + 2)^2}{2U} + \frac{[2(\mu - \varepsilon + 2)]^{\frac{3}{2}}}{6\pi} - \sum_{\vec{q}} \frac{1}{V\beta} \ln(1 - e^{-\beta E_{\vec{q}}^{(CS)}}) \quad (3.101)$$

**D=3** For  $D = 3$  we obtain a finite result with an analogous procedure:

$$P_0^{(G,CS)} = -\frac{[2(\mu - \varepsilon + 6)]^{\frac{5}{2}}}{30\pi^2} \quad (3.102)$$

note that this time we have a negative correction. The total pressure is given by:

$$P^{(CS)} = \frac{(\mu - \varepsilon + 6)^2}{2U} - \frac{[2(\mu - \varepsilon + 6)]^{\frac{5}{2}}}{30\pi^2} - \sum_{\vec{q}} \frac{1}{V\beta} \ln(1 - e^{-\beta E_{\vec{q}}^{(CS)}}) \quad (3.103)$$

---

<sup>2</sup>See Appendix D for more details.

**D=2** As we noted, there is a divergence because the Gamma function diverges for negative integers. By choosing  $U$  as the renormalized coupling and by using the same reasoning as in Appendix D, the divergence can be substituted by a logarithmic correction. For the total pressure we get:

$$P^{(CS)} = \frac{[\mu - \epsilon + 4]^2}{8\pi} \left[ \ln \left( \frac{q_0}{\sqrt{\mu - \epsilon + 4}} \right) + \frac{3}{4} - \frac{\gamma}{2} \right] - \sum_{\bar{q}} \frac{1}{V\beta} \ln(1 - e^{-\beta E_q^{(CS)}}) \quad (3.104)$$

where  $q_0$  is an ultraviolet cut-off.

Notice that these results are very similar to what was found in [27] for the non-relativistic weakly interacting gas in the superfluid phase.

# Conclusions

In this work we have studied the Bose-Hubbard model in the fully superfluid regime and in the regime near the Mott-superfluid transition. For both cases, we derived effective actions from which we computed, by expanding up to the Gaussian order in quantum fluctuations of the order parameter, the elementary excitations and the equation of state.

For the former regime, by using a basis of coherent states, we obtained a Bogoliubov-like spectrum which is characteristic of the non-relativistic superfluid weakly interacting gas. Also, with the aid of dimensional regularization technique we were able to find the equation of state both in the mean-field and with the inclusion of quantum fluctuations. Our results for this fully-superfluid regime are strikingly similar to what was found in [27] for the weakly non-relativistic gas.

In order to study the system near the transition line we started from treating the nearest-neighbor sites hopping as a perturbation above the the Mott configuration, the situation where that interaction is absent. By making a strong coupling random phase approximation (RPA), as in [26], we extracted two different effective theories characterized by the same form of the action. Also in this case, we computed the elementary excitations for both theories. We found that the predicted excitation gaps were in good agreement for both theory near the transition line, but one of them provided a better agreement far from the transition, especially in the Mott phase.

We noted that, however, our analytical results could be extended to a generic quantum phase transition and we computed the equation of state for a generic system. This effective action can be considered as a generalization of the familiar Ginzburg-Landau energy functional by the presence of linear and quadratic temporal derivatives. We have seen that the inclusion of the Gaussian quantum fluctuations modifies the form of both the pressure and its derivatives with the respect to the control parameter. In particular, for  $D = 2$  when both terms in temporal derivatives are present we obtained a change in the order of the quantum phase transition: while the mean-field predicts in all cases a second-order phase transition, with the inclusion of the fluctuations a first-order phase transition is predicted. When the linear temporal derivative is absent, for the same dimensionality we obtain a divergence in the second order derivative of the pressure with the respect to the control parameter, which is the analogous to what is found for the specific heat in the classical Ginzburg-Landau theory for the 3D case. A similar result is found, for the ordered phase only for  $D = 1$ , when the quadratic temporal derivative is absent.

When the divergences remained also after regularization, a renormalization procedure was employed. In this case, however, we were able to find the complete result for the pressure only in the ordered phase. Either when both the quadratic and the linear temporal derivatives are present or when the linear one is absent, we found that for  $D = 1$  the theory predicts asymptotic freedom with an infrared cut-off and that, instead, for  $D = 3$  a Landau Pole is predicted. Renormalization has also been used when the quadratic temporal derivative is absent for  $D = 2$ , where our theory predicts a Landau Pole.



# Appendices





# Appendix A

## Spontaneous symmetry breaking

In Condensed Matter physics phase transitions are modeled as a spontaneous symmetry breaking mechanism of a certain system. In fact, this mechanism can be used for classical phase transitions also in Landau theories [32, 33]. There, near the phase transition it is possible to write a thermodynamic potential, let us call it  $\mathcal{F}$ , as an expansion of the order parameter. As a simple example we can consider this function where the expansion is truncated at the fourth order and where the order parameter, be it  $\Phi$ , is space and time independent and complex:

$$\mathcal{F} = a_0 + a_2|\Phi|^2 + a_4|\Phi|^4 \quad (\text{A.1})$$

where we assume  $a_4 > 0$ . The coefficients of the expansion generally depend on the thermodynamical quantities of the system, like the temperature or the chemical potential. To find the value of the order parameter we need to minimize the potential. We find:

$$|\Phi| = \begin{cases} 0 & \text{if } a_2 > 0 \\ \sqrt{\frac{-a_2}{2a_4}} & \text{if } a_2 < 0 \end{cases} \quad (\text{A.2})$$

Therefore we see that the shift in sign of the coefficient of the quadratic term corresponds to a phase transition. Here, while the free energy is invariant under a phase redefinition of  $\Phi$ , the minimum is not when  $a_2 < 0$ , where the value of the order parameter is nonzero. When the minima are not invariant under the same symmetry of the action, we have a spontaneous symmetry breaking.

As another example of spontaneous symmetry breaking, let us consider a generic D-dimensional space-time and let us work in the Euclidean space formalism. Let  $\phi(\vec{r}, \tau)$  be a real scalar field. Suppose that the Lagrangian can be written as a sum of a kinetic term and a potential term:

$$\mathcal{L} = \partial_\mu\phi\partial_\mu\phi + V(\phi) \quad (\text{A.3})$$

where  $V(\phi)$  is:

$$V(\phi) = m^2\phi^2 + \frac{g}{4}\phi^4 \quad (\text{A.4})$$

where  $g$  is taken as a positive coupling and  $m^2$  can be either positive or negative. The minima of the potential represent the ground state of the system. If  $m^2 > 0$  there is only a minimum, namely:

$$\phi_0 = 0 \quad (\text{A.5})$$

In this case both the Lagrangian and the ground state are symmetric under a  $Z_2$  transformation:

$$\phi \rightarrow \phi' = -\phi \quad (\text{A.6})$$

If  $m^2 < 0$  the situation changes. The potential this time has two minima, namely:

$$\phi_{0,\pm} = \pm\sqrt{\frac{-m^2}{g}} \quad (\text{A.7})$$

and now while the Lagrangian is still invariant under a  $Z_2$  theory, the ground state is not. We have a spontaneous symmetry breaking of a theory. The choice of a particular minimum breaks the symmetry in

the states space. For example let us choose the positive minimum  $\phi_{0,+}$ . Let us now call  $\eta(\vec{r}, \tau)$  the fluctuations around the minimum:

$$\phi = \phi_{0,+} + \eta \quad (\text{A.8})$$

Expanding now the Lagrangian in the fluctuations we obtain:

$$\mathcal{L} = \frac{\phi_{0,+}^4}{\lambda} + \partial_\mu \phi \partial_\mu \phi + 2 \frac{\phi_{0,+}^2}{g} \eta^2 + g \phi_{0,+} \eta^3 + \frac{1}{4} \eta^4 \quad (\text{A.9})$$

Note that while the Lagrangian in the case of the total field respects the  $Z_2$  symmetry, this is not true for the fluctuations. This leads to the appearance of a cubic interaction otherwise forbidden.

Another interesting Lagrangian is the one of a complex scalar field invariant under a  $U(1)$  symmetry. Let  $\psi(\vec{r}, \tau)$  be the field. Suppose that the Lagrangian can be written as:

$$\mathcal{L} = \partial_\mu \psi^* \partial_\mu \psi + \mathcal{V}(\psi, \psi^*) \quad (\text{A.10})$$

where the potential  $\mathcal{V}(\psi, \psi^*)$  is given by:

$$\mathcal{V}(\psi, \psi^*) = m^2 |\psi|^2 + \frac{\lambda}{2} |\psi|^4 \quad (\text{A.11})$$

with  $\lambda > 0$ . Again for  $m^2 > 0$  the minimum of the potential is  $\psi_0 = 0$  and both the minimum and the Lagrangian are invariant under the  $U(1)$  transformation, defined as follows:

$$\psi \rightarrow \psi' = e^{i\nu} \psi \quad (\text{A.12})$$

where  $\nu$  is an arbitrary phase. The same is not true for  $m^2 < 0$ , where the potential has a circle of minima of radius  $|\psi_0|$  given by:

$$|\psi_0| = \sqrt{\frac{-m^2}{\lambda}} \quad (\text{A.13})$$

if we choose a particular vacuum state, let it be the real and positive one, we break the  $U(1)$  symmetry of the Lagrangian. Let us now define the fluctuations around the minimum as follows:

$$\psi = (\psi_0 + \rho) e^{i\theta} \quad (\text{A.14})$$

In particular  $\rho(\vec{r}, \tau)$  is the amplitude fluctuation field and  $\theta(\vec{r}, \tau)$  is the phase fluctuation field. If we expand the Lagrangian in the fluctuations we obtain:

$$\mathcal{L} = \frac{\phi_{0,+}^4}{\lambda} + \partial_\mu \rho \partial_\mu \rho + (\psi_0 + \rho^2)^2 \partial_\mu \theta \partial_\mu \theta - 4 \frac{\psi_0^2}{\lambda} \rho^2 + 2\lambda \psi_0 \rho^2 + \frac{\lambda}{2} \rho^4 \quad (\text{A.15})$$

again we note the presence of the constant term and the cubic interaction. Note also that we have a massive field, the amplitude fluctuations, and a massless field, the phase fluctuations. The first is called the ‘‘Higgs’’ field and the second one the ‘‘Goldstone’’ field [19].

## Appendix B

# The weakly interacting gas: phase transition

### B.1 The non-relativistic case

The shifted Hamiltonian of a weakly interacting bosonic gas of volume  $V$  is given by:

$$\hat{H} = \int_V d^D \vec{r} \hat{\psi}^\dagger \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \quad (\text{B.1})$$

where  $\hat{\psi}(\vec{r}, t)$  is the bosonic matter field,  $m$  is the mass of the particles of the gas and  $\mu$  is the chemical potential. We assumed also that the gas is sufficiently dilute in order to approximate the interaction potential, let call it  $V(\vec{r}, \vec{r}')$ , to a contact interaction, i.e.:

$$V(\vec{r}, \vec{r}') = g \delta(\vec{r} - \vec{r}') \quad (\text{B.2})$$

where  $g$ , the coupling constant, is given by:

$$g = \frac{4\pi \hbar^2 a_s}{m} \quad (\text{B.3})$$

where  $a_s$  is the scattering length of the interaction. In order to study the thermodynamical and dynamical properties of the gas, we have to write the action of the system, substituting the quantum fields with the classical used in the Path-Integral formulation. In particular in the real space the action is given by:

$$S_R = \int dt \int_V d^D \vec{r} \left\{ \psi^* \left( i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 + \mu \right) \psi - \frac{g}{2} |\psi|^4 \right\} \quad (\text{B.4})$$

where the superscript ‘‘R’’ stands for ‘‘real’’ time. In order to study the partition function, however, we need to perform a Wick rotation, i.e. we need to work in the Euclidean space and use an imaginary time,  $\tau$  defined as:

$$\tau = it \quad (\text{B.5})$$

Now the action (B.4) becomes for a system of absolute temperature  $T$ :

$$S = \int_0^{\hbar\beta} d\tau \int_V d^D \vec{r} \left\{ \psi^* \left( \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m} \nabla^2 - \mu \right) \psi + \frac{g}{2} |\psi|^4 \right\} \quad (\text{B.6})$$

where  $\beta$  is given by:

$$\beta = \frac{k_B}{T} \quad (\text{B.7})$$

where  $k_B$  is the Boltzmann constant. The partition function of the gas can be defined as:

$$Z = \int D[\psi, \psi^*] \exp\{-S[\psi, \psi^*]\} \quad (\text{B.8})$$

where  $D[\psi, \psi^*]$  is the measure of the fields, whereas  $S$  is the action in the Euclidean space for a gas of temperature  $T$ :

$$S = \int_0^{\hbar\beta} d\tau \int_V d^D \vec{r} \left\{ \psi^* \left( \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m} \nabla^2 - \mu \right) \psi + \frac{g}{2} |\psi|^4 \right\} \quad (\text{B.9})$$

The grand canonical potential is defined as:

$$\Omega = -\frac{1}{\hbar\beta} \ln(Z) \quad (\text{B.10})$$

As it is written in Appendix A, the phase transitions are explained as a spontaneous symmetry breaking mechanism of the system. To explain the transition between the normal gas and the superfluid phase we need however to find the minima the effective potential:

$$V_{eff} = -\mu|\psi|^2 + \frac{g}{2}|\psi|^4 \quad (\text{B.11})$$

which gives:

$$|\psi_0| = \begin{cases} 0 & \text{if } \mu < 0 \\ \sqrt{\frac{\mu}{g}} & \text{if } \mu > 0 \end{cases} \quad (\text{B.12})$$

Therefore for  $\mu < 0$  we the minimum is zero, whereas in the other case we have a circle of minima of radius  $\sqrt{\frac{\mu}{g}}$ . The choice of a particular minimum breaks the  $U(1)$  symmetry of the action. In particular we choose the real-valued positive minimum, i.e. the one with  $\psi_0 = \psi_0^* = |\psi_0|$  for the sake of simplicity. We now write the field as:

$$\psi = \psi_0 + \chi \quad (\text{B.13})$$

where  $\chi(\vec{r}, \tau)$  is the complex fluctuation around the minimum of the potential. Note that  $\psi_0$  can be interpreted as the order parameter of the phase transition. It is nonzero in the superfluid phase and is equal to zero at the transition and in the normal phase of the gas. We now expand the action up to the second order in the fluctuations:

$$S[\chi, \chi^*] = \int_0^{\hbar\beta} d\tau \int_V d^D \vec{r} \left\{ -\mu\psi_0^2 + \frac{1}{2}g\psi_0^4 + \chi^* \left( \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu + 2g\psi_0 \right) \chi + \frac{g}{2}\psi_0^2(\chi\chi + \chi^*\chi^*) \right\} \quad (\text{B.14})$$

We have ignored the linear parts because they do not contribute: the terms linear in the fluctuations cancel out each other whereas the linear terms in the derivatives do not contribute in the equation of motion. To proceed we now need to use the Fourier expansion

$$\chi = \sqrt{\frac{1}{V\hbar\beta}} \sum_{n, \vec{q}} \chi_{n, \vec{q}} e^{i(\omega_n \tau + \vec{q} \cdot \vec{r})} \quad (\text{B.15})$$

where  $\omega_n$  are the Matsubara frequencies:

$$\omega_n = \frac{2\pi n}{\hbar\beta} \quad n \in \mathbb{Z} \quad (\text{B.16})$$

We can split the action in the following way:

$$S[\chi, \chi^*] = S^{(MF)} + S^{(G)}[\chi, \chi^*] \quad (\text{B.17})$$

where  $S^{(MF)}$  is the part of the action independent of the fluctuations while  $S^{(G)}$  is the quadratic term. The constant term in the fluctuation gives the following contribution to the grand-canonical potential:

$$\Omega^{(MF)} = -V(-\mu\psi_0^2 + \frac{1}{2}g\psi_0^4) \quad (\text{B.18})$$

In order to find the contribution related to the Gaussian term, we will use the following relation:

$$\int_V d^D \vec{r} \frac{1}{V} e^{i(\vec{q} - \vec{q}') \cdot \vec{r}} = \delta_{\vec{q}, \vec{q}'} \quad (\text{B.19})$$

$$\int_0^{\hbar\beta} d\tau \frac{1}{\hbar\beta} e^{i(\omega_n - \omega_{n'}) \tau} = \delta_{n, n'} \quad (\text{B.20})$$

where  $\delta_{\vec{q}\vec{q}'}$  is the Kroenecker delta. We can write  $S^{(G)}$  as:

$$\begin{aligned}
S^{(G)} = \frac{1}{2} \sum_{n,\vec{q}} \sum_{n',\vec{q}'} \frac{1}{V\hbar\beta} \int_0^{\hbar\beta} d\tau \int_V d^D\vec{r} \{ & e^{i(\omega_n - \omega_{n'})\tau + i(\vec{q} - \vec{q}')\vec{r}} \chi_{n',\vec{q}'}^* [i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2] \chi_{n,\vec{q}} + \\
& e^{-i(\omega_n - \omega_{n'})\tau - i(\vec{q} - \vec{q}')\vec{r}} \chi_{-n',-\vec{q}'}^* [-i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2] \chi_{-n,-\vec{q}} + \\
& \frac{g}{2} \psi_0^2 (e^{i(\omega_n + \omega_{n'})\tau + i(\vec{q} + \vec{q}')\vec{r}} \chi_{n,\vec{q}} \chi_{n',\vec{q}'} + e^{-i(\omega_n + \omega_{n'})\tau - i(\vec{q} + \vec{q}')\vec{r}} \chi_{-n,-\vec{q}} \chi_{-n',-\vec{q}'} + \\
& e^{-i(\omega_n + \omega_{n'})\tau - i(\vec{q} + \vec{q}')\vec{r}} \chi_{n,\vec{q}}^* \chi_{n',\vec{q}'}^* + e^{i(\omega_n + \omega_{n'})\tau + i(\vec{q} + \vec{q}')\vec{r}} \chi_{-n,-\vec{q}}^* \chi_{-n',-\vec{q}'}^*) \} \quad (B.21)
\end{aligned}$$

Now if we use the the relations (B.19) and (B.20), we can write the quadratic terms in the following way:

$$S^{(G)} = \frac{1}{2} \sum_{n,\vec{q}} \begin{bmatrix} \chi_{n,\vec{q}}^* & \chi_{-n,-\vec{q}} \end{bmatrix} M \begin{bmatrix} \chi_{n,\vec{q}} \\ \chi_{-n,-\vec{q}}^* \end{bmatrix} \quad (B.22)$$

where  $M$  is the matrix given by:

$$M = \begin{bmatrix} i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2 & g\psi_0^2 \\ g\psi_0^2 & -i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2 \end{bmatrix} \quad (B.23)$$

The Gaussian contribution to the partition function is given by:

$$Z^{(G)} = \int D[\chi, \chi^*] \exp(-S^{(G)}[\chi, \chi^*]) \quad (B.24)$$

which gives the correction to the grand-canonical potential:

$$\Omega^{(G)} = -\frac{1}{\beta} \ln Z_2 = \frac{1}{2\beta} \sum_{n,\vec{q}} \ln(\det M) = \frac{1}{2\beta} \sum_{n,\vec{q}} \ln[\hbar^2 \omega_n^2 + (E_{\vec{q}})^2] \quad (B.25)$$

where  $E_{\vec{q}}$ , the spectrum of the elementary excitations is given by:

$$E_{\vec{q}} = \sqrt{\frac{\hbar^2 q^2}{2m} \left( \frac{\hbar^2 q^2}{2m} - 2\mu + 4g\psi_0^2 \right) + \mu^2 + 3g^2\psi_0^4 - 4g\psi_0^2\mu} \quad (B.26)$$

After the summation over Matsubara frequencies we can finally write:

$$\Omega^{(G)} = \sum_{\vec{q}} \left\{ \frac{E_{\vec{q}}}{2} + \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}}}) \right\} \quad (B.27)$$

Putting all parts of the grand canonical potential together:

$$\Omega = \Omega^{(MF)} + \Omega_0^{(G)} + \Omega_T^{(G)} \quad (B.28)$$

where  $\Omega^{(MF)}$  is the mean-field potential while  $\Omega_0^{(G)}$ , the zero-point energy, and  $\Omega_T^{(G)}$ , the thermodynamic fluctuation term, are given by:

$$\Omega_0^{(G)} = \sum_{\vec{q}} \frac{E_{\vec{q}}}{2} \quad (B.29)$$

$$\Omega_T^{(G)} = \sum_{\vec{q}} \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}}}) . \quad (B.30)$$

Until now, the calculations were completely general since we did not use a particular value for  $\psi_0$ .

**The normal gas phase** Let us consider the case of a normal gas, i.e.  $\psi_0 = 0$ . The spectrum becomes:

$$E_{\vec{q}} = \sqrt{\frac{\hbar^2 q^2}{2m} \left( \frac{\hbar^2 q^2}{2m} - 2\mu \right) + \mu^2} = \frac{\hbar^2 q^2}{2m} - \mu \quad (B.31)$$

whereas the mean-field contribution of the gran canonical potential,  $\Omega_0$ , goes to zero.

**The superfluid phase** For the superfluid phase  $\psi_0^2 = \frac{\mu}{g}$  the spectrum becomes:

$$E_{\vec{q}} = \sqrt{\frac{\hbar^2 q^2}{2m} \left( \frac{\hbar^2 q^2}{2m} + 2\mu \right)} \quad (\text{B.32})$$

This spectrum is known as the Bogoliubov spectrum [35]. The quantum fluctuation term of the grand canonical potential is in fact divergent. To tame such a divergence we can use the dimensional regularization approach and for  $D = 2$  a renormalization is needed. A study of the grand canonical potential can be found at [27].

## B.2 The relativistic case

Let us now consider the case of a weakly interacting relativistic gas. This time we will start directly the analysis from the action in the Euclidean space. Using the same approximation for the dilute gas as for the non-relativistic case, for a weakly-interacting relativistic gas the it is given by [36, 37, 38, 39]:

$$S = \int_0^{\hbar\beta} d\tau \int_V d^D \vec{r} \left( \frac{\hbar^2}{mc^2} \left| \frac{\partial}{\partial \tau} \psi \right|^2 + 2\hbar \frac{\mu_r}{mc^2} \psi^* \frac{\partial}{\partial \tau} \psi + \frac{\hbar^2}{m} |\nabla \psi|^2 + \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) |\psi|^2 + \frac{g}{2} |\psi|^4 \right) \quad (\text{B.33})$$

where  $\psi(\vec{r}, \tau)$  is the bosonic matter field. We introduced the relativistic chemical potential  $\mu_r$  which is given by:

$$\mu_r = \mu + mc^2 \quad (\text{B.34})$$

If we define again an effective potential  $V_{eff}$  such as:

$$V_{eff} = - \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) |\psi|^2 + \frac{g}{2} |\psi|^4 \quad (\text{B.35})$$

In particular the minima are given by:

$$|\psi_0| = \begin{cases} 0 & \text{if } \mu_r^2 - m^2 c^4 < 0 \\ \sqrt{\frac{\mu_r^2 - mc^2}{g}} & \text{if } \mu_r^2 - m^2 c^4 > 0 \end{cases} \quad (\text{B.36})$$

The first case corresponds to the normal phase, characterized by a mean value of order parameter equal to zero. The second corresponds to a superfluid phase, where the  $U(1)$  symmetry of the action is broken. In both cases, we choose the real and positive minimum  $\psi_0$ . Let us now call  $\chi(\vec{r}, \tau)$  the fluctuations around it. We expand now the action to the second order in the fluctuations, maintaining for generality the value of  $\psi_0$  implicit. We obtain:

$$S = V\hbar\beta \left[ - \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) \psi_0^2 + \frac{g}{2} \psi_0^4 \right] + \int_0^{\hbar\beta} d\tau \int_V d^D \vec{r} \left\{ \hbar \frac{\mu_r}{mc^2} (\chi^* \frac{\partial}{\partial \tau} \chi - \chi \frac{\partial}{\partial \tau} \chi^*) + \frac{\hbar^2}{mc^2} \left| \frac{\partial}{\partial \tau} \chi \right|^2 + \frac{\hbar^2}{m} |\nabla \chi|^2 - \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) |\chi|^2 + \frac{g}{2} \psi_0^2 (\chi \chi + \chi^* \chi^* + 4|\chi|^2) \right\} \quad (\text{B.37})$$

The constant term:

$$S^{(MF)} = V\hbar\beta \left( - \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) \psi_0^2 + \frac{g}{2} \psi_0^4 \right) \quad (\text{B.38})$$

gives a contribution to the grand canonical potential:

$$\Omega^{(MF)} = V \left( - \left( \frac{\mu_r^2}{mc^2} - mc^2 \right) \psi_0^2 + \frac{g}{2} \psi_0^4 \right) \quad (\text{B.39})$$

whereas, as we did in the previous Section, the second-order correction of the action can be written in a matrix form in the Fourier space (the sum over the index  $n$  refers to the sum over the Matsubara frequencies):

$$S^{(G)} = \frac{1}{2} \sum_{n, \vec{q}} \begin{bmatrix} \eta_{n, \vec{q}}^* & \eta_{-n, -\vec{q}} \end{bmatrix} \frac{1}{mc^2} M \begin{bmatrix} \eta_{\vec{q}} \\ \eta_{-\vec{q}}^* \end{bmatrix} \quad (\text{B.40})$$

where  $M$  is the matrix given by:

$$M = \begin{bmatrix} A & B \\ B & C \end{bmatrix} \quad (\text{B.41})$$

where:

$$A = \hbar^2 \omega_n^2 + 2\hbar \omega_n \mu_r + \hbar^2 c^2 q^2 - (\mu_r^2 - m^2 c^4) + 2g\psi_0^2 m c^2 \quad (\text{B.42})$$

$$B = g\psi_0^2 m c^2 \quad (\text{B.43})$$

$$C = \hbar^2 \omega_n^2 - 2\hbar \omega_n \mu_r + \hbar^2 c^2 q^2 - (\mu_r^2 - m^2 c^4) + 2g\psi_0^2 m c^2 \quad (\text{B.44})$$

The second order contribution to the grand canonical potential then results:

$$\Omega^{(G)} = \frac{1}{2\beta} \sum_{n, \vec{q}} \ln \left( \frac{1}{m^2 c^4} \det M \right) = \frac{1}{2\beta} \sum_{n, \vec{q}} \sum_{j=\pm} \ln \left[ \frac{1}{m^2 c^4} (\hbar^2 \omega_n^2 + E_{j, \vec{q}}^2) \right] \quad (\text{B.45})$$

where  $E_{\pm, \vec{q}}$  is given by:

$$E_{\pm, \vec{q}}^2 = \hbar^2 c^2 q^2 + (\mu_r^2 + m^2 c^4 + 2g\psi_0^2 m c^2) \pm \sqrt{4\mu_r^2 (\hbar^2 c^2 q^2 + m^2 c^4 + 2g\psi_0^2 m c^2) + g^2 \psi_0^4 m^2 c^4} \quad (\text{B.46})$$

Summing over the Matsubara frequencies we can finally write:

$$\Omega^{(G)} = \sum_{\vec{q}} \sum_{j=\pm} \left\{ \frac{E_{\vec{q}, j}}{2} + \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}, j}}) \right\} \quad (\text{B.47})$$

Putting all terms of the grand canonical potential density together we obtain:

$$\Omega = \Omega^{(MF)} + \Omega_0^{(G)} + \Omega_T^{(G)} \quad (\text{B.48})$$

where  $\Omega_0^{(G)}$ , the zero-point Gaussian grand canonical potential density, and  $\Omega_T^{(G)}$  is the fluctuation term, defined respectively as:

$$\Omega_0^{(G)} = \sum_{\vec{q}} \sum_{j=\pm} \frac{E_{\vec{q}, j}}{2} \quad (\text{B.49})$$

$$\Omega_T^{(G)} = \sum_{\vec{q}} \sum_{j=\pm} \frac{1}{\beta} \ln(1 - e^{-\beta E_{\vec{q}, j}}) \quad (\text{B.50})$$

**Normal phase** We now use  $\psi_0 = 0$ . In this case the spectrum becomes:

$$E_{\pm, \vec{q}} = \sqrt{\hbar^2 c^2 q^2 + m^2 c^4} \pm \mu_r \quad (\text{B.51})$$

As in the non-relativistic case the mean-field contribution to the grand-canonical potential goes to zero.

**Superfluid** We use  $\psi_0^2 = \frac{\mu_r^2 - m c^2}{m c^2 g}$  and therefore the spectrum becomes:

$$E_{\pm, \vec{q}}^2 = \hbar^2 c^2 q^2 + (3\mu_r^2 - m^2 c^4) \pm \sqrt{4\mu_r^2 \hbar^2 c^2 q^2 + (3\mu_r^2 - m^2 c^4)^2} \quad (\text{B.52})$$

### B.3 Analysis and comparison of the spectra

Let us now compare the results the spectra in both the phases.



**Normal Gas** In the case of a normal gas we have found for the non-relativistic case (B.31). In particular for high momenta this gives the non-relativistic free particle spectrum. The relativistic case (B.51) instead gives for low energies:

$$E_{\pm, \vec{q}} = mc^2 + \frac{\hbar^2 q^2}{2m} \pm \mu_r \quad (\text{B.53})$$

and using the definition of the relativistic chemical potential we obtain:

$$E_{+, \vec{q}} = 2mc^2 + \mu + \frac{\hbar^2 q^2}{2m} \quad (\text{B.54})$$

$$E_{-, \vec{q}} = \frac{\hbar^2 q^2}{2m} - \mu \quad (\text{B.55})$$

Therefore we have two gapped spectra and the second has the same form of the non-relativistic one. Let us now consider the chemical potential. In the non-relativistic case the constraint was  $\mu < 0$ . On the other hand in the relativistic case we had the constraint:

$$\mu_r^2 - m^2 c^4 = \mu(\mu - 2mc^2) < 0 \quad (\text{B.56})$$

which gives:

$$2mc^2 < \mu < 0$$

We however have to note that in the non-relativistic limit we have  $\mu \ll mc^2$  and therefore the two constraints are compatible to each other. At ultrarelativistic energies we have:

$$E_{\pm, \vec{q}} = \hbar c q \quad (\text{B.57})$$

i.e. linear in the momenta like a ultra-relativistic free particle.

**Superfluid** Let us now consider the Bogololiubov spectrum (B.32). In particular we note that for low momenta we have:

$$E_{\vec{q}} = \sqrt{\frac{\mu}{m}} \hbar q \quad (\text{B.58})$$

whereas for high momenta like the normal case we obtain a non-relativistic free particle spectrum. The non relativistic spectrum (B.52) for low energies gives:

$$\hbar \omega_- = \sqrt{\frac{\mu}{m}} \hbar q \quad (\text{B.59})$$

$$\hbar \omega_+ = 2mc^2 + \frac{\hbar^2 q^2}{2m} \quad (\text{B.60})$$

where we have used the condition  $\mu \ll mc^2$ . We have found therefore a gapped (also called ‘‘Higgs’’) mode, with the gap being  $2mc^2$ , and a quadratic dependency on the momenta and a gapless Goldstone mode which is exactly like the Bogoliubov spectrum at low energies. In order to recover the Bogoliubov spectrum let us now consider again the Goldstone (relativistic) mode,  $\hbar \omega_-$ . For small momenta it can be written as:

$$\hbar \omega_- = \sqrt{\hbar^2 c^2 q^2 - \frac{2\mu_r^2 \hbar^2 c^2 q^2}{3\mu_r^2 - m^2 c^4} + \frac{4\mu_r^4 \hbar^4 c^4 q^4}{(3\mu_r^2 - m^2 c^4)^3}} = \sqrt{\frac{\hbar^2 c^2 q^2}{3\mu_r^2 - m^2 c^4} \left( \frac{4\mu_r^2 \hbar^2 c^2 q^2}{(3\mu_r^2 - m^2 c^4)^2} + (\mu_r^2 - m^2 c^4) \right)} \quad (\text{B.61})$$

and now since we are interested in the non-relativistic case by imposing  $\mu \ll mc^2$  we obtain the Bogoliubov spectrum (B.32).

At high energies we have that the term involving the higher-degree momentum becomes dominant and modes are given by:

$$\hbar \omega_{\pm} = \hbar c q \quad (\text{B.62})$$

In this limit we have two free relativistic particles spectra: as in the non-relativistic case we obtained that at high energies the spectra are unaffected by the contact interaction

# Appendix C

## Green functions

In Section 1.4 the concept of Green function was introduced. The aim of this Appendix is to give a brief review of this concept<sup>1</sup>. In Condensed Matter Field Theory the path integral is identified with the partition function<sup>2</sup>:

$$Z = \int D[\psi] \exp\{-S[\psi]\} \quad (\text{C.1})$$

where  $\psi$  is the order parameter of the system,  $D[\psi]$  is the functional measure and  $S$  is the action in the Euclidean space. Let  $F[\psi]$  be a physical quantity which depends on the order parameter. In this formalism its mean-value is given by:

$$\langle F[\psi] \rangle_S = \frac{\int D[\psi] F[\psi] \exp\{-S[\psi]\}}{Z} \quad (\text{C.2})$$

where the subscript  $S$  indicates that we are computing the mean-value using the action  $S$ . Let us now assume that  $\psi$  is a generic complex parameter. If this is the case, the 2-points Green function<sup>3</sup> is given by:

$$G_{ij}^{(2)}(\vec{r}, \vec{r}', \tau, \tau') = \langle \psi_i(\vec{r}, \tau) \psi_j^*(\vec{r}', \tau') \rangle_S = \frac{\int D[\psi, \psi^\dagger] \psi_i(\vec{r}, \tau) \psi_j^*(\vec{r}', \tau') \exp\{-S[\psi, \psi^\dagger]\}}{Z} \quad (\text{C.3})$$

If we denote the point in space-time by  $r$ , i.e.:

$$r = (\vec{r}, \tau) \quad (\text{C.4})$$

the general 2N-point Green function is given by:

$$G_{i_1 \dots i_N j_N \dots j_1}^{(2N)}(r_1, \dots, r_N, r'_N, \dots, r'_1) = \langle \psi_{i_1}(r_1) \dots \psi_{i_N}(r_N), \psi_{j_N}^*(r_N) \dots \psi_{j_1}^*(r'_1) \rangle_S = \frac{\int D[\psi, \psi^\dagger] \psi_{i_1}(r_1) \dots \psi_{i_N}(r_N), \psi_{j_N}^*(r_N) \dots \psi_{j_1}^*(r'_1) \exp\{-S[\psi, \psi^\dagger]\}}{Z} \quad (\text{C.5})$$

Another way to compute the Green function is to introduce the external currents. In particular, we define:

$$Z[J, J^\dagger] = \int D[\psi] \exp\left\{-S[\psi] + \int_0^\beta d\tau \int_V d^D \vec{r} [J^\dagger \psi + h.c.]\right\} \quad (\text{C.6})$$

The generic Green function can be computed as:

$$G_{i_1 \dots i_N j_N \dots j_1}^{(2N)}(r_1, \dots, r_N, r'_N, \dots, r'_1) = \frac{\left( \frac{\delta}{\delta J_{i_1}^\dagger(r_1)} \dots \frac{\delta}{\delta J_{i_N}^\dagger(r_N)} \frac{\delta}{\delta J_{j_N}(r'_N)} \dots \frac{\delta}{\delta J_{j_1}(r'_1)} Z[J, J^\dagger] \right)_{J_{i_1}^\dagger(r_1)=\dots=J_{i_N}^\dagger(r_N)=J_{j_N}(r'_N)=\dots=J_{j_1}(r'_1)=0}}{Z} \quad (\text{C.7})$$

where we assumed that the fields are time ordered. These Green functions are, in general, not connected. In order to introduce them, we need to define the generator functional of Green connected functions which we call  $W[J, J^\dagger]$  which is defined by:

$$W[J, J^\dagger] = -\ln \left\{ \frac{Z[J, J^\dagger]}{Z} \right\} \quad (\text{C.8})$$

<sup>1</sup>For a more detailed discussion of the concepts used in this Appendix see for instance [15]

<sup>2</sup>We use the natural units  $\hbar = c = 1$

<sup>3</sup>Note that in the case of real order parameter we could have an odd number of points.

or alternatively:

$$\frac{Z[J, J^\dagger]}{Z} = \exp\{-W[J, J^\dagger]\} \quad (\text{C.9})$$

The connected Green functions are given by (assuming that the fields are time-ordered):

$$G_{i_1 \dots i_N j_N \dots j_1}^{(2N, C)}(r_1, \dots, r_N, r'_N, \dots, r'_1) = - \left( \frac{\delta}{\delta J_{i_1}^\dagger(r_1)} \dots \frac{\delta}{\delta J_{i_N}^\dagger(r_N)} \frac{\delta}{\delta J_{j_N}(r'_N)} \dots \frac{\delta}{\delta J_{j_1}(r'_1)} W[J, J^\dagger] \right)_{J_{i_1}^\dagger(r_1) = \dots = J_{i_N}^\dagger(r_N) = J_{j_N}(r'_N) = \dots = J_{j_1}(r'_1) = 0} \quad (\text{C.10})$$

conversely the expansion of the generating functional  $W[J, J^\dagger]$  is given by:

$$W[J, J^\dagger] = \frac{1}{(N!)^2} \sum_N \int d^{D+1}r_1 \dots d^{D+1}r_N d^{D+1}r'_N \dots d^{D+1}r'_1 \sum_{i_1 \dots i_N j_N \dots j_1} G_{i_1 \dots i_N j_N \dots j_1}^{(2N, C)} J_{i_1}^\dagger(r_1) \dots J_{i_N}^\dagger(r_N) J_{j_N}(r'_N) \dots J_{j_1}(r'_1) \quad (\text{C.11})$$

## C.1 Application: Green functions of the Local Limit of Bose Hubbard

In Section 1.4 we needed to compute the Green functions relative to the action of the Local Limit (see Section 1.3.1). In general action is given by<sup>4</sup>:

$$S_{loc}[a, a^*] = \int_0^\beta d\tau \left\{ a^* \frac{\partial}{\partial \tau} a - (\mu - \varepsilon) a^* a + \frac{U}{2} n(n-1) \right\} \quad (\text{C.12})$$

where:

$$n = a^* a \quad (\text{C.13})$$

The partition function is defined as:

$$Z_{loc} = \int D[a, a^*] \exp\{-S_{loc}[a, a^*]\} \quad (\text{C.14})$$

The two-point Green function is given by:

$$G_{loc}^{(2)} = \frac{\int D[a, a^*] a(\tau) a^*(\tau') \exp\{-S_{loc}[a, a^*]\}}{Z_{loc}} \quad (\text{C.15})$$

Now, formally the function  $a(\tau)$  is given by:

$$a(\tau) = \langle \Phi | e^{\tau h_{loc}} \hat{a} e^{-\tau h_{loc}} | \Phi \rangle \quad (\text{C.16})$$

Assuming now that  $\tau > \tau'$  we get:

$$a(\tau) a^*(\tau') = \langle \Phi | e^{(\tau - \tau') h_{loc}} \hat{a} \hat{a}^\dagger e^{-(\tau - \tau') h_{loc}} | \Phi \rangle \quad (\text{C.17})$$

Until now, however, we have said nothing about the nature of the states which in the Path Integral formulation above corresponds to an introduction of a constraint on the functional measure. In fact, the states are Fock states and therefore we have:

$$a^* a = \langle m | \hat{a}^\dagger \hat{a} | m \rangle = n \quad (\text{C.18})$$

$$\frac{\partial}{\partial \tau} a = \frac{\partial}{\partial \tau} (\langle m | \hat{a} | m \rangle) = 0 \quad (\text{C.19})$$

$$(\text{C.20})$$

and:

$$G_{loc}^{(2)}(\tau, \tau') = - \frac{\sum_m e^{-\beta \mathcal{E}_{loc}^{(m)}} \langle m | e^{(\tau - \tau') h_{loc}} \hat{a} \hat{a}^\dagger e^{-(\tau - \tau') h_{loc}} | m \rangle}{Z_{loc}} \quad (\text{C.21})$$

<sup>4</sup>We are using the same conventions of Section 1.3 and 1.4

if we introduce a completeness relation we find:

$$G_{loc}^{(2)}(\tau, \tau') = - \frac{\sum_m \sum_s e^{-[\beta - (\tau - \tau')] \mathcal{E}_{loc}^{(m)} - (\tau - \tau') \mathcal{E}_{loc}^{(s)}} \langle m | \hat{a} | s \rangle \langle s | \hat{a}^\dagger | m \rangle}{Z_{loc}} = \frac{\sum_m (m+1) e^{-[\beta - (\tau - \tau')] \mathcal{E}_{loc}^{(m)} - (\tau - \tau') \mathcal{E}_{loc}^{(m+1)}}}{Z_{loc}} \quad (C.22)$$

We note that the Green function is in fact a function of  $\tau - \tau'$ , i.e.:

$$G_{loc}^{(2)}(\tau, \tau') = G_{loc}(\tau - \tau') \quad (C.23)$$

The Fourier transform of the Green function is therefore given by:

$$G_{loc}^{(2)}(i\omega) = \int_0^\beta d\tau'' G_{loc}(\tau'') = \frac{\sum_m (m+1) \frac{e^{-\beta \mathcal{E}_{loc}^{m+1}} - e^{-\beta \mathcal{E}_{loc}^m}}{i\omega + \mathcal{E}_{loc}^m - \mathcal{E}_{loc}^{m-1}}}{Z_{loc}} \quad (C.24)$$

where:

$$\tau'' = \tau - \tau' \quad (C.25)$$

But at  $T \rightarrow 0$  we have also:

$$Z_{loc} = e^{-\beta \mathcal{E}_{loc}} \quad (C.26)$$

which gives:

$$G_{loc}^{(2)}(i\omega) = \frac{n+1}{i\omega + \mathcal{E}_{loc} - \mathcal{E}_{loc}^{(n+1)}} + \frac{n}{i\omega + \mathcal{E}_{loc}^{(n-1)} - \mathcal{E}_{loc}} = \frac{n+1}{i\omega + (\mu - \varepsilon) - Un} + \frac{n}{i\omega + (\mu - \varepsilon) - U(n-1)} \quad (C.27)$$

For the action:

$$S_0 = \sum_i S_{loc,i} \quad (C.28)$$

i.e. the total contribution of the local terms, if we label the two-point Green function for this action as  $G_0^{(2)}(i\omega)$ , it is straightforward to show that:

$$G_0^{(2)}(i\omega) = G_{loc}^{(2)}(i\omega) \quad (C.29)$$

Alternatively we can compute this Green function by adding a external currents in the partition Function, let us name them  $\psi_i$ :

$$Z[\psi, \psi^*] = \int D[a, a^*] \exp\{-S_0 + \int d\tau \sum_i [\psi_i^* a_i + c.c]\} \quad (C.30)$$

Let us call  $W_0$  the generator functional of connected Green function. For what we have seen before it can be written as:

$$W_0[\psi, \psi^*] = -\ln[\langle \int d\tau \sum_i [\psi_i^* a_i + c.c] \rangle_0] \quad (C.31)$$



## Appendix D

# Dimensional regularization and renormalization

In Chapter 3, in order to compute the pressure, we needed to use the dimensional regularization. This regularization technique is based on a shift in dimensionality as follows:

$$D \rightarrow \mathfrak{D} = D - \epsilon \quad (\text{D.1})$$

where  $\epsilon$  is a small complex number. As an example let us consider the case where both  $K_1$  and  $K_2$  are both non-vanishing as in Section 3.1. We found that the equation of state, in the ordered phase, is given by:

$$P^{(O)} = -\frac{\Omega^{(O)}}{L^D} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} - \frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^D \pi^{\frac{D}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{D}{2}-1} (1+Q)^{\frac{1}{2}} \quad (\text{D.2})$$

where  $q_{ph}$  a physical scale in the momenta is given by:

$$q_{ph} = \sqrt{\frac{K_1^2}{4K_2K_3} + \frac{|c_2|}{K_3}} \quad (\text{D.3})$$

If we now perform the shift in the dimensions we obtain:

$$\frac{P^{(O)}}{\kappa^\epsilon} = -\frac{\Omega}{L^\mathfrak{D}} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} - \frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^D \pi^{\frac{D}{2}} K_2^{\frac{1}{2}} \kappa^\epsilon \Gamma(\frac{D}{2})} \int_0^\infty dQ Q^{\frac{\mathfrak{D}}{2}-1} (1+Q)^{\frac{1}{2}} \quad (\text{D.4})$$

where  $\kappa$  is an arbitrary scale in the momenta. By using the analytic continuation of the Euler Beta function, i.e.:

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int dt t^{x-1} (1+t)^{-x-y} \quad (\text{D.5})$$

we obtain:

$$\begin{aligned} \frac{P^{(O)}}{\kappa^\epsilon} = -\frac{\Omega}{L^\mathfrak{D}} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} + \frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^{D+1} \pi^{\frac{D}{2} + \frac{1}{2}} K_2^{\frac{1}{2}} \Gamma(\frac{D}{2}) \kappa^\epsilon} \frac{\Gamma(\frac{\mathfrak{D}}{2}) \Gamma(-\frac{\mathfrak{D}}{2} - \frac{1}{2})}{\Gamma(-\frac{1}{2})} = \\ -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} + \frac{q_{ph}^{D+1} K_3^{\frac{1}{2}}}{2^{D+1} \pi^{\frac{D}{2} + \frac{1}{2}} K_2^{\frac{1}{2}} \kappa^\epsilon} \Gamma\left(-\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) \end{aligned} \quad (\text{D.6})$$

where we have considered that  $\epsilon$  is a small parameter. For odd dimensions the result is still divergent. The Euler Gamma function has poles for negative integers. The expansion for small  $\epsilon$  is given by:

$$\Gamma\left(-\frac{\mathfrak{D}}{2} - \frac{1}{2}\right) = \Gamma\left(-\frac{D}{2} - \frac{1}{2} + \frac{\epsilon}{2}\right) \simeq \frac{(-1)^{\frac{D+1}{2}} 2}{\frac{D+1}{2}!} \frac{2}{\epsilon} + \theta\left(\frac{D+1}{2} + 1\right) \quad (\text{D.7})$$

where  $\theta$  is the Euler Digamma function:

$$\theta(z) = \frac{\Gamma(z)'}{\Gamma(z)} \quad (\text{D.8})$$

therefore we have:

$$\begin{aligned} \frac{P^{(O)}}{\kappa^\epsilon} &= \frac{\mathcal{E}_0}{V} \frac{1}{\kappa^\epsilon} + \frac{c_2^2}{4c_4} + \frac{(-1)^{\frac{D+1}{2}} q_{ph}^{D+1} K_3^{\frac{1}{2}}}{\frac{D+1}{2}! 2^D \pi^{\frac{D}{2}+\frac{1}{2}} K_2^{\frac{1}{2}}} \frac{1}{\kappa^\epsilon} + \frac{(-1)^{\frac{D+1}{2}} q_{ph}^{D+1} K_3^{\frac{1}{2}}}{\frac{D+1}{2}! 2^{D+1} \pi^{\frac{D}{2}+\frac{1}{2}} K_2^{\frac{1}{2}}} \frac{1}{\kappa^\epsilon} \theta\left(\frac{D+1}{2} + 1\right) = \\ &= \frac{\mathcal{E}_0}{V} \frac{1}{\kappa^\epsilon} + \frac{c_2^2}{4c_4} + B \frac{1}{\kappa^\epsilon} + \frac{1}{2} B \theta\left(\frac{D+1}{2} + 1\right) \frac{1}{\kappa^\epsilon} \end{aligned} \quad (\text{D.9})$$

where  $B$  is given by:

$$B = \frac{(-1)^{\frac{D+1}{2}} q_{ph}^{D+1} K_3^{\frac{1}{2}}}{\left(\frac{D+1}{2}\right)! 2^D \pi^{\frac{D}{2}+\frac{1}{2}} K_2^{\frac{1}{2}}} \quad (\text{D.10})$$

We now can proceed with a renormalization, by interpreting  $c_4$  as a bare, unphysical coupling, rather than the observed one. We note that:

$$\begin{cases} B > 0 & \text{if } \frac{D+1}{2} = 2m \quad m \in \mathbb{N} \\ B < 0 & \text{if } \frac{D+1}{2} = 2m + 1 \quad m \in \mathbb{N} \end{cases} \quad (\text{D.11})$$

We now assume to be in the first case where  $B$  is positive. We now define the renormalized coupling constant  $c_{4,r}$  as:

$$\frac{1}{c_{4,r}(\kappa, \epsilon)} = \kappa^\epsilon \left( \frac{1}{c_4} + \frac{4}{c_2^2} B \frac{1}{\kappa^\epsilon \epsilon} \right) \quad (\text{D.12})$$

If we now derive the expression by  $\kappa$  we have:

$$-\frac{1}{c_2^2} \frac{\partial}{\partial \kappa} c_{4,r} = \frac{\epsilon \kappa^{\epsilon-1}}{c_4} - \frac{4}{c_2^2} B \kappa^{-1} \quad (\text{D.13})$$

and by multiplying by  $\kappa$  and taking the limit  $\epsilon \rightarrow 0$  we obtain the renormalization group equation for the running coupling constant (which is the  $\beta$  function):

$$\beta(c_{4,r}) = \kappa \frac{\partial}{\partial \kappa} c_{4,r} = \frac{4c_{4,r}^2}{c_2^2} B \quad (\text{D.14})$$

The beta function is positive and therefore  $c_{4,r}$  increases with the momenta. This means that the theory has a Landau Pole, a maximal scale in the momenta, which we call  $q_0$ , where the coupling diverges. This scale can be related to a minimal length of the system  $l$ , like the lattice spacing. By putting the constraint:

$$\frac{1}{c_{4,r}(q_0)} = 0 \quad (\text{D.15})$$

the solution of the equation of the renormalization group is given by:

$$\frac{1}{c_{4,r}(q_{ph})} = \frac{4}{c_2^2} B \ln \frac{q_0}{q_{ph}} \quad (\text{D.16})$$

Now, by writing the definition of the renormalized coupling (D.12) in terms of the bare coupling and by taking the  $\epsilon \rightarrow 0$  limit:

$$\frac{1}{c_4} = \frac{1}{c_{4,r}(q_{ph})} - \lim_{\epsilon \rightarrow 0} \frac{4}{c_2^2} B \frac{1}{\epsilon} \quad (\text{D.17})$$

and putting it into Equation (D.9) we have:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_{4,r}(q_{ph})} + \frac{1}{2} B \psi\left(\frac{D+1}{2} + 1\right) = -\frac{\mathcal{E}_0}{V} + B \ln \frac{q_0}{q_{ph}} + \frac{1}{2} B \theta\left(\frac{D+1}{2} + 1\right) \quad (\text{D.18})$$

For odd values of  $\frac{D+1}{2}$ ,  $B$  is negative. By following the same procedure as before we get the expression of the beta function:

$$\beta(c_{4,r}) = -\frac{4c_{4,r}^2}{c_2^2} |B| \quad (\text{D.19})$$

now the coupling decreases with the momenta, and therefore we have a divergence for an infrared cut-off, which we call again  $q_0$ . This scale can be related to the maximal length  $L$  of the system. We have therefore asymptotic freedom. If we now assume:

$$\frac{1}{c_{4,r}(q_0)} = 0 \quad (\text{D.20})$$

the solution of the renormalization group equation for  $\kappa = q_{ph}$  is given by:

$$\frac{1}{c_{4,r}(q_{ph})} = \frac{4}{c_2^2} |B| \ln \frac{q_{ph}}{q_0} \quad (\text{D.21})$$

therefore the expression of the pressure in the ordered phase is given by:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_{4,r}(q_{ph})} + \frac{1}{2} B \theta \left( \frac{D+1}{2} + 1 \right) = -\frac{\mathcal{E}_0}{V} + |B| \ln \frac{q_{ph}}{q_0} - \frac{1}{2} |B| \theta \left( \frac{D+1}{2} + 1 \right) \quad (\text{D.22})$$

Note that we have worked for the specific case when  $K_1 \neq 0$  and  $K_2 \neq 0$ . In fact, these results can be easily extended by using different expressions of the constant  $B$ . In particular, following the same steps it can be shown that there is an ultraviolet cut-off in the momenta for  $D = 3$  and  $K_1 = 0$  as well as for  $D = 2$  and  $K_2 = 0$ . Instead, for  $D = 1$  and  $K_2 = 0$  we have asymptotic freedom.

Note, also, that in the context of dimensional regularization the following equation is valid [29, 40, 27]:

$$\int_0^\infty dq q^{\lambda-1} (q^2)^{n-1} = 0 \quad (\text{D.23})$$

where  $\lambda \in \mathbb{C}$  and  $n \in \mathbb{N}$ . Hence, in this framework all polynomial integrals vanish.





## Appendix E

# Analogy with statistical classical mechanics

We will now compare what we have found with the results of classical Ginzburg-Landau theory. For the classical case we will only mention the relevant results: a treatment of Ginzburg-Landau theory is out of the scope of this study<sup>1</sup>. To begin, let us consider the transition between the ferromagnetic (ordered) and paramagnetic (disordered) phases. Let us call  $\psi(\vec{r})$  the magnetization. The Ginzburg-Landau Hamiltonian for a system of volume  $V$ , in  $D$  dimensions is given by:

$$\beta H = \int_V d^D \vec{r} \left\{ K |\vec{\nabla} \psi|^2 + a_2 \lambda |\psi|^2 + a_4 |\psi|^4 \right\} \quad (\text{E.1})$$

where  $K$  is the elastic coupling,  $a_2$  and  $a_4$  are the positive coefficients of the Landau Theory and  $\lambda$  is the reduced temperature:

$$\lambda = \frac{T - T_c}{T_c} \quad (\text{E.2})$$

where  $T_c$  is the critical temperature at which the transition takes place. Clearly for  $\lambda < 0$  (i.e.  $T < T_c$ ) there is a spontaneous symmetry breaking and we have the ordered phase. To this point, we write the magnetization as:

$$\psi(\vec{r}) = \psi_0 + \chi(\vec{r}) \quad (\text{E.3})$$

where  $\psi_0^2$  is the mean-field value of the magnetization. The Hamiltonian becomes, at the second order in the fluctuations:

$$H = H_0 + H_2 \quad (\text{E.4})$$

where  $H_0$ , the mean-field Hamiltonian is given by:

$$\beta H_0 = V a_2 \lambda \psi_0^2 + V a_4 \psi_0^4 \quad (\text{E.5})$$

whereas the contribution of the fluctuations is given by:

$$\beta H_2 = \int_V d^D \vec{r} \left\{ |\vec{\nabla} \chi|^2 + \chi^* (a_2 \lambda + 4 a_4 \psi_0^2) \chi + a_4 \psi_0^2 (\chi \chi + \chi^* \chi^*) \right\} \quad (\text{E.6})$$

The value of  $\psi_0$ , as usual, can be fixed by the minimization of  $H_0$ , and is given by:

$$\psi_0 = \begin{cases} 0 & \text{if } \lambda > 0 \\ \sqrt{\frac{-a_2 \lambda}{2 a_4}} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.7})$$

The partition function ( $Z$ ) and the free energy ( $\Omega$ ) are given by:

$$Z = \exp\{-\beta H\} \quad (\text{E.8})$$

$$\Omega = -\frac{1}{\beta} \ln Z \quad (\text{E.9})$$

<sup>1</sup>For a more extensive study of the classical case, see [30, 31]

<sup>2</sup>We take  $\psi_0$  real and positive, for simplicity.

Following the same procedure of Chapter 2, we find that the mean-field contribution to free energy is given by:

$$\Omega^{(MF)} = \begin{cases} 0 & \text{if } \lambda > 0 \\ -k_B TV \frac{a_2^2 \lambda^2}{4a_4} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.10})$$

and the contribution due to fluctuations:

$$\Omega^{(G)} = \begin{cases} k_B TV \int \frac{d^D q}{(2\pi)^D} \ln(K(q^2 + \xi_{DO}^{-2})) & \text{if } \lambda \geq 0 \\ k_B TV \int \frac{d^D q}{(2\pi)^D} \ln(K(q^2 + \xi_O^{-2})) & \text{if } \lambda < 0 \end{cases} \quad (\text{E.11})$$

are the wavenumbers,  $\xi_{DO}$  and  $\xi_O$  are, respectively, the correlation lengths for the disordered and ordered phases:

$$\xi_{DO} = \left( \frac{K}{a_2 \lambda} \right)^{\frac{1}{2}} \quad (\text{E.12})$$

$$\xi_O = \left( \frac{K}{-2a_2 \lambda} \right)^{\frac{1}{2}} \quad (\text{E.13})$$

We do not study the free energy, though, because the integral is not solvable. In fact, we will now study the specific heat at constant volume,  $c_V$ , given by:

$$c_V = -\frac{T}{V} \frac{\partial^2}{\partial T^2} \Omega \quad (\text{E.14})$$

The mean-field contribution to this quantity is then:

$$c_V^{(MF)} = \begin{cases} 0 & \text{if } \lambda > 0 \\ -k_B \frac{T}{T_c} \frac{a_2 \lambda}{a_4} - k_B \frac{T^2}{T_c^2} \frac{a_2^2}{2a_4} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.15})$$

whereas the contribution due to fluctuations:

$$c_V^{(G)} = \begin{cases} -2k_B \frac{T}{T_c} \frac{a_2}{K} \int d^D q \frac{1}{q^2 + \xi_{DO}^{-2}} - k_B \frac{T^2}{T_c^2} \frac{a_2^2}{K^2} \int d^D q \frac{1}{(q^2 + \xi_{DO}^{-2})^2} & \text{if } \lambda > 0 \\ -2k_B \frac{T}{T_c} \frac{(-2a_2)}{K} \int d^D q \frac{1}{q^2 + \xi_O^{-2}} - k_B \frac{T^2}{T_c^2} \frac{(-2a_2)^2}{K^2} \int d^D q \frac{1}{(q^2 + \xi_O^{-2})^2} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.16})$$

We are interested in the regime near the transition, hence we will make the approximation:

$$\frac{T}{T_c} \simeq 1 \quad (\text{E.17})$$

In this approximation we have a jump in the mean-field contribution at  $\lambda \rightarrow 0$ :

$$c_V^{(MF)} = \begin{cases} 0 & \text{if } \lambda > 0 \\ -k_B \frac{a_2^2}{2a_4} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.18})$$

This is reminiscent of what we have found for the second-order derivative of mean-field contribution the pressure of the quantum system, see Equation (3.20). To compute the contribution due to the correction, we write the integrals in polar coordinates and we introduce a ultraviolet cut-off, let us call it  $\Lambda$ , which is inversely proportional to the microscopic length of the system,  $l$ . The correction to the chemical potential is therefore given by:

$$c_V^{(G)} = \begin{cases} -k_B \frac{a_2}{K} \frac{1}{2^{D-2} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq \frac{q^{D-1}}{q^2 + \xi_{DO}^{-2}} - k_B \frac{a_2^2}{K^2} \frac{1}{2^{D-1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq \frac{q^{D-1}}{(q^2 + \xi_{DO}^{-2})^2} & \text{if } \lambda > 0 \\ k_B \frac{a_2}{K} \frac{1}{2^{D-3} \pi^{\frac{D}{2}}} \int_0^\Lambda dq \frac{q^{D-1}}{q^2 + \xi_O^{-2}} - k_B \frac{a_2^2}{K^2} \frac{1}{2^{D-3} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq \frac{q^{D-1}}{(q^2 + \xi_O^{-2})^2} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.19})$$

The above integrals do not have a divergence at high momenta, thanks to the cut-off. On the other hand, however, near the transition when  $q \rightarrow 0$  we might have a divergence due to the behavior of the correlation lengths. Hence, we now put:

$$k = q \xi_{DO, O} \quad (\text{E.20})$$

obtaining:

$$c_V^{(G)} = \begin{cases} -k_B \frac{a_2}{K} \frac{\xi_{DO}^{2-D}}{2^{D-2} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\xi_{DO}\Lambda} dk \frac{k^{D-1}}{k^2+1} - k_B \frac{a_2^2}{K^2} \frac{\xi_{DO}^{4-D}}{2^{D-1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\xi_{DO}\Lambda} dk \frac{k^{D-1}}{(k^2+1)^2} & \text{if } \lambda > 0 \\ k_B \frac{a_2}{K} \frac{\xi_O^{2-D}}{2^{D-3} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\xi_O\Lambda} dk \frac{k^{D-1}}{k^2+1} - k_B \frac{a_2^2}{K^2} \frac{\xi_O^{4-D}}{2^{D-3} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\xi_O\Lambda} dk \frac{k^{D-1}}{(k^2+1)^2} & \text{if } \lambda < 0 \end{cases} \quad (\text{E.21})$$

For both phases, the first term diverges for  $D < 2$  while the second term does the same for  $D < 4$  due to the divergence of the correlation length. At the same time, however, we note that in these units the integrals now diverge at the transition because the cut-off now goes to infinity. In particular we have that:

$$\int_0^{\xi_{DO}, O\Lambda} dk \frac{k^{D-1}}{k^2+1} \propto \xi_{DO, O}^{D-2} \Lambda^{D-2} \quad (\text{E.22})$$

$$\int_0^{\xi_{DO}, O\Lambda} dk \frac{k^{D-1}}{(k^2+1)^2} \propto \xi_{DO, O}^{D-4} \Lambda^{D-4} \quad (\text{E.23})$$

So, it seems that the first term has an ultraviolet divergence for  $D > 2$ , while the second has it for  $D > 4$ . However, we have seen that such a divergence was not present before the substitution in the integrals, i.e. when the integrals were written in their physical units. This means that this divergence is dominated by the vanishing of the opposite of the length correlation. Hence, for  $D < 2$  both terms diverge, while for  $2 \leq D < 4$  only the second diverges and finally for  $D \geq 4$  both are finite. This means that the mean-field theory is a very good approximation for dimensions higher than the the upper critical dimension,  $D = 4$ . On the other hand for  $D < 2$ , which is the lower critical dimension, the theorem of Mermin-Wagner implies that the inclusion of the fluctuations breaks the order at long range, and therefore there is no phase transition. Finally, for the intermediate case the fluctuations produce a divergence.

These results might be compared to the pressure computed in a generic theory of action (3.2) for the case  $K_1 = 0$ . In that case the pressure was given by:

$$P = - \begin{cases} \frac{\xi_0}{V} + \frac{1}{(2\pi)^D} \int d^D q \sqrt{K_3 q^2 + |c_2|} & \text{if } \lambda \geq \lambda_c \\ \frac{\xi_0}{V} - \frac{c_2^2}{4c_4} + \frac{1}{2(2\pi)^D} \int d^D q \sqrt{K_3 q^2 + 2|c_2|} & \text{if } \lambda < \lambda_c \end{cases} \quad (\text{E.24})$$

if we introduce a cut-off in the momenta, let us call it  $\Lambda$ , and we write the pressure in polar coordinates:

$$P = - \begin{cases} \frac{\xi_0}{V} + \frac{1}{2^{D-1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq q^{D-1} \sqrt{K_3 q^2 + |c_2|} & \text{if } \lambda \geq \lambda_c \\ \frac{\xi_0}{V} - \frac{c_2^2}{4c_4} + \frac{1}{2^D \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq q^{D-1} \sqrt{K_3 q^2 + 2|c_2|} & \text{if } \lambda < \lambda_c \end{cases} \quad (\text{E.25})$$

and its second derivative to the respect to  $\lambda$  (which is the analogous to the specific heat) is given by:

$$\frac{\partial^2}{\partial_x^2} P = \begin{cases} \frac{A^2}{2^{D+1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq q^{D-1} (K_3 q^2 + |c_2|)^{-\frac{3}{2}} & \text{if } \lambda > \lambda_c \\ \frac{A^2}{2c_4} \frac{A^2}{2^D \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^\Lambda dq q^{D-1} (K_3 q^2 + 2|c_2|)^{-\frac{3}{2}} & \text{if } \lambda < \lambda_c \end{cases} \quad (\text{E.26})$$

For the mean-field we have a discrete jump. Regarding the corrections, for high momenta the integrals have the following behavior:

$$\int_0^\Lambda dq q^{D-1} (q^2 + |c_2|)^{-\frac{3}{2}} \propto \Lambda^{D-3} \quad (\text{E.27})$$

which of course is not divergent. Divergences, if any, are at low momenta near the transition when  $|c_2| \rightarrow 0$ . To see when it happens, let us make a substitution in the integral, namely:

$$\tilde{q} = \begin{cases} \frac{q}{q_{ph}} & \text{if } \lambda > \lambda_c \\ \frac{q}{\sqrt{2}q_{ph}} & \text{if } \lambda < \lambda_c \end{cases} \quad (\text{E.28})$$

where  $q_{ph}$ , the typical scale in the momenta is given by:

$$q_{ph} = \sqrt{\frac{|c_2|}{K_3}} \quad (\text{E.29})$$

which leads to:

$$\frac{\partial^2}{\partial \lambda^2} P^{(G)} = \begin{cases} \frac{A^2 q_{ph}^{D-3} K_3^{\frac{1}{2}}}{2^{D+1} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\frac{\Lambda}{q_{ph}}} d\tilde{q} \tilde{q}^{D-1} (\tilde{q}^2 + 1)^{-\frac{3}{2}} & \text{if } \lambda > \lambda_c \\ \frac{A^2 q_{ph}^{D-3} K_3^{\frac{1}{2}}}{2^{\frac{D}{2}-\frac{3}{2}} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\frac{\Lambda}{q_{ph}}} d\tilde{q} \tilde{q}^{D-1} (\tilde{q}^2 + 1)^{-\frac{3}{2}} & \text{if } \lambda < \lambda_c \end{cases} \quad (\text{E.30})$$

Close to the transition we have  $q_{ph} \rightarrow 0$ . This means that for  $D < 3$  the theory predicts a divergence in the second derivative. Indeed, we proved that it is indeed the case for  $D = 2$  in Section 3.2. In the normalized units, the integrals now diverge for  $D \geq 3$ , but this divergence is dominated by the vanishing of  $q_{ph}$ . Hence, there is no divergence for  $D > 3$ . Similarly if we, instead, neglect the second order derivatives we have for the ordered phase<sup>3</sup>:

$$P^{(O)} = -\frac{\mathcal{E}_0}{V} + \frac{c_2^2}{4c_4} - \frac{1}{2(2\pi)^D} \int d^D q \sqrt{K_3 q^2 (K_3 q^2 + 2|c_2|)} \quad (\text{E.31})$$

By introducing a cut-off in the momenta, it is possible to find that the second derivative to the respect to  $x$  is given by:

$$\frac{\partial^2}{\partial \lambda^2} P^{(O)} = \frac{A^2}{2c_4} + \frac{A^2 q_{ph}^{D-2} K_3^{\frac{1}{2}}}{2^{\frac{D}{2}} \pi^{\frac{D}{2}} \Gamma(\frac{D}{2})} \int_0^{\frac{\Lambda}{\sqrt{2}q_{ph}}} d\tilde{q} \tilde{q}^D \sqrt{\tilde{q}^2 + 1} \quad (\text{E.32})$$

The mean-field, as usual, produces a jump discontinuity (the value of the second derivative for the disordered phase is zero.). We note that the contribution of the fluctuations is divergent for  $D < 2$ . Indeed, this confirms what we found in Section 3.3, where we have seen that for  $D = 1$  we had a divergence and for  $D = 3$ , instead, a finite result.

The results found are quite interesting. We have seen that, for the mean-field, the specific heat in the classical system has a jump discontinuity just like the quantum systems. If we include the fluctuations the specific heat has a divergence at the transition for  $D < 4$ . This is true, also, for the second derivative of the pressure for  $D < 3$  we can neglect  $K_1$  and for the ordered phase for  $D < 2$  when we can neglect  $K_2$ .

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<sup>3</sup>The fluctuations do not contribute for the ordered phase in this regime.

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