Bosons and Fermions in Mixed-dimensional Optical Lattices: Phase equilibria and Quantum Phase Transitions

A thesis submitted to the University of the Basque Country to obtain the degree of Doctor in Physics by

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-Disclaimer, in basque:

# Contents

Acknowledgements  
List of Figures  
List of Tables  
List of Symbols  

Introduction  

1 The physics of ultracold gases  
1.1 The atomic interaction  
1.2 Optical lattices  
1.2.1 The dipole force  
1.2.2 Periodic lattice potentials  
1.2.3 Negligible kinetic energy limit ("atomic limit")  
1.2.4 Tight binding approximation  
1.3 From lattices to sites  
1.3.1 The Bose-Hubbard model  
1.4 One dimensional systems  

2 Phase equilibria  
2.1 Introduction  
2.2 Model  
2.2.1 Bose-Fermi interaction: mean-field  
2.2.2 Zero-temperature free energy  
2.3 Phase diagram  
2.3.1 Mixed dimensions  
2.3.2 Pure 1D limit  
2.4 Conclusions and Outlook  

3 Superfluid to insulator transition in mixed dimensionality Bose-Fermi mixtures  
3.1 Introduction  
3.2 Basic model  
3.2.1 Hamiltonian  
3.2.2 Integrating out the fermions  
3.2.3 Low-energy effective theory  
3.3 Renormalization Group Analysis
3.3.1 Integer Lattice filling \hfill 70  
3.3.2 Half-Integer Lattice filling \hfill 71  
3.4 Commensurate - Incommensurate transition in the Presence of Dissipation \hfill 74  
3.4.1 Integer filling \hfill 74  
3.4.2 Half-integer filling \hfill 75  
3.5 Conclusions \hfill 75  

Appendices \hfill 81  

A Phase equilibria \hfill 81  
A.1 Mean-field approximation \hfill 81  
A.2 Character of the transitions for which the Fermi density changes \hfill 82  

B Superfluid to insulator transition in mixed dimensionality Bose-Fermi mixtures \hfill 87  
B.1 Relating $\chi_R^F(x,\omega)$ to $\chi_F(x,\tau)$ \hfill 87  
B.2 Fermion bath response function \hfill 88  
B.3 RG analysis at half-filling \hfill 94  
\hspace{1em} B.3.1 First order terms \hfill 96  
\hspace{1em} B.3.2 Second order terms \hfill 98  
B.4 SCHA \hfill 101  

Bibliography \hfill 109
List of Figures

1 Optical lattice vs Real crystal .......................... 17
1.1 Effective interatomic potential and partial waves .... 21
1.2 $s$-wave scattering length in a square well ........ 21
1.3 Optical lattice shapes ................................ 25
1.4 Periodic potentials in the "atomic limit" .......... 26
1.5 Band structure in optical lattices .................... 30
1.6 Phase diagram of the Bose-Hubbard model at T=0 .... 33
1.7 Bose-Hubbard depiction in an egg carton-like lattice . . 34
1.8 Schematic figure of the field $\hat{\phi}(x)$ .......... 35

2.1 Schematic representation of a mixed-dimensionality BF system 38
2.2 Phase diagram for the repulsive and attractive quasi-1D system 46
2.3 Phase diagram for the repulsive and attractive quasi-1D system in density space ..................... 49
2.4 Phase diagram for the repulsive and attractive 1D system . 51
2.5 Representation of the free energy in function of the boson density ........................................ 53
2.6 Phase diagram for the repulsive and attractive 1D system in density space ..................... 54

3.1 Schematic representation of the system ............. 58
3.2 A single tube depiction ................................ 64
3.3 Static response function ................................ 68
3.4 Imaginary part of the response function ........... 69
3.5 Phase diagram at half-filling ......................... 72
3.6 RG flow of the couplings $g_u$ and $g_D$ .......... 73
3.7 Mott gapp in the presence/absence of dissipation .... 74
3.8 Schematic phase diagram of a 1D Boson system embedded in a Fermi Gas ................................. 76
List of Tables

1.1 Hopping matrix elements to nearest neighbors $J$ and bandwidth $W$ in units of recoil energy $E_r$ for different potential depths. .............................................. 30
List of Tables
List of Symbols

- \( a_s \) : s-wave scattering length
- \( m_r \) : Reduced mass
- \( m_B \) : Mass of the bosonic atom
- \( m_F \) : Mass of the fermionic atom
- \( \lambda_T \) : de Broglie thermal wavelength
- \( R_0 \) : Spatial range of the interatomic potential
- \( E_B \) : Energy of the bound state
- \( E_{BE} \) : Binding energy
- \( g \) : Coupling constant
- \( d \) : Induced dipole moment
- \( \alpha(\omega) \) : Complex polarizability
- \( I(\mathbf{r}) \) : Field intensity
- \( \omega_0 \) : Characteristic oscillation frequency
- \( \Delta \) : Detuning
- \( V_0 \) : Maximum lattice potential depth
- \( E_r \) : Recoil energy
- \( k_L \) : Wavevector of the laser beam
- \( \lambda_L \) : Wavelength of the laser beam
- \( \omega \) : Quantum oscillator frequency
- \( \hat{n}_{j,n} \) : Number of particles operator on site \( j \) and energy level \( n \)
- \( \hat{b}_{j,n}^\dagger (\hat{b}_{j,n}) \) : Creation (and destruction) operators on site \( j \) and energy level \( n \)
- \( U \) : Interaction parameter
- \( \mathbf{k} \) : Bloch wavevector
- \( \mathbf{K} \) : Reciprocal lattice vector
- \( \psi_{n,k}(\mathbf{r}) \) : Bloch functions with pseudo-momentum \( k \) and band index \( n \)
- \( w_{n,R}(\mathbf{r}) \) : Wannier functions on site \( R \) and band index \( n \)
- \( j,t \) : Hopping parameter
- \( \varepsilon_n(\mathbf{k}) \) : Bloch band energy with band index \( n \)
- \( z \) : Number of nearest neighbor connections
- \( \hat{\phi}(x) \) : Labeling index in the harmonic fluid approach
- \( \phi(x) \) : Field that stands for the displacements of the particles from the exact crystalline lattice positions
- \( g_{\alpha,\beta} \) : Bose-Fermi interaction strength
- \( \varphi_{R}(\mathbf{r}_\perp) \) : Wannier functions on site \( R \) in the lowest band
- \( g_{1D}^{BB} \) : One-dimensional boson coupling
- \( \mu_{BB}^{1D} \) : One-dimensional boson chemical potential
- \( \phi_{k_\perp}(\mathbf{r}_\perp) \) : Lowest Bloch band function for fermions
- \( \varepsilon(\mathbf{k}) \) : Fermion dispersion
- \( H^{mf} \) : Mean-field Hamiltonian
\( f \) : Free energy potential
\( e(\gamma) \) : Dimensionless function related to the
  ground state energy obtained by the Bethe ansatz
\( \Omega \) : Thermodynamic grand canonical free energy
\( V_{BB}(r) \) : Boson interaction potential
\( Z \) : Partition function
\( S \) : Effective action of the system
\( A, B_m \) : Amplitudes that depend on the microscopic details of the model
\( \chi_F(r, r', \tau) \) : Density response function
\( \chi_F(x - x', \tau) \) : Fermion density correlation function
\( \chi_F^R(x - x', \omega) \) : Retarded fermion density correlation function
\( \Gamma(x - x', \tau) \) : Dissipative kernel
\( g_u, g_{uD}, g_{bD}, g_D \ldots \) : Dimensionless couplings
\( l \) : Constant as a function of logarithm the ratio between
  the system cut-off and the temperature
\( \eta, \Delta \) : Dimensionless self-consistent parameters in the SCHA
Introduction

The experimental achievement of Bose-Einstein condensation (BEC) in 1995 [1–3] opened the gates to a qualitatively new regime of exploration. An exceptional way of investigating quantum phenomena in a macroscopic scale was facilitated, following Bose and Einstein’s prediction that a gas of non-interacting bosonic atoms would, below a certain condensation temperature, develop a macroscopic population in the lowest energy quantum mechanical state. Certain physical systems were already known for exhibiting striking properties related to quantum degeneracy, such as superfluidity in helium ($^4$He). However, in a superfluid liquid of $^4$He, bosons are so constricted that the interaction between the helium atoms is very strong, thus making it difficult to obtain detailed properties of the macroscopic quantum state and allowing only a small fraction of the particles to occupy the Bose condensed state.

It took 70 years to experimentally realize BEC in dilute gases of alkali atoms, and it implied the development of powerful methods such as laser cooling and evaporative cooling. This was required in order to observe quantum phenomena in trapped alkali atomic clouds with a typical particle density of $10^{13}$–$10^{15}$ cm$^{-3}$ - in contrast to the density of molecules in air at room temperature and atmospheric pressure which is about $10^{19}$ cm$^{-3}$ - it is necessary to cool the atomic cloud down to temperatures of the order of $10^{-5}$ K or less [4].

For many years, the main focus in the field of cold atoms had been the exploration of the wealth of phenomena associated with the existence of coherent matter waves. Typically, condensates were confined to featureless magnetic traps, and the experiments were mainly aimed at demonstrating the macroscopic quantum coherence in these new physical systems.

Nevertheless, two fundamental advances would be needed so that the range of physical phenomena that were accessible with ultracold gases would definitely expand: the possibility of changing the dimensionality with optical and magnetic potentials and, in particular, of generating strong periodic potentials for cold atoms using optical lattices and the ability to tune the interaction strength in cold gases by Feshbach resonances. These two developments, either individually or in combination, have allowed to enter a regime in which the interactions even in extremely dilute gases can no longer be described by a picture based on non-interacting quasiparticles. The appearance of such phenomena is characteristic of the physics of strongly correlated systems. For a long time, this area of research was confined to the study of quantum liquids as Helium, electrons in solids, or the nuclear matter in heavy nuclei and neutron stars. By contrast, gases - almost by definition -
were never thought to exhibit strong correlations. Thus, it was found that loading ultracold atoms into versatile light traps, such as the optical lattices mentioned above, atomic wave functions could exhibit strongly correlated behavior. An exceptional example of this was the realization of a quantum phase transition from a superfluid to a Mott-insulating state by loading a BEC into an optical lattice and increasing its depth [5, 6].

Furthermore, in general, an optical lattice gives the opportunity to increase control over system parameters allowing us to explore a whole range of fundamental phenomena that would be extremely difficult - or impossible - to study in a real material, as well as giving the possibility of matching better with the model in question. Ultracold quantum gases in optical lattices could in fact be considered as quantum simulators, in a similar way to Feynman’s conception of a quantum computer: a powerful simulator in which a highly controllable quantum system could be used to simulate the dynamical behaviour of another complex quantum system [7].

An illustrative example would be that of the crystal lattice of a solid. Its small dimensions - the interatomic spacing is of the order of 1Å-, the fact that it involves a band structure that has to be determined, the difficulty to account for the Coulomb interactions of the electrons and the existence of disorder in addition to lattice vibrations impede a proper description of the real system. An optical lattice allows us to obtain an enlarged - and simplified - version of the actual system: it is a crystal formed by interfering counter-propagating laser beams, with a typical dimension about 1,000 times larger than that of a conventional crystal - in the order of 100 nm-. Here, ultracold atoms in the lattice play the role of electrons in the solid; they tunnel quantum-mechanically between lattice sites just as single or paired electrons (Cooper pairs) tunnel through the periodic potential wells created by positive ions in crystalline materials.

With the feasibility of changing the dimensionality of the system through optical lattices, further directions in the regime of strong correlations were opened with the suggestions of realizing interacting boson systems confined in one dimension [9, 10], as strong correlations play a dominant role in low-dimensional systems. Moreover, the possibility of achieving a Luttinger liquid with cold fermionic atoms was pointed out too [11], with the subsequent prospect of analyzing spin-charge separation. Even the realization of a rapidly-rotating two dimensional BEC, where the physics resembles that of fractional quantum Hall effect [12].

The ability to tune the interaction strength in cold gases by Feshbach resonances turned out to be indispensable in order to achieve Fermi degeneracy in trapped ultracold dilute gases [13–15] shortly after BEC was first realized. These degenerate clouds of fermionic atoms were applied to investigation into the crossover between Bardeen-Cooper-Schrieffer superfluidity and Bose-Einstein condensation (BCS-BEC crossover). Here, as superfluids are fundamentally associated with the quantum statistical properties of
bosons, pairing in the Fermi gas of atoms happens to be crucial. Thus, two ways of pairing are manifest, one is a two-body bound state of two fermions, forming a composite boson and the other one is Cooper pairing. As the interaction between fermions is increased a continual change, or crossover, happens between a BCS state and a BEC of diatomic molecules [16].

Nonetheless, it was observed that new insights could be attained by mixing bosonic and fermionic species. The possibility of sympathetic cooling of fermions with bosons has lead to several recent experiments on trapped ultracold Bose-Fermi mixtures. Although the main goal of these experiments was, in principle, to achieve the previously mentioned BCS transition in atomic Fermi gases, a growing interest has arisen towards the physics of ultracold Bose-Fermi mixtures themselves, including the analysis of the ground-state properties, stability, excitations, and the effective fermion-fermion interaction mediated by the bosons.

Lately, the attention has been brought towards the behavior of these mixtures in optical lattices [17] and lower dimensional geometries [18]. Bose-Fermi mixtures in analogous setups to the ones used for bosonic atoms loaded into an optical lattice in order to observe the quantum phase transition from a superfluid to a Mott insulator [6] -as mentioned before-, manifest a much
more complex and richer behavior at low temperatures.
1 The physics of ultracold gases

1.1 The atomic interaction

A general approach to dilute ultracold atomic gases consists in treating them in such a way that, as we can assume from the word \textit{dilute}, there is a large mean inter-particle distance. This regime can be more specifically characterized by the condition that the atomic de Broglie thermal wavelength \( \lambda_T = \sqrt{\hbar^2/2\pi mk_B T} \) is much larger than the spatial range \( R_0 \) of the inter-atomic potential, i.e. \( \lambda_T \gg R_0 \). In addition to this, being in the ultracold regime also implies that the typical atomic momentum fulfills the condition \( kR_0 \ll 1 \), the importance of which will become manifest later on.

It is common to study the behavior of the interactions in these systems by first understanding the few-body problem, and more specifically, as it comprises most of the relevant results, by the two-body problem, i.e. understanding the scattering process in two-body collisions. As it is known from scattering theory \cite{19, 20} the time-independent scattering processes take the Lippman-Schwinger equation as a starting point, leading to the result in the asymptotic limit (\(|r| \gg R_0\)) for the relative-motion wave function or collision state:

\[
\psi_k(r) \propto e^{ikr} + f(k, n, n') e^{ikr}/r,
\]

(1.1)

where \( n = k/k \) and \( n' = r/r \). In this form, we can understand the \textit{collision state} as the superposition of the original incident plane wave propagating in direction \( n \) with momentum \( k \) and of an outgoing scattered spherical wave function with an amplitude \( f(k, n, n') \). The definition of this amplitude can be found in e.g. \cite{19}, however, here it will only be noted that its relation to the differential cross-section is given by \( d\sigma/d\Omega = |f(k, n, n')|^2 \).

Nevertheless, everything is considerably simplified when dealing with an isotropic (i.e. spherically symmetric) potential \( V(r) = V(r) \). In order to take advantage of this symmetry, we employ the partial wave decomposition. Taking into account that as the free-particle Hamiltonian is just the kinetic energy term that commutes with the (relative) angular momentum operator, we can thus expand the \textit{collision state} wave function in the basis set of
Chapter 1. The physics of ultracold gases

eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$, such that:

$$\psi_k(r) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\theta, \phi) \frac{u_l(r)}{r}, \quad (1.2)$$

where $\phi$ is the azimuthal angle around the $z$ axis and the $Y_l^m(\theta, \phi)$ are the spherical harmonic functions. $u_l(r)/r$ is the radial wave-function which obeys the radial 1D-Schrödinger equation for the relative motion:

$$\left[ -\frac{\hbar^2}{2m_r} \frac{d^2}{dr^2} + V(r) + \frac{l(l+1)}{r^2} - \frac{k^2}{2m_r} \right] u_l(r) = 0 \quad (1.3)$$

In the asymptotic limit ($|r| \gg R_0$) the collision state can be written in such a way following the partial wave expansion:

$$\psi_k(r) \propto \frac{1}{2ikr} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta)((-1)^{l+1}e^{-ikr} + e^{2i\delta_l}e^{ikr}), \quad (1.4)$$

where $P_l(\cos \theta)$ are the Legendre polynomials and the coefficients $e^{2i\delta_l}$ have a modulus equal to 1, i.e. the phase shifts $\delta_l$ (defined here modulo $\pi$) are real.

Nonetheless, it is at low energies where the utility of the partial wave expansion becomes clear. In this situation, as long as the potential decreases fast enough at infinity, the scattering process is isotropic, a condition that is described by the aforementioned $kR_0 \ll 1$, or equivalently, $E \ll \hbar^2/(2m_rR_0)$. Furthermore, we can assume qualitatively that the scattering mediated by the interatomic potential $V(r)$ goes to zero for all partial waves but $l = 0$ at sufficiently low energy, that is, we should only consider the $s$-wave scattering. This can be seen in Fig. 1.1, where for low energies and $l > 0$, the effective potential $V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2m_r r^2}$ becomes insurmountable.

It is reasonable to think that, although it is notably different from a realistic interatomic potential, the square well is a useful rudimentary model as many of its features are common to more complicated finite range potentials. Thus, in the low energy regime it is enough to deal with the $s$-wave scattering and to look at the behavior of the radial wave function. The shape of the latter can be fixed by solving the modified radial 1D-Schrödinger equation, which for small momenta ($k \approx 0$) and $r > R_0$ is given by $d^2u/dr^2 = 0 \to u(r) \propto (r - a_s)$. Considering that the outside wave function has to behave like $u(r)/r = \frac{\sin(kr + \delta_0)}{kr}$ as it can be deduced from the hard-sphere scattering [19], leads to $\lim_{k \to 0} k \cot \delta_0 \to -1/a_s$, where the quantity $a_s$ is defined as the s-wave scattering length. The physical meaning of $a_s$ is the intercept of the $r$ axis (see Fig. 1.2) of the outside asymptotic wave-function.
1.1 The atomic interaction

Figure 1.1: The effective interatomic potential for \( l = 0 \) in green and higher values of \( l \) in red. An incident energy equal to \( E \) (blue) is not enough to overcome the centrifugal barrier \( \hbar^2 l(l+1)/(2m_r r^2) \) when \( l > 0 \).

Figure 1.2: The shape of the radial wave function times \( r \) in green shows a change in magnitude and sign of the scattering lengths, reflected in the intercept of the \( r \) axis depending on the depth of the square well, which is deeper in \( b \) than in \( a \). The blue dashed line accounts for the asymptotic behavior of \( u(r) \), while the red horizontal line shows the energy level of a bound state of energy \( E_B = -\hbar^2/(2m_r a_s^2) \).

Even though \( a_s \) has the same dimensions as the range of the interatomic potential \( R_0 \), they may differ by orders of magnitude. In particular, for an attractive potential, the magnitude of the scattering length can be much greater than the range of the potential. For a shallow attractive potential, for example, we can expect the intercept to be on the negative side (see Fig. 1.2(a)). However, if the depth of the potential is increased, the asymptote of the curve of the wave function can again cross the \( r \) axis on the positive side. This sign change is related to the development of a bound state (see Fig. 1.2(b)), the energy of which can be determined to be \( E_B = -\hbar^2/(2m_r a_s^2) \). Note that it is also reasonable to define the binding energy from the opposite perspective, \( E_{BE} = \hbar^2/(2m_r a_s^2) \), with the opposite sign.
Of course, interactions between atoms have a complex form and it is not an easy task to determine the interatomic potential precisely. Nevertheless, they can be characterized by two main factors: on the one hand, there is the strong repulsion that happens at short distances due to the overlap of the electron clouds that surround the nuclei, and on the other hand, the van der Waals attractive interaction at larger atomic separations:

\[ V(r) = \begin{cases} +\infty & \text{if } r < R_0 \\ -C_6/r^6 & \text{if } r \geq R_0 \end{cases} \]  

where \( C_6 \) is a constant coefficient. The scattering properties of such an interatomic potential can be elucidated following the above explained partial wave expansion due to its relative simplicity and isotropy.

However, from the two-body viewpoint, all short range potentials are equivalent as long as they have the same scattering length [21]. This convenient characteristic becomes crucial for simplifying the representation of the scattering processes, as we can use an idealized zero-range potential (pseudo-potential) that shares the same scattering length as a more elaborate interatomic potential. Thus, it is common to describe atomic interactions by a Lee-Huang-Yang contact pseudo-potential [22–25]:

\[ V(r) \approx g\delta(r)\partial_r(r) \]  

where \( g \) is a coupling constant related to the \( s \)-wave scattering length \( a_s \) by \( g = 2\pi\hbar^2 a_s/m_r \). Note that this relation is often written in function of the atomic mass \( m \) instead of the reduced mass \( m_r \) of the two-body problem by \( g = 4\pi\hbar^2 a_s/m \). Hence, this potential has a range \( R_0 = 0 \), and a scattering amplitude given by \( f(k) = -1/(a_s^{-1} + ik) \). Moreover, in a similar way as for the square well potential it has a bound state with the binding energy \( E_{BE} = \hbar^2/(2m_r a_s^2) \). The differential operator \( \partial_r(r) \) is placed to eliminate the singular \( 1/r \) short-range behavior of the wave function \( u_l(r)/r \) [20, 25].

This contact potential is useful in a wide range of systems, describing the weakly interacting BEC [22, 26], the BCS-BEC crossover in fermionic mixtures [25], as well as many other systems loaded in optical lattices as the ones that will be studied in the next chapters.

1.2 Optical lattices

In order to trap neutral atoms at very low temperatures we rely on the use of different approaches and techniques, discarding the most disadvantageous ones in favor of the optical dipole trapping that will be explained in detail below. Charged atoms will be left aside as they usually require different procedures due to their Coulomb interaction and other specific properties of ion traps.
On the one hand, radiation-pressure traps [27, 28] were used for this purpose, however, the lowest attainable temperature was limited because of the photon recoil and the achievable density was reduced due to light-assisted inelastic collisions.

And on the other hand, magnetic traps [29, 30] were also explored, which seem to be ideal for Bose-Einstein condensation experiments. But the arrangement of coils and magnets that are necessary restrict considerably the range of geometries that can be studied with these traps.

However, it should be noted that none of these methods have been abandoned, but are often complementary to the nowadays prevalent optical dipole trapping. In the latter, many disadvantages of the previously mentioned methods are overridden, and optical excitations can be kept low as well as having the possibility of realizing highly anisotropic or multi-well potentials.

From a historical perspective, the feasibility of using optical dipole forces as a confining mechanism in a so called dipole trap, was first considered by Askar’yan in 1962. However, the real possibility of trapping atoms with this forces was considered by Letokhov (1968), but it took 18 years from this for the first realization of an optical trap for neutral atoms by S. Chu [31].

### 1.2.1 The dipole force

The optical dipole force arises from the interaction between the atomic dipole moment induced on the atom and the intensity gradient of the light field. That is, the electron cloud surrounding the atom and the protons in the nucleus under an inhomogeneous light field experience an alternating electric field gradient, which induces a dipole moment $d$ that oscillates at the driving frequency $\omega$. The latter can be assumed from the description of the applied electric field in the usual complex notation $E(r, t) = E(r)e^{-i\omega t}\hat{n} + c.c.$ and $p(r, t) = d(r)e^{-i\omega t}\hat{n} + c.c.$, where $\hat{n}$ is the unit polarization vector. Furthermore, the amplitude of the dipole moment and the electric field amplitude are related by $d = \alpha(\omega)E$, where $\alpha$ is the complex polarizability. As it is usual in the theory of electromagnetism, the interaction potential resulting from the induced dipole moment and the electric field is given by:

$$V_{dip}(r) = -(1/2)\langle d \cdot E \rangle = -\frac{1}{2\varepsilon_0 c} \text{Re}[\alpha(\omega)] I(r),$$

where the angular brackets denote the time average over the rapid oscillating terms, the field intensity is $I = 2\varepsilon_0 |E|^2$, and the factor $1/2$ is related to the fact that the dipole moment is an induced, not a permanent one. Because of its conservative character, we can derive the force from the gradient of the potential, and thus the dipole force can be written as:

$$F_{dip}(r) = -\nabla V_{dip}(r) = \frac{1}{2\varepsilon_0 c} \text{Re}[\alpha(\omega)] \nabla I(r).$$

(1.7)
Thus, the calculation of the polarizability is only left. The simplest way to do this is by considering the atom in Lorentz’s model of a classical oscillator, where in this picture an electron (here to be the valence electron when dealing with alkali atoms) is considered to be bound to the nucleus with a characteristic oscillation frequency $\omega_0$. From this, inserting the obtained polarizability [32] it is possible to rewrite the interaction potential and the dipole force:

$$V_{\text{dip}}(r) = -\frac{3\pi e^2}{2\omega_0^3} \left( \frac{\Gamma}{\omega_0 - \omega} + \frac{\Gamma}{\omega + \omega_0} \right) |I(r)| \ll \omega_0 \approx 3\pi e^2 \frac{\Gamma}{2\omega_0} |\Delta I(r)|,$$  \hspace{1cm} (1.9)

where $\Gamma$ is the damping rate on resonance. The last part of the equation is a valid approximation when the laser is tuned close enough to the resonance, such that the detuning $\Delta \equiv \omega - \omega_0$ is small enough in comparison to the characteristic frequency $\omega_0$. We can also deduce from here that if the detuning is small the complex polarizability $\alpha(\omega)$ becomes big. However, the phase with which the induced dipole moment oscillates does not necessarily coincide with the phase of the electric field. For red-detuned lasers ($\Delta < 0$) the dipole potential is negative and the interaction thus attracts atoms into the light field, so that potential minima are therefore found at positions with maximum intensity. On the contrary, for blue-detuned lasers ($\Delta > 0$) the positive dipole interaction repels atoms out of the field, and potential minima correspond to minima of the intensity.

### 1.2.2 Periodic lattice potentials

A lattice potential that consists of a periodic dipole trap array can be realized by making two coherent laser beams propagating in opposite directions interfere with each other. This is usually realized by retro-reflecting a Gaussian laser beam so that the interfering counterpropagating beams create a standing wave pattern. This results in a trapping potential of the form:

$$V(r, z) \simeq -V_0 e^{-2r^2/\omega^2} \sin^2(k_L z) $$  \hspace{1cm} (1.10)

where $k_L = 2\pi/\lambda_L$ is the wavevector associated with the lattice laser wavelength $\lambda_L$, corresponding to a lattice period $a = (2\pi/k_L)/2 = \pi/k_L = \lambda_L/2$. The $1/2$ factor comes from the fact that we have two counterpropagating lasers. $\omega$ represents the waist of the beam i.e. the radius at which the intensity has dropped of to $1/e^2$ of its maximum value. And $V_0$ stands for the maximum lattice potential depth, usually given in units of the recoil energy $E_r = \hbar^2 k_L^2 / 2m$ (m being the mass of a single neutral atom), which is a natural energy scale for neutral atoms in periodic optical lattices. The potential depth $V_0$ is four times higher than what is shown in Eq. (1.9) for a running wave trap. This due to the fact that the constructive interference doubles the intensity of the laser beam [33].
1.2 Optical lattices

Figure 1.3: A setup of two standing waves placed orthogonally can tightly confine the atoms into 1D cigar-like tubes. (Although, neglecting the harmonic confinement, they are often considered infinite in the longitudinal direction.) Whereas, three orthogonal standing waves can create a simple cubic array of isotropic traps at each lattice site. [34].

Consequently, we can expand the arrangement of retro-reflecting laser beams. Thus, two orthogonal optical standing waves can create an array of 1D potential tubes (see figure 1.3(a)), in which the atoms can only move along the confining axis of the potential tube, thus realizing a 1D quantum behavior, with the radial motion being completely frozen out for low-enough temperatures i.e when \( \omega \) is big enough. Whereas three orthogonal optical standing waves would correspond to a 3D simple cubic crystal (see figure 1.3(b)), in which each trapping site acts as a tightly confining harmonic oscillator potential. It should be noted that, these setups may lead to unwanted cross-interferences between the orthogonal standing waves, however, this is usually avoided by choosing orthogonal polarization vectors or by using slightly different wavelengths for the three standing waves.

It is of particular interest a geometry for the optical lattice that lays between both configurations, as it will be studied throughout the following chapters. It consists of a very anisotropic three-dimensional lattice of the following shape:

\[
V(r) = V(x, y, z) = V_{0\parallel} \sin^2 k_L x + V_{0\perp} (\sin^2 k_L y + \sin^2 k_L z) \tag{1.11}
\]

where the potential depth in the perpendicular \( y \) and \( z \) directions is much bigger than along the longitudinal \( x \) direction (\( V_{0\perp} \gg V_{0\parallel} \)).
1.2.3 Negligible kinetic energy limit ("atomic limit")

The limit of considering a very deep optical potential is of special interest. In this situation, the kinetic energy of the particles trapped in the minima of the potential can be considered irrelevant. That is, the particles will remain mostly localized around one of the minima of the potential (see Fig. 1.4). More precisely, the overlap between the wavefunctions localized in neighboring sites decreases. This limit is often called the "atomic limit" in concordance to the condensed matter context, where the particles are considered to stay localized around the "atoms" or discrete units. Therefore, the usual sinusoidal expression for the optical lattice created by standing waves is no longer necessary and we can approximate each minimum by a harmonic potential that results from the series expansion \( V(x) = V_0 \sin^2(kx) \) (in one-dimension). Thus, the system can be studied in analogy to the 1D quantum harmonic oscillator problem, by solving around each minimum the Schrödinger equation:

\[
\frac{-\hbar^2}{2m} \frac{d^2\psi_{j,n}}{dx^2} + V_0k_L^2x^2\psi_{j,n} = E\psi_{j,n},
\]

where \( \psi_{j,n}(x) = \psi_{j,n}(x - x_j) \), with \( x_j = aj \), being \( a \) the separation between the minima, the lattice period. And \( n \) refers to the \( n \)th energy level following with the comparison to the quantum oscillator, as it can be seen with \( \frac{1}{2}m\omega^2x^2 = V_0k_L^2x^2 \):

\[
E = \hbar\omega(n + \frac{1}{2}), \quad \omega = \sqrt{\frac{2k_L^2V_0}{m}}
\]
This can also be described by using the second quantization representation [35] and by introducing the common creation (and destruction) operators \( \hat{b}_{j,n}^{\dagger} \) (\( \hat{b}_{j,n} \)), so that it is possible to write the Hamiltonian in the “atomic limit”:

\[
\hat{H} = \sum_{j,n} \hbar \omega (n + \frac{1}{2}) \hat{b}_{j,n}^{\dagger} \hat{b}_{j,n}. \tag{1.14}
\]

The assumption that wavefunctions do not overlap, which justifies the fact that in the second order representation interaction can only involve operators on a given site, can be seen more rigorously by resorting to the groundstate wavefunction of the harmonic oscillator: \( \psi_0(x) = \left( \frac{m \omega / (\pi \hbar)}{\sqrt{\pi}} \right)^{1/4} e^{-\frac{m \omega}{2 \hbar} x^2} \).

As the width of the Gaussian (the standard deviation) is defined by \( c = \sqrt{\hbar/(m \omega)} \propto V_0^{1/4} \) with Eq. (1.13) it can be expected that a deep potential may easily result in a regime where the range of the wavefunction probability is much smaller that the intersite (i.e. interminima) distance \( a \) (see Fig. 1.4).

In addition to this, it is meaningful to look at the hypothetical situation where two particles were coinciding on the same site. For this, it can be adopted the simple contact interaction model that in Eq. (1.6) and then extend the expression for the groundstate wavefunction to the three-dimensional case for completeness. Thus, we obtain that the energy cost of having two-particles in the same site is:

\[
U = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 U(\mathbf{r}_1 - \mathbf{r}_2)|\psi_0(\mathbf{r}_1)|^2 |\psi_0(\mathbf{r}_2)|^2 = \frac{g}{2\sqrt{2}} (\sqrt{m \omega \hbar \pi})^{3/2} \tag{1.15}
\]

And the interaction term of the Hamiltonian can thus be written in such a form:

\[
\hat{H}_{int} = \frac{U}{2} \sum_{j} \hat{n}_{j,0}^{\dagger} (\hat{n}_{j,0}^{\dagger} - 1), \tag{1.16}
\]

where \( \hat{n}_{j,0}^{\dagger} \) is the number of particles operator, for the site \( j \) and always in the groundstate \( n = 0 \). At this point, it should be remarked that, as we are dealing with the groundstate of the harmonic potential only, the previous considerations are solely valid when the temperature is smaller that the magnitude of the quantum oscillator interlevel separation \( T \ll \omega \). But also the interaction parameter \( U \) has to be much smaller than \( \omega \) (i.e. \( U \ll \omega \)), as in the contrary, interlevel transitions would be favorable to the on-site interaction that is being described.

### 1.2.4 Tight binding approximation

The previous limit where the more general optical lattice potential is replaced by a harmonic potential is an oversimplification, the constraints of which, can be surpassed by considering that there is some (non-zero) overlap between the wavefunctions on different sites. Namely, tunneling is possible
between neighboring sites and the kinetic energy of the atoms is not restricted to zero.

However, it is interesting not to leave aside the fact that the wavefunctions are highly localized, together with the fact that the optical lattice is periodic. Taking into account the latter, based only in the periodicity of the lattice as a prerequisite, Bloch functions become suitable as they are exact eigenstates of these systems. Bloch’s well known theorem states that the energy eigenfunction for a periodic system may be written as the product of a plane wave envelope function and a periodic function \( u_{n,k}(r) = u_{n,k}(r + R) \), such that we have the following expression for the Bloch functions:

\[
\psi_{n,k}(r) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,k}(r),
\]

and as a consequence, the corresponding energy eigenvalues \( \varepsilon_n(k) = \varepsilon_n(k + K) \) are periodic with a periodicity \( K \), where \( K \) is the reciprocal lattice vector.

On the other hand, considering the localization of the wavefunctions in our system, although it is not a necessary requirement for this, we can take advantage of the Wannier functions for the tight binding representation. Wannier functions \( w_{n,R}(r) = w_n(r - R) \) are connected to Bloch functions by a Fourier transform, and are characterized by a discrete band index \( n \) (not a mere energy level anymore as before) and a pseudo-momentum \( k \) within the first Brillouin zone of the reciprocal lattice [33, 36]):

\[
\psi_{n,k}(r) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} w_n(r - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad w_n(r - \mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \psi_{n,k}(r) e^{-i\mathbf{k} \cdot \mathbf{R}}.
\]

They are thus appropriate as they depend only on the relative distance \( r - \mathbf{R} \), and, at least for the lowest bands where their profile is still localized around the periodic minima, they can be regarded as being centered around the lattice sites \( \mathbf{R} \). Note that \( x_j \) sites previously introduced in one-dimension have now been replaced by the more general \( \mathbf{R} = (m,n,l)\lambda_L/2 \). These Wannier functions form a complete orthonormal basis and can be used to expand the field operator \( \hat{\psi}(r) \) which destroys a particle in the position \( r \). Therefore,

\[
\hat{\psi}(r) = \sum_{n,\mathbf{R}} w_n(r - \mathbf{R}) \hat{a}_{n,\mathbf{R}},
\]

where \( \hat{a}_{n,\mathbf{R}} \) is the annihilation operator for particles in the corresponding Wannier states. With the help of this representation we can now write the kinetic energy part of the Hamiltonian that was suppressed in the ”atomic limit” in Sec. (1.2.3), in this form:

\[
\hat{H}_{\text{kin}} = \sum_{n,\mathbf{R},\mathbf{R}'} J_n(\mathbf{R} - \mathbf{R}') \hat{a}^\dagger_{n,\mathbf{R}} \hat{a}_{n,\mathbf{R}'},
\]

here, \( J_n(\mathbf{R} - \mathbf{R}') \) stands for the hopping parameter between arbitrary \( \mathbf{R},\mathbf{R}' \) lattice sites. It is worth noting that the diagonalization of this Hamiltonian
through Bloch states shows that the hopping matrix elements $J_n(R)$ are uniquely determined by the Bloch band energies $\varepsilon_n(k)$ via [33]:

$$\varepsilon_n(k) = \sum_{R} J_n(R)e^{ikR}$$

(1.21)

It is specially illustrative to show the band structure that can be obtained for an optical lattice potential with a $V(x) = V_0\sin^2(k_Lx)$ shape (in one-dimension for simplicity) by following the above explained methodology.

Bearing in mind that the periodic potential and $u_{n,k}(x)$ share the same periodicity by Bloch’s theorem, a Fourier expansion can be performed on them so that:

$$V(x) = \sum_{m} V_m e^{i2mqx}, \quad u_{n,k}(x) = \sum_{l} c_{l,n,k} e^{i2lqx},$$

(1.22)

where $m$ and $l$ are integers. And, furthermore, as the optical potential can be rewritten as:

$$V(x) = V_0\sin^2(k_Lx) = \frac{V_0}{4}(2 - e^{2iqx} - e^{-2iqx})$$

(1.23)

which inserting into the Schrödinger equation for the periodic function $\hat{H}u_{n,k}(x) = E_n,k u_{n,k}(x)$, with $\hat{H} = \hbar^2/(2m)\nabla + V_0\sin^2(k_Lx)$ results in:

$$\sum_{l} e^{i(k+2lx)} \left[ \left( \frac{(k + 2lhq)^2}{2m} - \varepsilon_{n,k} \right) c_{l,n,k} + \sum_{m} V_m c_{l-m,n,k} \right] = 0.$$ 

(1.24)

Solving these system of equations independently, as each term in the sum must be zero, enables the calculation of the energy bands. (See figure 1.5).

From the eigenvalue equation $\varepsilon_{n,k} = -2J\cos(ka)$ we can find that the $4J$ is the height (named as width, $W$) of the lowest Bloch band [5]. However, there is a simpler analytical expression for calculating the hopping parameter in the deep potential limit. It can be obtained from the width $W$ of the lowest band by in the 1D Mathieu equation [33]:

$$J \simeq \frac{4 \sqrt{\pi}}{V_0} \frac{E_r}{E_r^{3/4}} e^{-2\sqrt{V_0/E_r}}$$

(1.25)

(See table 1.1 for comparisons).

1.3 From lattices to sites

As a starting point, it will be introduced the most general possible Hamiltonian for a system of $N$ bosons in 1D interacting through a generic two-body potential $V_{int}$ and under the influence of a general external potential $V_{ext}$, without giving any specifications. Bosons will be considered only here as in
Chapter 1. The physics of ultracold gases

Figure 1.5: Band structure of a one-dimensional system under a periodic potential with a depth such that \( V_0 = 3E_r \).

the next chapters they will be strictly confined to effective one-dimensional tubes. However, many of the results will be of general importance, because the quantum statistics of the atoms in these systems is less relevant in 1D, in comparison to higher dimensions.

\[
\hat{H} = \sum_{i=1}^{N} \left[ \frac{\hat{p}_i}{2m} + V_{\text{ext}}(\hat{x}_i) \right] + \sum_{i<j=1}^{N} V_{\text{int}}(\hat{x}_i - \hat{x}_j)
\]  

(1.26)

where \( \hat{p}_i = -i\hbar(\partial/\partial x_i) \) is the momentum operator for the \( i \)th particle.

<table>
<thead>
<tr>
<th>( V_0/E_r )</th>
<th>( J/E_r ) approx.</th>
<th>( J/E_r ) fitting to cosine</th>
<th>( W/E_r ) by the author</th>
<th>( J/E_r ) by M. Holthaus</th>
<th>( W/E_r ) by M. Holthaus</th>
</tr>
</thead>
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</tr>
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<td>0.00185154</td>
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<td>—</td>
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</tbody>
</table>

Table 1.1: Hopping matrix elements to nearest neighbors \( J \) and bandwidth \( W \) in units of recoil energy \( E_r \) for different potential depths. The data by M. Holthaus [33] shown in the table for comparison coincides almost exactly with the calculations obtained by the author when the width \( W \) is calculated without approximations.
1.3 From lattices to sites

Or equivalently by:

\[ \hat{H} = \frac{\hbar^2}{2m} \int dx \partial_x \hat{\psi}^\dagger(x) \partial_x \hat{\psi}(x) + \int dx \hat{V}_{\text{ext}}(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \]
\[ + \frac{1}{2} \int dx \int dx' \hat{\psi}^\dagger(x) \hat{\psi}(x) V(x - x') \hat{\psi}^\dagger(x') \hat{\psi}(x') \]  
(1.27)

First of all, following the path taken in the previous chapter, we can focus on treating the external potential as given by an optical lattice. Moreover, the habitually regarded situation where the particles are under the presence of a deep potential can lead to simplified expressions that are common to some interesting models already studied. Or from the opposite perspective, some rich models that have been long studied can be characterized by a rather simple (although general) Hamiltonian (Eq. (1.26)) with an external potential described by an optical lattice.

Thus, with a deep lattice potential (see Sec. (1.2.4)) we can make the assumption that the Wannier orbitals in the lowest Bloch band are enough to describe the field operators in a system with such characteristics. More accurately, the following conditions must be fulfilled: a) both the thermal and mean interaction energies at a single site are much smaller than the separation \( \omega \) to the first excited band, that is, \( V_0 \) is the largest energy scale in the problem; and b) the Wannier functions decay essentially within a single lattice constant. With this, we could try a projected field operator such that:

\[ \hat{\psi}(x) \approx \sum_{i=1}^{L} w_0(x - x_i) \hat{b}_i \]  
(1.28)

with \( x_i = ai \), being \( a \) the lattice constant. Note that this is nothing but Eq. (1.19) in one-dimension. Inserting this projected field operator in the general Hamiltonian in Eq. (1.27) we obtain the following simplified expression:

\[ \hat{H} = \sum_{i,j=1}^{L} \left[ - t_{i,j} \hat{b}^\dagger_i \hat{b}_j + \sum_{k,l=1}^{L} V_{\text{int}}^i_{j,k,l} \hat{b}_i^\dagger \hat{b}_k \hat{b}_j \right] \]  
(1.29)

where the interlatice hopping paramter is given by \( t_{i,j} = -\int dx w_0^*(x - x_i)(\hbar^2/2m) \partial_x^2 + V_{\text{ext}}(x) w_0(x - x_j) \) and the interaction parameter is defined by \( V_{\text{int}}^i_{j,k,l} = \int dx dx' w_0^*(x - x_i) w_0^*(x - x_k) V_{\text{int}}(x - x') w_0(x - x_j) w_0(x - x_l) \). Furthermore, if the aforementioned overlap between adjacent Wannier orbitals is allowed to be finite but very small, as it is for deep potentials, we obtain the Extended Bose-Hubbard model (EBHM). Here, hopping is only permitted between neighboring sites:

\[ \hat{H}_{\text{EBHM}} = \sum_{i=1}^{L} \left[ - t (\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}) - \mu \hat{n}_i + \frac{U}{2} \hat{b}_i^\dagger \hat{b}_i \hat{b}_i + V \hat{n}_i \hat{n}_{i+1} \right] \]  
(1.30)

where \( \mu \) is the chemical potential. The first term represents the kinetic energy of the bosons in the tight-binding approximation, whereas the last two
terms describe an on-site interaction of strength $U$ and a nearest-neighbor interaction of strength $V$. In practice, optical lattices allow for the possibility of easily tuning the amplitude $j$, while $U$ is usually controlled by tuning the scattering length of the two-body interactions by Feshbach resonances. Thus a total control of the ratio $U/t$ can be gained.

### 1.3.1 The Bose-Hubbard model

Moreover, we can go one step further and forbid the nearest neighbor hopping $V = 0$. This can be expected from making the lattice even deeper. And this results in the well-known Bose-Hubbard model:

$$
\hat{H}_{BHM} = \sum_{i=1}^{L} \left[ -t(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}) - \mu \hat{n}_i + \frac{U}{2} \hat{b}_i^\dagger \hat{b}_i \hat{b}_i^\dagger \hat{b}_i \right]
$$

(1.31)

Note that the interaction term is often written in the equivalent form $\frac{U}{2} \hat{n}_i (\hat{n}_i - 1)$ recalling the boson commutation relations: $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$. This model cannot be solved exactly for finite values of the ratio $U/t$, however, its properties are well understood.

It is interesting to introduce first the 3D case of the Bose-Hubbard model, as studying this case by using mean-field approximation clarifies many of the most important aspects, including the Mott phenomenon. One approach is to write particle creation operators as the average plus the fluctuations such that $\hat{b}_i^\dagger \hat{b}_i^\dagger \rightarrow \hat{b}_i^\dagger \langle \hat{b}_{i+1} \rangle + \langle \hat{b}_i^\dagger \rangle \hat{b}_{i+1} - \text{const.}$, neglecting the second order fluctuation terms. Thus, after applying a perturbative analysis around the zero-hopping Hamiltonian we can obtain the critical boundary for a fixed average (integer) density $n$ as a function of the chemical potential (see blue lined lobes in Fig. 1.6):

$$
\frac{zt}{U} = \frac{(n - \mu/U)(\mu/U - n + 1)}{1 + \mu/U}
$$

(1.32)

where $z$ stands for the number of nearest neighbor connections (e.g. $z = 6$ in 3D (and $z = 2$ in 1D)). If $t/U$ is smaller than a critical value that is determined by the tip of the lobe corresponding to $n$ integer number of bosons per site on average, bosons localize on the lattice sites, and quantum fluctuations are reduced. This conforms the Mott-insulator. However, it should be remarked that for chemical potential values such as: $\mu = Un$ ($n \in \mathbb{N}$) there is a degeneracy of the ground state which will always lead to small but unavoidable fluctuations that result in superfluidity. This can be seen in the reentrant behavior of the lobes on the vertical axis in Fig. 1.6. For higher values of the hopping amplitude to interaction strength ratio $t/U$, the delocalization is also favored leading to a superfluid phase, as it will be seen more clearly below.
Alternatively, although equivalent to the mean field, we can use a variational approach to study the competition of the $t/U$ ratio, and propose an ansatz for the ground state wavefunction. In the limit where the interactions dominate ($t/U$ is small) we can assume that each site is occupied by a single atom (see Fig. 1.7(a)) and that the ground state wavefunction is built by applying the particle creation operator to the vacuum in each site. Thus, there is no long range coherence due to the strong local repulsion, which corresponds to a Mott-insulating phase:

$$\hat{\Psi}_{\text{MI}} = \prod_i |n_i\rangle = \frac{1}{\sqrt{n_i!}} (\prod_i \hat{b}_i^\dagger)^n |0\rangle$$

However, in the opposite limit, when the on-site interaction is negligible, we can expect that all the particles are in the lowest momentum possible in the ground state. This can be written in terms of the creation operators as:

$$\hat{\Psi}_{\text{SF}} = \frac{1}{\sqrt{N!}} (\hat{b}_{k=0})^N |0\rangle = (\sum_i \hat{b}_i^\dagger)^N |0\rangle$$

Or similarly, as global coherence should be expected in this limit, it is reasonable to write the ground state wavefunction as a product of coherent states on each site:

$$\hat{\Psi}_{\text{SF}} = \prod_i |\alpha_i\rangle = (\sum_i \hat{b}_i^\dagger)^N |0\rangle$$

where $|\alpha\rangle = e^{\alpha^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\alpha\rangle$ is an eigenstate of the annihilation operator $\hat{a}, \hat{a}^\dagger |\alpha\rangle = \alpha |\alpha\rangle$. 

**Figure 1.6:** Phase diagram of the Bose-Hubbard model as a function of the chemical potential and hopping amplitude.
Chapter 1. The physics of ultracold gases

Figure 1.7: A naïve atomic representation of the Superfluid to Mott-insulator quantum phase transition for an ultracold commensurate gas in an egg carton-like lattice. a) Shows the Mott-insulator phase where all particles are localized due to the strong on-site repulsion, whereas b) shows the superfluid phase, where particles are itinerant and there is a long range coherence.

Therefore, we can adopt the variational ansatz that describes an intermediate state between the two limits above:

\[ \hat{\Psi}_{\text{VAR}} = \prod_i \left[ \sum_n c_n |n\rangle_i \right] \] (1.36)

Thus, it represents a state for an arbitrary value of the ratio \( t/U \) and by the use of the variational principle we can determine the coefficients \( c_n \).

The properties of the one-dimensional limit of this model are qualitatively similar to the higher dimensional counterparts. However there are considerable differences specially when the ratio \( t/U \) gets bigger. The mean-field formulation starts losing its validity when phase fluctuations are strong, which is especially the case for one-dimensional systems. For this purpose, characteristic techniques have been developed taking into account the peculiarities of the 1D.

1.4 One dimensional systems

Following F.D.M. Haldane’s introduction of the harmonic fluid approach in 1981 [37–40], a usual starting point is by defining a density operator such that:

\[ \hat{\rho}(x) = \sum_i \delta(x - x_i), \] (1.37)

where \( x_i \) refers to the position of the \( i \)th particle (not site). However, we could also write \( x_i \) in relation to a fixed equilibrium position that would
1.4 One dimensional systems

Figure 1.8: Schematic figure of the field $\hat{\phi}_l(x)$, red circles represent atoms along one-dimension.

correspond to perfect crystalline lattice with inter-site distance $a = 1/\rho_0$, so that $x_i = ai + \delta_i$, where $\rho_0$ is the average density of particles in one-dimension. It is possible to rewrite the Eq. (1.37) in a more convenient way without loss of generality by temporarily using the labeling field $\hat{\phi}_l(x)$ that takes the value of $\hat{\phi}_l(x_i) = 2\pi i$ at the position of the $i$th particle. This results in a monotonically increasing function that has been depicted schematically in Fig. 1.8. Therefore, we can rewrite the equation Eq. (1.37):

$$\hat{\rho}(x) = \sum_i \delta(x - x_i) = \sum_n |\nabla \hat{\phi}_l(x)| \delta(\hat{\phi}_l(x) - 2\pi n).$$

By taking into account that $\hat{\phi}_l(x)$ is monotonically increasing and Poisson’s expression for Dirac’s delta, we have:

$$\hat{\rho}(x) = \frac{\partial_x \hat{\phi}_l(x)}{2\pi} \sum_p e^{ip\hat{\phi}_l(x)}$$

(1.38)

where $p$ is an integer number. Following this approach, the field $\hat{\phi}_l(x)$ is usually redefined by introducing a new field $\hat{\phi}$ relative to the crystal lattice positions, as it has been done before for the position operator $x_i$, so that: $\hat{\phi}_l(x) = 2\pi \rho_0 x - 2\hat{\phi}(x)$. Thus, yielding to the following expression for the density operator:

$$\hat{\rho}(x) = \left[\rho_0 - \frac{\partial_x \hat{\phi}(x)}{\pi}\right] \sum_p e^{ip(x\rho_0 - \hat{\phi}(x))}$$

(1.39)

There is a semiclassical explanation to this expression as shown in [40], the field $\hat{\phi}(x)$ stands for the displacements of the particles from the exact crystalline lattice positions (i.e. the $\delta_i$ introduced before). The $p=0$ term is the standard elastic representation of the particle density. And on top of this, density waves add up with the corresponding $2\pi \rho_0 p$ wavevectors. Thus, if the density is averaged over large distances in comparison to the mean interparticle distance $a$, the oscillating terms in the exponential of Eq. (1.39) can be neglected, and we can assume that the lowest Fourier component at around $q \simeq 0$, that is only the term with $p = 0$ remains:

$$\hat{\rho}(x) \simeq \rho_0 - \frac{\partial_x \hat{\phi}(x)}{\pi}$$

(1.40)
Chapter 1. The physics of ultracold gases

Now, we can write the the collective boson field operator $\hat{\Psi}(x)$ in polar form:

$$\hat{\Psi}^\dagger(x) = \sqrt{\hat{\rho}(x)} e^{-i\hat{\theta}(x)}$$  \hspace{1cm} (1.41)

having introduced the phase $\hat{\theta}(x)$. The boson commutation relations and the quantum mechanical nature of the harmonic fluid approach require that the following relations must be fulfilled:

$$[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')] = \delta(x - x') \iff [\hat{\rho}(x), e^{-i\hat{\theta}(x')}]) = \delta(x - x') e^{-i\hat{\theta}(x')}$$  \hspace{1cm} (1.42)

The right hand side term accounts for the well-known fact from the theory of superfluids, in which the density and phase are canonically conjugated fields [26]. Finally, from Eqs. (1.39) and (1.41), we have that the field operator can be written as:

$$\hat{\Psi}^\dagger(x) = \left[\rho_0 - \frac{\partial_x \hat{\phi}(x)}{\pi}\right]^{1/2} \sum_p e^{ip(\pi\rho_0 x - \hat{\phi}(x))} e^{-i\hat{\theta}(x)}$$  \hspace{1cm} (1.43)

Therefore, the low-energy behavior of Hamiltonians such as the one presented in Eq. (1.27) can be expressed by using the definitions Eqs. (1.39) and (1.41), we have that the field operator can be written as:

$$\hat{\Psi}^\dagger(x) = \left[\rho_0 - \frac{\partial_x \hat{\phi}(x)}{\pi}\right]^{1/2} \sum_p e^{ip(\pi\rho_0 x - \hat{\phi}(x))} e^{-i\hat{\theta}(x)}$$  \hspace{1cm} (1.43)

Thus, we see that only two parameters $K$ and $v$ are relevant to describe the behavior of the system at low-energies. Or as it is often done, a combination of both: $v_J = vK$ and $v_N = v/K$. What is more, they are able to characterize the low-energy properties of massless 1D systems, without knowing precisely the form of the microscopic Hamiltonian. This is called the Luttinger liquid theory [37–40].
2 Phase equilibria

2.1 Introduction

The quest for lower temperatures in ultracold gases has led to the development of many ingenious techniques to cool several atomic and molecular species. In particular, the explosion of activity concerning ultracold Fermi gases has become possible largely owing to the success of sympathetic cooling, which allows to efficiently cool fermions by mixing them with bosons [4]. At the same time, this procedure has stimulated the investigation, both experimental and theoretical, of Bose-Fermi mixtures. Here, the possibility of tuning the inter-species interaction strength using Feshbach resonances [33, 41, 42], has led to the exploration of many interesting phenomena such as collapse and phase separation [43, 44], as well as boson-mediated Cooper pairing [4]. Furthermore, Feshbach resonances can also be used to generate heteronuclear molecules, which can exhibit large electric dipole moments. This opens the interesting possibility of studying dipole-dipole interactions in quantum degenerate gases [45–51].

Meanwhile, the advent of optical-lattice confinement [6, 33] has turned ultracold atomic gases into unique environments where to simulate and understand strongly correlated phenomena relevant to condensed matter systems. This has been made it possible, for example, by confining the atomic clouds in reduced dimensions, such as a one dimensional (1D) array of two-dimensional (2D) planes or a 2D array of 1D tubes. Whereas the former has enabled the study of interesting phenomena occurring in two-dimensions [52, 53], the latter has provided us with an amazingly tunable tool to explore the physics of interacting 1D quantum systems [26, 54–56], of which it is much more difficult to find faithful realizations in a more conventional condensed matter context.

Optical lattice confinement has also allowed to envisage the realization of new types of quantum systems. One such example, analyzed in this chapter, is provided by mixtures of interacting particles in mixed-dimensional lattices. In recent years, these systems have attracted an increasing amount of theoretical attention [57, 58], and very recently they have been also experimentally realized [59, 60]. Besides its intrinsic interest as a new category of quantum many-body systems, they may also offer advantages for reducing few-body losses and enhancing stability in strongly interacting regimes [61].

In recent years, there has been a growing interest in understanding the properties of mixtures of ultracold Bose and Fermi gases. In particular,
Chapter 2. Phase equilibria

Figure 2.1: Schematic representation of the system studied in this chapter, namely a mixed dimensionality Bose-Fermi system. The Bose-Fermi cloud is loaded in an anisotropic optical lattice that produces a two-dimensional $N_y \times N_z$ array of one-dimensional (1D) tubes of length $L$. The fermions are light enough to hop between the tubes whereas bosons, which are assumed to be much heavier, are confined in the 1D tubes. The bosonic and fermionic Wannier functions ($\phi_R(r_\perp)$ and $w_R(r_\perp)$, respectively) are also displayed.

Binary mixtures of bosons and spin-polarized fermions have been studied in three-dimensions (3D) [17, 43, 44, 62–64], 2D [65] and 1D [18, 66–69]. Note that the 1D geometry has a special relevance because of the central role played by quantum fluctuations and the fact that there is neither broken continuous symmetry nor, consequently, off-diagonal long-range order. The equilibrium phase diagram of 1D Bose-Fermi mixtures has been considered by many authors [18, 66–69], while the case of a Bose-Fermi system in an anisotropic optical lattices was studied by one of us in Ref. [61].

In addition to dimensionality issues, the significant interest in studying the stability of binary mixtures comes also from the possibility of tuning the Bose-Fermi scattering length via the Feshbach resonance mechanism. Indeed, in the repulsive interaction regime, the spatial overlap between bosons and spin-polarized fermions is reduced, thus ensuring the stability of the system [70, 71]. When the repulsion is increased, the two components tend instead to phase separate, rather than uniformly mix: In the particular case of a 3D geometry, phase separation occurs either between a mixed phase and a purely fermionic phase or between two pure phases [44]. In the regime where the interaction between bosons and fermions is attractive, a significant reduction of the interatomic distance can lead to a collapse of the mixture, because of three-body recombination processes [72]. As discussed later, the stability of the mixture towards a collapsed phase can be enhanced...
2.1 Introduction

in one-dimensional geometries [61].

In this chapter, we study the phase stability of a Bose-Fermi mixture embedded in a mixed-dimensional optical lattice of an array of one-dimensional tubes [5, 73] (see Fig. 3.8). The mixed-dimensionality comes from the fact that, while bosons are longitudinally confined along the tubes and strictly move in 1D, fermions are not constrained to 1D and are allowed to hop between tubes in the transverse directions. This assumption can be justified based on the fact that many realizations of Bose-Fermi mixtures consider bosonic species that are much heavier than the fermionic ones. We do also assume that, while bosons interact with each other, as well as with fermions, the fermionic component is polarized in a single hyperfine state and thus is non-interacting at very low temperatures.

As already mentioned, one motivation to study this geometry is that, by confining bosons in 1D, the mixture stability is enhanced [61]. Note that, even for purely bosonic gases, the spatial overlap between bosons has been experimentally shown to be strongly suppressed by the strong correlations emerging in 1D [74]. In addition, mixed-dimensional systems allow to study interesting few-body [75] and many-body [58, 76] phenomena. We should stress that the results reported here are relevant to several experimental realizations. The simplest is, for example, a mixture of light fermions and heavy bosons. In particular, in order to make contact with ongoing and future experiments [77–79], we explicitly consider a mixture of $^6$Li (a light fermion) and $^{173}$Yb (a heavy boson) atoms. An alternative realization could be given by an originally imbalanced mixture of fermions in two hyperfine states [80]: Bosons are then formed by associating fermions into Feshbach molecules [80], leaving out from the pairing the spin polarized excess majority fermions. When the fermions belong to the same atomic species, the Feshbach molecules have twice the mass and twice the polarizability of the fermionic atoms. Therefore, it should be relatively easy to confine the bosons in 1D by loading them into a two-dimensional optical lattice. On the same lattice, the remaining majority fermions behave as the light component.

We find that, since bosons are confined to strictly 1D, they can undergo fermionization. This means that, as they mix with fermions, they form a Tonks-Girardeau gas whose energy per unit length grows as third power of the lineal density. As a result, we find that the nature of the transition from the pure Fermi gas to a mixture is always first order, implying phase separation in density space. Note that this is a very different result from the one obtained by assuming that bosons form a (quasi-)condensate, with the energy density growing as the square of the boson lineal density. The latter situation applies either to a high density Bose gas in 1D or to a gas of bosons that can hop in 3D. We also find that, in the mixed dimensionality lattice, the transition between pure boson and mixed phases is continuous, while it becomes first order when the fermions are also confined in 1D.

The rest of this chapter is organized as follows: In Sec. 2.2 we intro-
duce the model for the Bose-Fermi mixture and discuss methods and approximations employed to derive the system phase diagram. In particular, in Sec. 2.2.1, we explain how a mean-field approximation is applied solely to the boson-fermion interaction, whereas the boson-boson interaction is treated non-perturbatively using the Bethe ansatz in Sec. 2.2.2. In Sec. 2.3, we derive the phase diagram and interpret the origin of the discontinuous character of the transitions between the pure fermion and mixed phases in terms of an expansion of the free energy for small values of the boson density. We first describe the results obtained for the case of mixed dimensions in Sec. 2.3.1 and later for the pure 1D limit in Sec. 2.3.2. Finally, in Sec. 2.4, we present the main conclusions of our study and discuss the limitations of our approach, as well as some directions for future work. Some technical aspects of our derivations are provided in the appendices.

2.2 Model

We consider a mixture of interacting bosonic (B) and single-component fermionic (F) atoms described by the following Hamiltonian (in $\hbar = 1$ units):

$$\hat{H} = \hat{H}_B + \hat{H}_F + \hat{H}_{BF},$$

$$\hat{H}_B = \int dr \hat{\Psi}_B^\dagger \left[ -\frac{\nabla^2}{2m_B} + V_B(r) - \mu_B + \frac{g_{BB}}{2} \hat{\rho}_B \right] \hat{\Psi}_B,$$

$$\hat{H}_F = \int dr \hat{\Psi}_F^\dagger \left[ -\frac{\nabla^2}{2m_F} + V_F(r) - \mu_F \right] \hat{\Psi}_F,$$

$$\hat{H}_{BF} = g_{BF} \int dr \hat{\rho}_B(r) \hat{\rho}_F(r),$$

where the density operators are $\hat{\rho}_\alpha(r) = \hat{\Psi}_\alpha^\dagger(r) \hat{\Psi}_\alpha(r)$, with $\alpha = B, F$. We have approximated all interaction potentials by contact interactions, which are parameterized by an $s$-wave scattering length $a_{\alpha\beta}$:

$$g_{\alpha\beta} = \frac{4\pi a_{\alpha\beta}}{m_{\alpha\beta}},$$

being $m_{BB} = m_B$ and $m_{BF} = 2m_B m_F / (m_B + m_F)$. For thermodynamic stability reasons, the bosons are assumed to repel each other (i.e., $a_{BB} > 0$). The value of $a_{BB}$ can be tuned by, e.g., controlling the strength of the transverse confinement [9]. The sign of the Bose-Fermi interaction strength is determined by $a_{BF}$, which can be controlled independently from $a_{BB}$ by resorting to an inter-species Feshbach resonance. Below we consider both the repulsive ($a_{BF} > 0$) as well as the attractive ($a_{BF} < 0$) case. At ultracold temperatures, interactions between identical fermions can be safely neglected.
2.2 Model

The Bose-Fermi mixture is loaded into an anisotropic optical lattice formed by a 2D \( N_y \times N_z \) square array of 1D “tubes” of length \( L \) directed along the \( x \)-direction and equally spaced by a distance \( d \) (see Fig. 3.8). This can be described by an optical potential of the form \( V_\alpha(\mathbf{r}_\perp) = V_0^\alpha[\sin^2(\pi y/d) + \sin^2(\pi z/d)] \), where \( \mathbf{r}_\perp = (y, z) \). The strength of the optical potential \( V_0^B \) (\( V_0^F \)) is determined by both the laser intensity and the boson (fermion) atomic polarizability, allowing the possibility of mixed dimensionality for the mixture. In particular, we assume that the bosons are tightly confined in 1D tubes and thus move strictly in 1D, while fermions can hop between the tubes. We will derive the thermodynamic phase diagram for this geometry, thus neglecting the harmonic confinement. By making use of the local density approximation, information about the experimentally relevant trapped case can be extracted from the homogeneous phase diagram plotted in chemical potential space.

Because the bosons in the mixture are assumed to be more massive than fermions and/or to experience a more confining lattice potential \( V_B(\mathbf{r}_\perp) \), they are tightly confined along the “tubes”, a configuration often refereed to as a two-dimensional optical lattice \([6, 26, 55, 73, 81, 82]\). Thus, the field operator \( \hat{\Psi}_B(\mathbf{r}) \) can be expressed in terms of Wannier functions \( \varphi_R(\mathbf{r}_\perp) \) localized at the tube site \( \mathbf{R} = (i_y, i_z) d \) (see, e.g., \([33]\) and references therein) and the tube boson operator \( \hat{\Psi}_{BR}(x) \):

\[
\hat{\Psi}_B(\mathbf{r}) = \sum_R \varphi_R(\mathbf{r}_\perp) \hat{\Psi}_{BR}(x).
\] (2.3)

The Wannier functions form an orthonormal basis. By neglecting the interactions between tubes with \( R \neq R' \), we can rewrite the bosonic Hamiltonian \( \hat{H}_B \) in (2.1) as a sum of decoupled 1D Hamiltonians,

\[
\hat{H}_B = \sum_R \int d\mathbf{x} \hat{\Psi}_{BR}^\dagger(\mathbf{x}) \left[ -\frac{\partial^2}{2m_B} - \mu_1^B + \frac{g_{BB}^{1D}}{2} \hat{\rho}_{BR}(x) \right] \hat{\Psi}_{BR}(x), \quad (2.4)
\]

where \( \hat{\rho}_{BR}(x) = \hat{\Psi}_{BR}^\dagger(x) \hat{\Psi}_{BR}(x) \) is the single-tube boson density operator, \( g_{BB}^{1D} \) is the one-dimensional boson coupling, which, for weak boson-boson interaction, takes the form:

\[
g_{BB}^{1D} = g_{BB} \int d\mathbf{r}_\perp |\varphi_R(\mathbf{r}_\perp)|^4, \quad (2.5)
\]

and \( \mu_1^B \) is the 1D boson chemical potential:

\[
\mu_1^B = \int d\mathbf{r}_\perp \varphi_R^\ast(\mathbf{r}_\perp) \left[ \frac{\nabla_\perp^2}{2m_B} - V_B(\mathbf{r}_\perp) + \mu_B \right] \varphi_R(\mathbf{r}_\perp).
\]

Note that, as we will see later, for strong boson-boson interactions, the expression of the 1D boson coupling \( g_{BB}^{1D} \) is instead given by Eq. (2.28) \([9]\) rather than Eq. (2.5).
Chapter 2. Phase equilibria

In contrast, we assume the fermions to be more weakly confined than bosons along each tube due to their smaller mass and/or a weaker optical potential. Yet, the lattice confinement is strong enough so that the description of the Fermi field in terms on the lowest Bloch band $\phi_{k_\perp}(\mathbf{r}_\perp)$ is accurate and we can expand:

$$\hat{\Psi}_F(\mathbf{r}) = \frac{1}{\sqrt{L}} \sum_k e^{ik_x x} \phi_{k_\perp}(\mathbf{r}_\perp) \hat{f}_k,$$

(2.6)

where $\mathbf{k} = (k_x, k_\perp)$. Here, whereas the motion along the $x$ direction is free, the motion in the transverse directions $\mathbf{r}_\perp = (y, z)$ is described by $\phi_{k_\perp}(\mathbf{r}_\perp)$, which is a Bloch wavefunction belonging to the lowest Bloch band characterized by a crystal momentum $k_\perp$. Projecting the fermion Hamiltonian onto this band yields:

$$\hat{H}_F = \sum_k [\varepsilon(k) - \mu_F] \hat{f}_k \hat{\dagger} f_k,$$

(2.7)

where the Fermion dispersion reads as:

$$\varepsilon(k) = \frac{k_x^2}{2m_F} + \varepsilon(k_\perp)$$

(2.8)

$$\varepsilon(k_\perp) = 2t \left[ 2 - \cos(k_y d) - \cos(k_z d) \right].$$

(2.9)

Thus, summarizing, in the geometry studied here, the bosons are tightly confined to move in 1D, whereas the fermions can hop between the tubes, although the optical lattice potential does affect their dispersion relation. Under these conditions, it is known [26] that, at low temperatures, the bosonic atoms lose their individuality and the low-energy long-wavelength excitations are 1D phonons. For arbitrary values of $g_{BB}^{1D} > 0$, the ground state properties of such an interacting bosonic gas are exactly described by the Bethe ansatz solution obtained by Lieb and Liniger [83]. The lack of individuality and the highly correlated behavior brought about by the 1D confinement calls for a treatment of the problem that treats the boson-boson interactions in a non-perturbative way. Since a mean-field approximation fails to capture the fundamental bosonic correlations in 1D, we apply it only to the interactions between the fermions and the bosons, as we explain in what follows.

2.2.1 Bose-Fermi interaction: mean-field

In order to render the above model tractable, we apply a mean-field approximation to the Bose-Fermi interaction term. We do this in such a way that the different 1D tubes become decoupled at the expense of introducing self-consistent shifts of both the boson and fermion chemical potentials. To this end, we first observe that the tight confinement of the bosons in 1D allows
us to neglect the overlap between Wannier functions localized at different 1D tubes (see Fig. 3.8) and thus we can approximate the density operator of the bosons as

$$\hat{\rho}_B(r) \simeq \sum_R |\varphi_R(r_\perp)|^2 \hat{\rho}_{BR}(x).$$

In this limit, the Bose-Fermi interaction term $\hat{H}_{BF}$ of the Hamiltonian (2.1) can be written as

$$\hat{H}_{BF} \simeq g_{BF} \sum_R \int dx \hat{\rho}_{BR}(x) \hat{\rho}_{FR}(x), \quad (2.10)$$

where $\hat{\rho}_{FR}(x)$ is a projection of the 3D Fermi density operator $\hat{\rho}_F(r)$ on the $R$-th tube:

$$\hat{\rho}_{FR}(x) = \int dr_\perp |\varphi_R(r_\perp)|^2 \hat{\rho}_F(r). \quad (2.11)$$

We note that this approximation does not decouple the different tubes yet because, even if bosons cannot hop from one tube to another, the interaction between bosons belonging to different tubes is mediated by the hopping fermions, i.e., the operator $\hat{\rho}_{FR}(x)$. However, if we rely on a mean-field approximation to replace the operator $\hat{\rho}_{FR}(x)$ by its expectation value (which, as shown in detail in Appendix A.1, is a constant), the different tubes become decoupled, which allows for a solution of the model introduced above. We emphasize again that this kind of mean-field approximation is different from the standard treatment (for example employed in Ref. [61]), where also the boson density in the boson-boson interaction term is replaced with its expectation value. Instead, here the boson interaction is treated non-perturbatively using the Bethe ansatz, emphasizing that the fundamental entities subject to the mean-field interaction are the 1D tubes and not the bosons themselves.

Thus, in Eq. (2.10), we write the density operators $\hat{\rho}_{\alpha R}(x)$ as their quantum averages plus fluctuations, i.e., $\hat{\rho}_{\alpha R}(x) = \langle \hat{\rho}_{\alpha R}(x) \rangle + \delta \hat{\rho}_{\alpha R}(x)$. Hence, the mean-field approximation is obtained by substituting these expressions into Eq. (2.10) and by neglecting the second order terms in the fluctuations, which leads to:

$$\hat{H}_{BF} \simeq H_{BF}^{mf} = g_{BF} \sum_R \int dx [-\langle \hat{\rho}_{BR}(x) \rangle \langle \hat{\rho}_{FR}(x) \rangle + \hat{\rho}_{BR}(x) \langle \hat{\rho}_{FR}(x) \rangle + \langle \hat{\rho}_{BR}(x) \rangle \hat{\rho}_{FR}(x)]. \quad (2.12)$$

In absence of harmonic confinement along the tubes, translational invariance along the $x$-direction requires that the averages

$$\langle \hat{\rho}_{BR}(x) \rangle = \rho_0^B, \quad \langle \hat{\rho}_{FR}(x) \rangle = A \rho_0^F. \quad (2.13)$$
are constants independent on the tube index $\mathbf{R}$. Here, the constant

$$A \simeq N \int d\mathbf{r}_\perp |\varphi_{\mathbf{R}}(\mathbf{r}_\perp)|^2 |\phi_{\mathbf{k}_\perp}(\mathbf{r}_\perp)|^2,$$

(2.14)

it is obtained in the limit where the transverse confinement for the bosons is tight (see App. A.1 for the details of the derivation). Also, we have introduced the following lineal densities:

$$\rho^0_\alpha = \frac{N_\alpha}{NL},$$

(2.15)

where $N = N_y N_z$ is the total number of 1D tubes. Thus, within this mean-field approximation, the system Hamiltonian (2.1) can be written as

$$\hat{H} \simeq \hat{H}^{mf} = \hat{H}^{mf}_B + \hat{H}^{mf}_F - \sum_{\mathbf{R}} g_{BF} A \rho^0_B \rho^0_F,$$

(2.16)

where $\hat{H}^{mf}_B$ is defined as the bosonic Hamiltonian from Eq. (2.4) with the chemical potential shifted as $\mu^{1D}_B \rightarrow \mu^{1D}_B - g_{BF} A \rho^0_F$:

$$\hat{H}^{mf}_B = \sum_{\mathbf{R}} \int dx \hat{\Psi}_B^{\dagger}(x) \left[ -\frac{\partial^2}{2m_B} - \mu^{1D}_B + g_{BF} A \rho^0_F + \frac{g^{1D}_{BB}}{2} \hat{\rho}_B(x) \right] \hat{\Psi}_B(x),$$

(2.17)

and $\hat{H}^{mf}_F$ is the fermion Hamiltonian from Eq. (2.7) with a chemical potential shifted as $\mu_F \rightarrow \mu_F - g_{BF} A \rho^0_B$:

$$\hat{H}^{mf}_F = \sum_{\mathbf{k}_\perp} \left[ \varepsilon(\mathbf{k}) - \mu_F + g_{BF} A \rho^0_B \right] \hat{f}_{\mathbf{k}}^{\dagger} \hat{f}_{\mathbf{k}}$$

(2.18)

We would like to stress that we are not applying a mean-field approximation to the boson-boson interaction term $\hat{\rho}^2_{BR}(x)$. On the contrary, as shown in the next section, we shall treat this term exactly using the Bethe ansatz solution of Eq. (2.17) due to Lieb and Liniger [83].

### 2.2.2 Zero-temperature free energy

Starting from the mean-field Hamiltonian defined by equations (2.16), (2.17), and (2.18), we can evaluate the grand-canonical free energy density at zero temperature. Note that, by virtue of the mean-field approximation and the translational invariance, the bosonic $\hat{\Psi}_{BR}$ and fermionic $\hat{f}_{\mathbf{k}}$ field operators in Eq. (2.16) have become decoupled and therefore we can separate the bosonic and a fermionic contributions to the free energy potential $f = f(\mu^{1D}_B, \mu_F, \rho^0_B)$, which can be written as:

$$f = \frac{(\rho^0_B)^3}{2m_B} \gamma(\gamma) - \mu^{1D}_B \rho^0_B - \frac{1}{N} \sum_{\mathbf{k}_\perp \in BZ} \frac{k^3_{Fz}(\mathbf{k}_\perp)}{3\pi m_F},$$

(2.19)
where \( BZ \) stands for the 2D Brillouin zone, i.e., the region of \( k_{\perp} \)-space where 

\[
|k_{y,z}| \leq \pi/d
\]

In evaluating this expression, we have relied upon the Bethe ansatz solution \([26, 83]\) of the interacting 1D boson Hamiltonian, \( \hat{H}^{mf}_{BB} \). It is worth noting that the constant term \( g_{BF}A\rho_{BF}^{0} \) in Eq. (2.16) cancels exactly the mean-field shift of the bosonic chemical potential, \( \mu_{B}^{1D} \rightarrow \mu_{B}^{1D} - g_{BF}A\rho_{BF}^{0} \), in Eq. (2.17).

In Eq. (2.19), the dimensionless function \( e(\gamma) \), where \( \gamma = m_{B}g_{BF}^{D}/\rho_{B}^{0} \), is determined by numerically solving the following system of coupled integral equations:

\[
e(\gamma) = \frac{3}{l^{4}} \int_{-1}^{1} du u^{2} g(u), \tag{2.20}
\]

\[
2\pi g(u) = 1 + 2l \int_{-1}^{1} du' \frac{g(u')}{(u-u')^{2} + l^{2}}, \tag{2.21}
\]

where \( l = \gamma \int_{-1}^{1} du g(u) \). The fermionic contribution to the free energy can be expressed as an integral over the transverse momentum, which leads to the last term in Eq. (2.19), where we have defined:

\[
k_{Fx}(k_{\perp}) = \text{Re} \sqrt{2m_{F} [\mu_{F} - g_{BF}A\rho_{BF}^{0} - \epsilon(k_{\perp})]}.
\]

Finally, the thermodynamic grand-canonical free energy density is obtained by finding the global minimum of the potential \( f(\mu_{B}^{1D}, \mu_{F}, \rho_{0}^{B}) \) with respect to the boson density \( \rho_{0}^{B} \):

\[
\Omega(\mu_{B}^{1D}, \mu_{F}) = \min_{\rho_{0}^{B}=n_{B}} f(\mu_{B}^{1D}, \mu_{F}, \rho_{0}^{B}), \tag{2.22}
\]

where \( n_{B} \) denotes the equilibrium lineal boson density. Note that, since Bose-Einstein condensation is not allowed in 1D interacting boson systems \([26]\), the boson density cannot be regarded as the condensate density, i.e., the square of the condensate order parameter. In addition, the equilibrium 1D fermionic density can be evaluated from

\[
n_{F} = \frac{1}{N} \sum_{k_{\perp} \in BZ} \frac{k_{Fx}(k_{\perp})}{\pi}. \tag{2.23}
\]

As explained in the next section, we can thus now evaluate the system equilibrium phase diagram either in chemical potential or in density space.

### 2.3 Phase diagram

In this section, we obtain the phase diagram of the mixed-dimensionality system by minimizing the free energy introduced above in Eq. (2.19) with respect to the boson density \( \rho_{0}^{B} \) for fixed \( \mu_{B}^{1D} \) and \( \mu_{F} \). The free energy
Figure 2.2: Zero temperature phase diagrams for a repulsive ($a_{BF} > 0$, top panel) and attractive $a_{BF} < 0$ (bottom panel) Bose-Fermi mixture with fixed dimensionless hopping amplitude $\tilde{t} = 37.8$ and fixed interaction parameter $\zeta = 0.23$ (the parameters of this calculation correspond to a $^{174}$Yb-$^6$Li system, see main text). The diagrams are plotted vs. the boson $\mu_{B}^{D}/\varepsilon_{R_{B}}$ and fermion $\mu_{F}/\varepsilon_{R_{B}}$ chemical potentials, where $\varepsilon_{R_{B}}$ is the boson recoil energy — note that $\mu_{B}^{D}/\varepsilon_{R_{B}} \ll 1$, thus ensuring that the bosons remain confined to 1D throughout. The thin solid black lines correspond to 2nd order (i.e. continuous) phase transitions between either the vacuum and the pure boson/fermion phases or between the pure boson and the homogeneous mixed phase. The thick solid (red) line corresponds to a first order transition between the pure fermion and the mixed phase. Second and first order lines meet at at the tricritical point at $\mu_{F} = \mu_{B} = 0$ (filled blue circle). The region with finite boson density is the light gray shaded region. In both cases phase separation can only occur between a mixed and pure fermion phases.

$f(\mu_{B}^{1D}, \mu_{F}, \rho_{B}^{0})$ also depends on several other parameters, such as $g_{BF}$, $g_{BB}^{1D}$, and $t$, as well as the particle masses $m_{B}, m_{F}$. Thus, it is convenient to simplify the description of the system by considering the following minimal set of four independent dimensionless parameters:

$$\tilde{\mu}_{B}^{1D} = \frac{2m_{B}\mu_{B}^{1D}}{c^{2}}, \quad \mu_{F} = \frac{2m_{F}^{1/3}m_{B}^{2/3}\mu_{F}}{c^{2}},$$

$$\tilde{\rho} = \frac{2m_{F}^{1/3}m_{B}^{2/3}t}{c^{2}}, \quad \zeta = \frac{c}{2m_{B}g_{BB}^{1D}},$$

where $c = 2A m_{F}^{1/3} m_{B}^{2/3} |g_{BF}|$. Thus, the dimensionless interaction parameter $\gamma$ can we rewritten as $\gamma = (2\tilde{\rho}_{B}^{0})^{-1}$, with the dimensionless boson density given by $\tilde{\rho}_{B}^{0} = \rho_{B}^{0}/c$. In terms of the above dimensionless quantities, the
free energy takes the form:

\[ \tilde{f} = (\tilde{\rho}_B^0)^3 \epsilon(\gamma) - \tilde{\mu}_B^0 \tilde{\rho}_B^0 - \frac{1}{N} \sum_{k_\perp \in BZ} \frac{\tilde{k}_{Fx}^3(k_\perp)}{3\pi m_F}, \]  

(2.26)

where \( \tilde{k}_{Fx}(k_\perp) = \text{Re}\sqrt{\tilde{\mu}_F - \text{sign}(g_{BF})\tilde{\rho}_B^0 - \tilde{c}(k_\perp)} \) and \( \tilde{c}(k_\perp) = 2\tilde{t}[2 - \cos(k_y d) - \cos(k_z d)] \).

### 2.3.1 Mixed dimensions

We explicitly consider here the case of mixed dimensions, while later in Sec. 2.3.2, we will derive the phase diagram for the case of pure 1D. We have numerically minimized \( \tilde{f} \) by fixing the value of the dimensionless interaction parameter, \( \zeta \), and hopping amplitude, \( \tilde{t} \). In order to make contact with ongoing as well as future experiments \([77–79] \), we consider the specific case of a Bose-Fermi system consisting of a light fermionic species such as \( ^6\text{Li} \) and a heavy bosonic species like \( ^{174}\text{Yb} \). When this system is loaded in a sufficiently deep 2D optical lattice, the large boson to fermion mass ratio \( (m_B/m_F \simeq 29) \) is enough to suppress the hopping between tubes of bosons, while allowing fermions to hop between the tubes. This makes it possible to realize our initial assumption of mixed dimensionality for the system. Indeed, in the limit of a deep lattice, the fermion hopping amplitude in the tight-binding approximation of Eq. (2.7) can be expressed in terms of the optical potential strength \( V_F^0 \) and the Fermi recoil energy \( E_{RF} \), where \( E_{RF} = 2\pi^2/(m_\alpha \lambda^2) \) and \( \lambda = 2d \) is the wavelength of the laser generating the optical lattice potential [33]:

\[ t \approx \frac{4E_{RF}}{\sqrt{\pi}} \left( \frac{V_F^0}{E_{RF}} \right)^{3/4} e^{-2\sqrt{V_F^0/E_{RF}}} . \]  

(2.27)

For a laser wavelength \( \lambda = 1064 \text{ nm} \), the deep lattice condition is achieved by making \( V_F^0 \simeq 40E_{RB} \) (for this system \( V_F^0 \simeq 2V_B^0 \) \([77, 84]\)). Furthermore, the boson-boson scattering \( \ell_{BB} \) length has been experimentally estimated to be \( a_{BB} = 104.9 \text{ a}_0 \) \([85] \) (where \( a_0 \) is the Bohr radius). The 1D interaction strength \( g_{BB}^D \) can be obtained from [9]:

\[ \frac{1}{g_{BB}^D} = \frac{m_B \ell_B}{2} \left( \frac{\ell_B}{a_{BB}} - C \right) , \]  

(2.28)

where \( C \simeq 1.0326 \) and \( \ell_B = 67.34 \text{ nm} \). For these parameters, \( \ell_F = 131.40 \text{ nm} \), and therefore, using Eq. (A.6), \( A = 1.46017 \times 10^{13} \text{ m}^{-2} \). Finally,

---

1 Note that, approximating the confining optical lattice as harmonic, one has that the trapping frequencies for bosons and fermions are given by \( \omega_\alpha = \ell_\alpha^2/(m_\alpha) = 2E_{Ra}\sqrt{V_\alpha^0/E_{Ra}} \).
we set $|a_{BF}| = 13 a_0$ [77], and allow for both positive and negative signs for $a_{BF}$, i.e. for the Bose-Fermi interactions to be repulsive or attractive. Using these values, the dimensionless interaction and hoping parameters are $\tilde{t} = 37.8$ and $\zeta = 0.23$.

The phase diagrams for repulsive ($a_{BF} > 0$) and attractive ($a_{BF} < 0$) Bose-Fermi interactions are shown in Fig. 2.2 as a function of the boson and fermion chemical potentials. In both cases, a qualitatively similar structure emerges: The transition between the pure fermion and the phase where boson and fermions form a homogeneous mixture (mixed phase) is first order (thick solid red line). For the particular values of parameters chosen in Fig. 2.2 to describe the $^{174}$Yb-$^6$Li mixture, we numerically find that the transition is weakly first order close to the origin $(\mu_F, \mu_B^D) = (0,0)$, i.e., the chemical potential values for which the slope of the free energy at $\rho_B^0 = 0$ changes sign are very close to the values of chemical potentials at the transition. On the other hand, the transition between the pure boson and the mixed phases (thin solid black line) is second order, i.e. continuous. This transition coincides with the locus of points where the system first develops a Fermi surface, i.e., $\tilde{\mu}_F - \text{sign}(g_{BF})\tilde{\rho}_B^0 = 0$, and therefore $\mu_F > 0$ ($\mu_F < 0$) for repulsive (attractive) interactions. In Appendix A.2, we carry on an expansion for small fermion density which allows to establish the nature of the phase transitions where the number of Fermi surfaces changes from zero to one. There, we argue that this transition is continuous because of the scaling that the Fermi kinetic energy has with the fermion density in 3D, while it would be first order if the fermion would also move in strictly 1D like the bosons. This result is also in agreement with the conclusion reached by Viverit et al. for Bose-Fermi mixtures in 3D [63], where they show that phase separation between a mixed phase and a pure boson phase cannot be realized in 3D.

Finally, the transitions between the vacuum, corresponding to zero density of both fermions and bosons, and either the pure boson or fermion phases (thin solid black lines in Fig. 2.2) are continuous, as they correspond to the filling of a band [86]. Therefore, the first order line separating the pure fermion and mixed phases terminates at the origin $(\mu_F, \mu_B^D) = (0,0)$ in a tricritical point (filled blue circle), where the first order transition becomes second order.

A first order transition in the phase diagram in chemical potential space implies that the system exhibits phase separation in density space, where, rather than fixing the chemical potentials $\mu_F$ and $\mu_B^D$, one fixes the boson $n_B$ and fermion $n_F$ densities (see Fig. 2.3). We obtain therefore that, for finite inter-tube hopping $t$, phase separation is only possible between pure fermion and mixed phases (dot-dashed black lines in Fig. 2.3). In Sec. 2.3.2, we will see that this fact is related to the dimensionality where fermions move and that the situation drastically changes for strictly 1D, e.g., when the hopping $t$ for fermions is reduced to zero. Note also that, for attractive
2.3 Phase diagram

Figure 2.3: Phase diagrams in the density plane ($\tilde{n}_B, \tilde{n}_F$). In order to obtain a more accurate estimate of the phase boundaries, we have used the parameters $\tilde{t} = 0.023$ and $\zeta = 0.27$. The corresponding phase diagrams in the chemical potential plane (not shown for brevity) display the same features and phase topology as the diagrams shown Fig. 2.2, which are computed for the experimentally relevant $^{174}$Yb-$^6$Li system, but for which the phase boundary in the density plane proved much harder to determine numerically. The top panel corresponds to a repulsive Bose-Fermi interactions, whereas in the bottom corresponds to attractive interactions. In both cases, the system can either be in a uniform mixed phase (lightly gray shaded region) or, by undergoing a first order transition, it can be in a phase separated state (dark gray shaded region), where a pure fermion and mixed phase coexist. The dot-dashed lines connect points on the first order boundary with the same values of the chemical potentials.

interactions, in contrast to a 3D Bose-Fermi mixtures in the absence of the lattice [4, 44], the system is found to exhibit phase separation rather than collapse. This result was also obtained in Ref. [61], by treating the boson-boson interactions within the mean-field approximation. However, different from that work, the non-perturbative treatment of the boson interactions employed here, yields a first order transition between the pure fermion and mixed phases.

The absence of a continuous phase transition between the pure fermion and any phase with a finite density of bosons can be qualitatively understood by making an analogy with the Landau theory of phase transitions and considering the series expansion of the free energy $\tilde{f}$ in (2.26) for small values of the boson density $\tilde{\rho}_B$. In this limit, for fixed $\zeta^{-1} \propto n_B^{2D}$, we have that $\gamma = (2\zeta \tilde{\rho}_B)^{-1} \gg 1$, and therefore the Bose gas is essentially fermionized and close to a Tonks gas. Thus, we can use the following asymptotic formula
for the boson energy [83, 87]:

$$e(\gamma) \simeq e_{TG} \left[1 - \frac{4}{\gamma} + O(\gamma^{-2})\right],$$

where $e_{TG} = \pi^2/3$. Note that this expression implies that the boson contribution to the free energy grows as $(\rho_B^0)^3$. This yields the following series expansion for the free energy at small boson density:

$$\tilde{f} = \tilde{f}_0 + \tilde{f}_2 \rho_B^0 + \tilde{f}_2 (\tilde{\rho}_B^0)^2 + \tilde{f}_6 (\tilde{\rho}_B^0)^3 + \cdots,$$

(2.29)

where the coefficients of the expansion are given by:

$$\tilde{f}_2 = \text{sign}(g_{BF}) C_1 - \tilde{\mu}_B^{1D},$$

$$\tilde{f}_4 = -C_{-1}/4,$$

$$\tilde{f}_6 = e_{TG} - \text{sign}(g_{BF}) C_{-3}/24,$$

and where $C_n = \frac{1}{N} \sum_{k \in BZ} \text{Re} \left[ \sqrt{\mu_F - i(k_\perp)} \right]^n \geq 0 (|n| \text{ is odd})$. In addition, note that $C_n = 0$ if $\mu_F = 0$. Thus, for $\mu_F > 0$, a continuous phase transition cannot take place because the coefficient $\tilde{f}_4$ of the above expansion is always negative meaning that for $\tilde{f}_2 > 0$ the free energy must eventually decrease away from the origin where $\tilde{\rho}_B^0 = 0$ before it can rise again ($\tilde{f}_6 > 0$ is assumed, for stability). Thus, the free energy develops a local minimum for $\tilde{\rho}_B^0 \neq 0$, which eventually can be tuned to be degenerate with the local minimum at $\rho_B^0 = 0$. It is worth comparing this situation with the result of the mean-field treatment of bosons interactions carried out by one of us in Ref. [61], where it was found that $\tilde{f}_4 = (2 - \zeta C_{-1})/(4 \zeta)$, thus allowing both second and first order phase transitions to occur for $\mu_F > 0$ by tuning $\tilde{f}_2 = 0$ and $\tilde{f}_4 = 0$.

In addition, we can use the above expressions to understand the emergence of a tricritical point, which corresponds to the conditions $\tilde{f}_2 = 0 = \tilde{f}_4$ while $\tilde{f}_6 > 0$ for stability. Since $C_n = 0$ only for $\mu_F = 0$, we can conclude that a stable tricritical point can only exist at the origin of the chemical potential plane, i.e. for $(\mu_F, \mu_B^{1D}) = (0, 0)$. Close to the tricritical point, the shape of the first order line can also obtained analytically using the conditions $\tilde{f}_2 > 0$ and $\tilde{f}_4 = -2 \sqrt{\tilde{f}_2 \tilde{f}_6}$. Note that for the choice of parameters done to describe the $^{174}\text{Yb}^{6}\text{Li}$ mixture, we find that, the true first order transition obtained numerically stays very close to the one found analytically here. In addition, the transition is weakly first order because of the large values of the coefficient $\tilde{f}_6$ for which $\tilde{f}_2 \to 0$.

### 2.3.2 Pure 1D limit

Next, we focus on the pure 1D limit, i.e., the limit where the fermions, like the bosons, cannot hop between the tubes (i.e. $t = 0$). The phase diagram
Figure 2.4: Zero temperature phase diagrams for a repulsive ($a_{BF} > 0$, top panel) and attractive ($a_{BF} < 0$, bottom panel) Bose-Fermi $^{174}$Yb-$^6$Li mixture in 1D, i.e., for zero hopping amplitude $t = 0$, and for $\zeta = 0.23$. Differently from the finite $t$ case (cf. Fig. 2.2), the transition between the pure boson and mixed phase becomes first order (thick red solid line), meeting with the other two first order transition lines (one between the pure fermion and mixed phase and the other between the pure fermion and the pure boson phases) at a triple point (filled violet square), where the three phases coexists. Bottom panel: For an attractive mixture there is neither a triple point nor a tricritical point, rather the first order line crosses the second order line at two critical end-points (filled [red] diamond) delimiting the region of phase separation between the vacuum and a mixed phase.

in chemical potential resulting from minimizing the free energy is shown in Fig. 2.4, for both repulsive and attractive Bose-Fermi interactions. It can be seen that, in the pure 1D limit, for both repulsive and attractive interspecies interactions, all transitions (except for the trivial ones from the vacuum phase) are discontinuous. In particular, the transition between the pure boson to the mixed phases, which was found to be continuous in the mixed dimensional system, becomes discontinuous as soon as the fermions are confined to 1D. In App. A.2 we carry on an expansion for small fermion density that allows us to establish the nature of the phase transitions where the number of Fermi surfaces changes from zero to one. As shown there, the main difference between the mixed-dimensional case illustrated in the previous section and the pure 1D limit analyzed here can be traced down to the different scaling of the Fermi kinetic energy with the lineal fermion density $\rho_F^0$ in 1D and 3D. In particular, whereas in 1D the Fermi kinetic energy scales as $(\rho_F^0)^3$, in 3D it scales more slowly as $(\rho_F^0)^{5/3}$.

Furthermore, similarly to what was found in the previous section, the fermionization of bosons in 1D also renders the transition between the pure
fermion and mixed phases discontinuous. These results are compatible with the previous results obtained by Das in Ref. [18], where was found that the transition between the pure boson and fermion phases is discontinuous thus leading to phase separation.

The main difference between the repulsive and the attractive cases is the way the transitions across which the density of fermions changes connect with the transition between the pure fermion and mixed phase. In particular, in the repulsive case (upper panel of Fig. 2.4), the three first order transition lines (thick red solid curves) between pure boson-pure fermion, pure fermion-mixed, and pure boson-mixed phases meet at a triple point (filled violet square symbol). At this triple point, the three phases coexist since the free energy exhibits three degenerate local minima (see Fig. 2.5). On the other hand, for the attractive case (see lower panel of Fig. 2.4), the triple point is absent. Instead, two critical end points (filled red diamonds) appear. In the density phase diagram, the critical end points delimit a triangularly-shaped region (see bottom panel of Fig. 2.6), where phase separation occurs between the vacuum and mixed phases. Similarly to conclusion reached in Ref. [61], this region can be regarded as a remnant of the collapse that occurs in the absence of a lattice in 3D Bose-Fermi mixtures with sufficiently large attractive interactions [4, 44].

Let us finally remark that 1D Bose-Fermi mixtures in the exactly solvable limit of equal masses (i.e. \( m_B = m_F \)) and equal interactions strengths (\( g_{BB}^{1D} = g_{BF} \)) have been analyzed in Ref. [69]. By relying on a linear stability analysis, which requires that the compressibility matrix must be positively defined for any strength of the interactions, the authors of Ref. [69] concluded that the system is always stable against demixing. However, here, by globally minimizing the system free energy, i.e., by looking for the global energy minima, we find that phase separation occurs in a rather broad region of the density phase diagram and, in particular, it always occurs for small bosons and fermion densities in the pure 1D limit.

2.4 Conclusions and Outlook

To summarize, we have studied the equilibrium phase diagram of a Bose-Fermi system in a mixed-dimensional geometry of an array of coupled 1D tubes, where bosons are strongly localized along the 1D tubes, while fermions can hop between the tubes. Because we treat the boson interaction term non-perturbatively using the Bethe ansatz, we have found that the transition between the pure Fermi phase and the mixed phase is always first order. This implies that, for this system, phase separation can take place between a pure fermion and a mixed phase. However, the phase transition between pure boson and mixed phases is found to be continuous for finite hoping amplitude of the fermions and phase separation cannot take place between
2.4 Conclusions and Outlook

Figure 2.5: Dimensionless free energy density $\tilde{f}$ plotted versus the dimensionless bosonic density $\tilde{n}_B = \tilde{\rho}_B$ for fixed dimensionless hopping strength $\tilde{t} = 0.023$, fixed interaction parameter $\zeta = 0.27$, and a 1D repulsive Bose-Fermi system, corresponding to the density phase diagram shown in the top panel of Fig. 2.6. The values of the chemical potentials are fixed at the three different first order transition lines near the triple point $(\mu_D/\tilde{E}_B, \mu_F/\tilde{E}_B) \simeq (35.3,11.2)$, which describes the state where phase separation occurs between the three phases, pure boson, pure fermion and mixed phase: (1) $\simeq (36.3,11.4)$ describes phase separation between pure fermion and mixed phase; (2) $\simeq (33.9,10.8)$ phase separation between pure fermion and pure boson; finally (3) $\simeq (38.1,12.4)$ phase separation between mixed and pure boson.

these two phases. This contrasts with the results obtained by assuming that the bosons form a quasi-condensate and thus applying a standard mean-field treatment where the boson density is replaced with its expectation value [61]. In that case, the free energy the transition between the pure fermion and a mixed phases can be continuous as well as discontinuous, depending on the system parameters.

In the pure 1D limit, we found that the all transitions are first order, except for the trivial ones between the vacuum state and the pure fermion or boson phases. The main differences introduced by the sign of the interaction are the existence of a triple point for repulsive interactions, and the appearance of two critical end points delimiting a first order line between the mixed and the vacuum phases.

Thus, the main difference between the 1D limit and the mixed dimensional system is the change in the character of the transition between the pure boson and mixed phases. We have argued (see App. A.2) that this difference is a consequence of the different scaling of the Fermi gas kinetic energy contribution to the free energy function with the fermion density.

Before commenting on the relevance of our findings for the experiments using $^{174}$Yb-$^6$Li mixtures, it is interesting to note that, because we have applied the Bethe ansatz to the 1D Bose Hamiltonian $\hat{H}_{B}^{mf}$ (2.17), we can extend our analysis to to Fermi-Fermi system consisting of a light and a
Chapter 2. Phase equilibria

Figure 2.6: Phase diagrams in the density plane \((\tilde{n}_B, \tilde{n}_F)\) for \(\zeta = 0.27\) and zero hopping strength \(t = 0\) (same remarks as for Fig. 2.3 apply). Top panel: for repulsive interactions in the 1D limit, phase separation occurs, not only between a pure fermion and a mixed phase, but also between a pure boson and pure fermion phase, as well as between a pure boson and a mixed phase. Bottom panel: In contrast, for the attractive case, there is no phase separation between pure phases, rather, it exists a region of phase separation between the vacuum and a mixed phase.

heavy atom. In fact, in the limit \(g_{BB} \to +\infty\) where \(\gamma \to \infty\), the boson energy, \(e(\gamma)\) becomes identical to that of a free Fermi gas [88]. By taking this limit of the Bethe-energy in Eq. (2.26), we found that the phase diagrams for both repulsive and attractive Fermi-Fermi interactions evaluated in the same way as before are qualitatively similar to those displayed in Fig. 2.2 for the Bose-Fermi mixture and that the differences are small and only quantitative.

The actual experimental systems are rendered inhomogeneous by the existence of harmonic trapping. For mixed dimensionality systems, in general, and the \(^{174}\text{Yb}^{6}\text{Li}\) system [77–79] loaded in an anisotropic optical lattice in particular, we can rely on the local density approximation and deduce the main implications for experiments from the phase diagrams in the chemical potential space shown in Fig. 2.2 and in Fig. 2.4. For a given trap frequency and total atom numbers \(N_F\) and \(N_B\), it is possible to determine the range

\[^{2}\text{In particular, we have checked that for fixed interaction parameter } \zeta = 0.23, \text{ the relative difference between the exact Bethe-ansatz energy } e(\gamma) \text{ and the Tonks gas limit } e_{TG} \text{ can be only roughly up to } 12\% \text{ for typical densities } \tilde{\rho}_B^{0} \text{ involved in the first order transition. As a result, we obtain that the phase diagrams for both repulsive and attractive interactions maintain the same qualitative features.}\]
of values of the chemical potentials $\mu_F$ and $\mu_D^{1D}$ of the phase diagrams in Figs. 2.2 and 2.4 being sampled by the trapped system. This range determines a region in the chemical phase diagram that contains the possible phases that will coexist in the trap.

Lastly, we comment on the accuracy of the above mean-field approach that we have employed for the Bose-Fermi interaction term. Indeed, as any other mean-field theory, it neglects fluctuations. We expect fluctuations to be especially important close to a phase transition. Nevertheless, as shown later in Sec. 2.3, our calculations indicate that many of the phase transitions in the mixed dimensionality Bose-Fermi system (cf. 2.3.1) and in the pure 1D limit are discontinuous. This means that, even very close to the transition point, fluctuations of the boson and fermion densities are typically suppressed and thus it can be expected that the mean-field theory to give a reliable picture. However, we also numerically observed that some of the transitions are only weakly first order. In other cases, however, the transition was found to be continuous. Therefore a careful assessment of the effect of fluctuations will be required but will not be pursued here.

Furthermore, within the above mean-field approach, we also have neglected the inter-tube couplings as well as the effect of the bosons on the fermion properties, which are as a non-interacting Fermi gas. These are also concerns that deserve to be investigated in the future work. Here, we have assumed that such effects are relatively weak and can only become important only for large values $|a_{BF}|$ and/or very low temperatures that may not be easily achievable under current experimental conditions.

Beyond the assessment the accuracy of the present mean-field approach, another interesting direction is to apply the methods developed here to mixed dimensionality systems where the 1D bosons interact via longer range interactions, such as dipolar gases or are tuned to the so-called the super-Tonks regime [21, 26, 89–92].
3 Superfluid to insulator transition in mixed dimensionality Bose-Fermi mixtures

3.1 Introduction

The interest in systems of interacting bosons and fermions has been a recurrent and central topic in the study of the many-body problem. Many early studies were concerned with dilute solutions of $^3$He in $^4$He (see e.g. [93], for a review) as well as with the problem of electrons coupled to phonons in solids (see e.g. [94]). This research led to the understanding of important phenomena such like the polaron and Cooper pairing [94]. More recently, these concepts have reemerged in the context of ultracold atomic gases [33], where new types of interacting Bose-Fermi mixtures have been experimentally realized [17, 59, 70, 95–103]. Indeed, such experiments with ultracold gases have made it possible to study and envision Bose-Fermi systems [18, 61, 67, 68, 104–119] that can exhibit very different properties from their condensed-matter counterparts.

Thus far, much research has focused on understanding how interactions with the bosonic component of the mixture influences the properties of the fermions and, in particular, how the interactions mediated by the bosons can possibly induce fermion superfluidity (see e.g. [33, 113, 118] and references therein). The complementary problem, namely, understanding how the properties of bosons are modified by their interaction with fermions in a mixture has only recently attracted interest, especially motivated by a series of ground-breaking experiments with Bose-Fermi mixtures loaded in optical lattices [95, 98, 99, 120, 121].

Within this setup, in recent years a number of groups have addressed the problem of how the addition of fermions to a Bose gas in an optical lattice affects the phase transition from superfluid to Mott insulator in the latter [17, 95, 98, 99, 107, 108, 121, 122]. Thus, experimental observations have been reported indicating that fermions effectively decrease the quantum coherence of the bosons, thus making it easier for the latter to become Mott insulating [17, 95, 98, 99, 121]. In the case of attractive interactions between bosons and fermions, this effect has been explained by a ‘self-trapping’ effect:
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures

Figure 3.1: Schematic representation of the system studied in this chapter: A mixture of light fermions and heavy bosons loaded in an anisotropic optical lattice. Being the bosons heavier, they can be easily confined to one dimension by the lattice potential.

the bosons move in the lattice potential that effectively becomes deeper by the addition of fermions to which the bosons are attracted. This ‘self-trapping’ would have the opposite effect in the case of repulsive boson-fermion interactions. However, in this case, the two components do not mix in a deep lattice.

In connection with the experiments referred to above, there has been some theoretical discussion on other, perhaps more subtle, effects of adding fermions to an interacting boson system [107, 108]. These effects concern the physics of polarons, where one particle (in this case, the bosons) is dressed by its interactions with other particles (i.e. the fermions). The bosons interact via screened interactions, which are much less repulsive, but also undergo dissipative effects, which involve the creation of particle-hole pairs and/or (if they exist) zero-sound modes. Indeed, as discussed below within a weak coupling approach, whereas the ‘self-trapping effect’ arises at first order, the polaronic effects arise at second order in the coupling strength between fermions and bosons.

Going beyond mean-field theory, Yang [122] has studied the effect of the boson-fermions interaction on the superfluid (SF) to Mott insulator (MI) transition in a three dimensional Bose-Fermi mixture. He found that the properties of the transition at the particle-hole symmetric point (i.e. at the tip of the ‘Mott lobes’) is modified and becomes either a first order transition or a different (i.e. not XY) second order transition. However, in this chapter
we find that in a mixed dimensionality system, the universality class of the transition (2D XY) is not modified by the boson-fermion coupling for integer filling. The latter only introduces screening of the external periodic potential and the boson-boson interactions. Whereas the former tends to make the system less (more) superfluid for attractive (repulsive) boson-fermion interactions, the screening of the boson interactions always favors superfluidity. On the other hand, for a half-filled lattice, we find that the quantum phase transition from the SF to the charge-density wave (CDW) phase is modified by the presence of the fermions. However, transition remains continuous and belongs to the 2D XY universality class.

The outline of this chapter is as follows. In the following section, we introduce the basic model of a Bose-Fermi mixture that will be subsequently analyzed. There we also outline the derivation of its effective low-energy description. In Sect. 3.3 we consider the effect of the Fermi gas on the Mott insulator to superfluid transition of a Bose gas confined to one dimension. The perturbative renormalization group is used to analyze the low-energy properties of the effective low-energy model, the effect of the fermions on the superfluid to insulator quantum phase transition is studied. Depending on the lattice filling and the boson-boson interactions, the Mott insulator can be stabilized at integer or half-integer filling, and the effects of the Fermi gas are very different on both transitions. Thus, we have separated the discussion into two subsections, 3.3.1 and 3.3.2. Finally, in Sect. 3.5 the main conclusions of this chapter are summarized.

3.2 Basic model

3.2.1 Hamiltonian

The system under study is an ultracold mixture of bosonic atoms (mass \(m_B\)) and single-species fermionic atoms (mass \(m_F\)) loaded in an optical lattice (see Fig. 3.1). The repulsive interaction between bosons is described by an interaction potential \(v_{BB}(r - r')\). The latter can be either the Lee-Yang-Huang pseudo-potential, which accounts for the s-wave scattering of ultracold atoms (as for alkali or alkaline earth atoms), or a dipolar potential (as for Chromium or polar bosonic molecules). Furthermore, fermions and bosons are assumed to interact only via a short-range potential, which is also described by the Lee-Yang-Huang pseudo-potential. Inter-fermion interactions are negligible because, by the Pauli principle, the dominant scattering channel for single-species fermions is p-wave, which, away from resonances, is very weak at ultracold temperatures. The optical lattice potential \(U_{B(F)}(r) = U_{0\parallel}^{B(F)} \sin^2 k_L x + U_{0\perp}^{F(B)} (\sin^2 k_L y + \sin^2 k_L z)\), where \(k_L = 2\pi/\lambda_L\) and \(\lambda_L\) is the laser wavelength. It is further assumed that \(U_{0\parallel}^B \ll U_{0\perp}^B\), that is, the bosons move in a strongly anisotropic two-dimensional lattice. We
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures

further assume that the bosons are heavier (i.e., \( m_F/m_B \ll 1 \)), which means that their motion along two directions (here \( y \) and \( z \)) is strongly suppressed beyond zero-point motion, thus effectively confining them to one dimension for at least the duration of the experiment. However, the fermions, being lighter, can hop in all three dimensions but the large laser intensity required for at least the duration of the experiment. However, the fermions, being beyond zero-point motion, thus effectively confining them to one dimension. Thus, the Hamiltonian reads:

\[
\hat{H} = \hat{H}_B + \hat{H}_F + \hat{H}_{BF},
\]

\[
\hat{H}_B = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m_B} \nabla \hat{\Psi}_B^\dagger(\mathbf{r}) \nabla \hat{\Psi}_B(\mathbf{r}) + U_B(\mathbf{r}) \rho_B(\mathbf{r}) \right] + \frac{1}{2} \int d\mathbf{r}' \rho_B(\mathbf{r}) V_{BB}(\mathbf{r} - \mathbf{r}') \hat{\rho}_B(\mathbf{r}'),
\]

\[
\hat{H}_F = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m_F} \nabla \hat{\Psi}_F^\dagger(\mathbf{r}) \nabla \hat{\Psi}_F(\mathbf{r}) + U_F(\mathbf{r}) \rho_F(\mathbf{r}) \right],
\]

\[
\hat{H}_{BF} = g_{BF} \int d\mathbf{r} \hat{\rho}_B(\mathbf{r}) \rho_F(\mathbf{r}),
\]

where \( \hat{\Psi}_B(\mathbf{r}) \) is the boson (fermion) field operator, which obeys \( [\hat{\Psi}_B(\mathbf{r}), \hat{\Psi}_B(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \) (anti-)commuting otherwise; \( \hat{\rho}_B(\mathbf{r}) = \hat{\Psi}_B^\dagger(\mathbf{r}) \hat{\Psi}_B(\mathbf{r}) \) is the boson (fermion) density operator and \( N_B = \int d\mathbf{r} \rho_B(\mathbf{r}) \) the boson (fermion) number operator. The boson-fermion interaction is parametrized by the coupling \( g_{BF} = 2\pi \hbar^2 a_{BF}/M_{BF} \), where \( M_{BF} = m_B m_F/(m_B + m_F) \) is the reduced mass and \( a_{BF} \) is the s-wave scattering length. Since we are interested in the ground state phase diagram in the thermodynamic limit of the above system, we have neglected the harmonic trapping potential, which is also present in the experiments. Note that an implicit assumption of our analysis below is that the bosons and fermions are mixed. For short range interactions between the bosons (i.e. for \( V_{BB}(\mathbf{r}) = g_{BB} \delta(\mathbf{r}) \)) the problem of phase equilibria has been previously studied in Ref. [119]. One conclusion of this chapter is that the uniform mixed phase in this Bose-Fermi system is always stable provided the density of bosons and fermions is sufficiently high, for both attractive and repulsive interactions (see Ref. [119] for further details).

The Hamiltonian introduced in equations ((3.1), (3.2), (3.3)), and (3.4) contains too much information about energy scales in which we are not interested. Since our goal is to analyze the ground state and low-lying excitations of the system, we next derive an effective Hamiltonian that is much more appropriate to this end. The first step is to project the Bose and Fermi fields onto the lowest Bloch band of the lattice potential. Thus, we expand \( \hat{\Psi}_B(\mathbf{r}) \approx \sum_{\mathbf{R}} w_B(\mathbf{r}_\perp - \mathbf{R}) \hat{\Psi}_{B\mathbf{R}}(x) \) where \( w_B(\mathbf{r}_\perp - \mathbf{R}) \) are the Wannier orbitals describing particles localized round the site \( \mathbf{R} = \frac{1}{2}(m,n)\lambda_L \) of a 2D
(square) lattice. For the fermions, \( \hat{\Psi}_F(r) \approx \sum_k \varphi_k(r) \hat{f}_k \), where \( \varphi_k(r) \) are the Bloch states of the lowest band. Note the differences in treatment of the Bose and Fermi fields, which reflects their differences in mobility introduced by the conditions discussed above. Hence, upon neglecting terms coupling different lattice sites, the bosons are described by

\[
\hat{H}_B = \sum_R \int dx \left[ \frac{\hbar^2}{2m_B} \left| \frac{\partial_x \hat{\Psi}_{BR}(x)}{\partial x} \right|^2 + U_B(x) \hat{\rho}_{BR}(x) \right] + \frac{1}{2} \sum_R \int dx dx' V_{BB}(x-x') \hat{\rho}_{BR}(x) \hat{\rho}_{BR}(x').
\] (3.5)

However, the fermions are described by:

\[
\hat{H}_F = \sum_k \epsilon(k) \hat{f}_k \hat{f}_k^\dagger.
\] (3.6)

where the sum is over \( k \) belonging to the first Brillouin zone and \( \epsilon(k) = \epsilon_{\parallel}(k) + \epsilon_{\perp}(k) \approx \frac{\hbar^2 k^2}{2m_F} - 2t_{\perp}(\cos k_y b_0 + \cos k_z b_0) \), where \( b_0 = \frac{\pi}{k_F L} \) is the lattice parameter, and we have assumed that the periodic potential along the \( x \) direction is so weak that effectively amounts to a renormalization of the fermion mass. Finally, the boson-fermion interactions are described by:

\[
\hat{H}_{BF} = g_{BF} \sum_R \int dx |w_0(r_{\perp} - R)|^2 \hat{\rho}_{BR}(x) \hat{\rho}_F(r),
\] (3.7)

where \( r = (x, y, z) = (x, r_{\perp}) \). In the above expression we have approximated the boson density operator \( \hat{\rho}_B(r) = \hat{\rho}_B(x, r_{\perp}) \approx \sum_R |w_0(r_{\perp} - R)|^2 \hat{\rho}_{BR}(x) \).

### 3.2.2 Integrating out the fermions

The total Hamiltonian obtained upon projection onto the lowest Bloch band \( H = H_B + H_F + H_{BF} \) is still too complicated to solve. Since we are mainly interested on the low-temperature properties of the heavier bosons, which are much slower, a first step towards understanding the latter is integrating out the fermion degrees of freedom. To this end, we rely on the path integral representation of the partition function \( Z = \text{Tr} e^{-\beta [H - \mu_B N_B - \mu_F N_F]} \) for the Hamiltonian, \( H = H_B + H_F + H_{FB} \), which allows us to write:

\[
Z = \int [d\hat{\psi}_B d\hat{\psi}_F d\hat{\bar{\psi}}_F d\hat{\bar{\psi}}_B] e^{-S[\hat{\psi}_B, \hat{\bar{\psi}}_B, \hat{\bar{\psi}}_F, \hat{\psi}_F]},
\] (3.8)
where
\[ S = S_B + S_F + S_{BF}, \]
\[ S_B = \sum_R \int dx \int_{0}^{\beta} d\tau \bar{\psi}_{BR}(x,\tau) \partial_{\tau} \psi_{BR}(x,\tau) + \int_{0}^{\beta} \frac{d\tau}{\hbar} H_B(\tau) \]
\[ - \frac{\mu_B}{\hbar} \sum_R \int dx \int_{0}^{\beta} d\tau |\psi_{BR}(x,\tau)|^2, \]
\[ (3.9) \]
\[ S_F = \sum_k \int_{0}^{\beta} d\tau f(x,k) \left[ \partial_{\tau} f(k,\tau) - \frac{\mu_F}{\hbar} f(k,\tau) \right] + \frac{1}{\hbar} \int_{0}^{\beta} d\tau H_F(\tau), \]
\[ (3.10) \]
\[ S_{BF} = \frac{1}{\hbar} \int d\tau H_{BF}(\tau). \]
\[ (3.11) \]

where \( \beta = (k_B T)^{-1} \) is the inverse of absolute temperature and \( k_B \) is Boltzmann’s constant. Thus, the effective action for the bosons is defined by the following equation:
\[ e^{-S_{\text{eff}}[\bar{\psi}_B,\psi_B]} = \int [d\bar{f}df] e^{-S_B - S_F - S_{BF}} = Z_F^0 e^{-S_{BF}}F, \]
\[ (3.12) \]

where \( \langle \ldots \rangle_F = \text{Tr} \hat{\rho}_F \ldots \) and \( \hat{\rho}_F = Z_F^{-1} e^{-\beta(H_F - \mu N_F)} \), being \( Z_F = \text{Tr} e^{-\beta(H_F - \mu N_F)} \) the non-interacting fermion partition function. To make further progress, we shall assume that the interaction between the bosons and the fermions is perturbatively small. Therefore, the above functional integral can be performed using the cumulant expansion, which yields:
\[ \langle e^{-S_{BF}} \rangle_F = e^{-(S_{BF}) + \frac{1}{2}(S_{BF}^2 - (S_{BF})^2) + \ldots} \]
\[ (3.13) \]

The leading term is
\[ \langle S_{BF} \rangle_F = \frac{g_{BF}}{\hbar} \sum_R \int_{0}^{\beta} d\tau \int d\mathbf{r} |w_0(\mathbf{r} - \mathbf{R})|^2 \rho_{BR}(x,\tau) \rho_{F}^0(\mathbf{r}), \]
\[ (3.14) \]

where \( \rho_{F}^0(\mathbf{r}) = \langle \rho_F(\mathbf{r},\tau) \rangle_F \) is the equilibrium density of the Fermi gas (in the absence of the bosons). Since \( \rho_{F}^0(\mathbf{r}) \) is periodic, Eq. (3.14) amounts to a correction to the periodic potential that the boson gas undergoes. The correction has the same sign as the coupling \( g_{BF} \), which means that e.g. for attractive boson-fermion interactions, the effective potential seen by the bosons is deepened by its (mean-field) interaction with the fermions. This effect has been termed ‘self-trapping’ and has been studied both theoretically [98] and experimentally [95, 99, 121]. We shall not study it any further here. Instead, we focus on the second order term, which leads to much
more interesting physics. Neglecting the coupling between different sites \( R \) (i.e. terms where \( R' \neq R \)) yields:

\[
-\frac{1}{2} (S_{BF}^2 - \langle S_{BF} \rangle^2) = \frac{g_{BF}^2}{2\hbar} \sum_R \int dr d\tau dr' d\tau' \rho_{BR}(x, \tau) \chi_F(x-x', \tau-\tau') \rho_{BR}(x', \tau'),
\]

(3.15)

where \( r = (x, r\perp), r' = (0, r'\perp) \). After defining \( F_0(r\perp, r\perp') = |w_0(r\perp)|^2 |w_0(r'\perp)|^2 \), we introduce

\[
\chi_F(x, \tau) = \int dr_\perp dr'_\perp F_0(r_\perp, r'_\perp) \chi_F(r, r', \tau),
\]

\[
\chi_F(r, r', \tau) = -\frac{1}{\hbar} \langle \delta \rho_F(r, \tau) \delta \rho_F(r', 0) \rangle_F.
\]

(3.16)

Thus, up to \( O(g_{BF}^2) \), we obtain the following effective action for the bosons:

\[
S_{\text{eff}}[\psi_B, \psi_B] = \sum_R S_{\text{eff}, R}
\]

\[
S_{\text{eff}, R} = \int_0^{\beta_0} d\tau \int dx \psi^*_B R(x, \tau) \partial_\tau \psi_B R(x, \tau) + \int_0^{\beta_0} d\tau \int dx \frac{\hbar}{2m_B} |\partial_x \psi_B R(x, \tau)|^2
\]

\[
+ \int_0^{\beta_0} d\tau \int dx [\tilde{U}_{B\parallel}(x) - \mu_B] |\psi_B R(x, \tau)|^2
\]

\[
+ \frac{1}{2} \int_0^{\beta_0} d\tau \int dx dx' |\psi_B R(x, \tau)|^2 V_{BB}(x-x') |\psi_B R(x', \tau)|^2
\]

\[
+ \frac{g_{BF}^2}{2\hbar} \int dx d\tau dx' d\tau' |\psi_B R(x, \tau)|^2 \chi_F(x, x', \tau-\tau') |\psi_B R(x', \tau')|^2,
\]

(3.17)

where \( \tilde{U}_{B\parallel}(x) = U_{B\parallel}(x) + g_{BF} \int dr_\perp |w_0(r_\perp)|^2 \rho_0^F(x, r_\perp) \). Note that we have thus reduced the problem to a set of one dimensional systems independently coupled to a fermionic bath. Therefore, in what follows we shall drop the lattice index \( R \) and study the phase diagram of a generic 1D system coupled to the fermionic bath.

However, one important caveat is in order when considering the applicability of the effective action, Eq. (3.17). In what follows, we will not treat the bosons and the fermions on equal footing. Such a treatment would require to also account for the effect of the bosons on the fermionic component of the mixtures, which may modify the density response \( \chi_F(r, r', \tau) \). Nevertheless, below we shall assume that \( \chi_F(r, r', \tau) \) is well described by the non-interacting limit where we take \( g_{BF} = 0 \). Indeed, this assumption is qualitatively correct as long as the Fermi component of the mixture remains a Fermi liquid, which is reasonable given that the fermions are much lighter, interact with the bosons weakly, and therefore their energy is dominated by
Figure 3.2: In the limit of strong one-dimensional (1D) confinement, the inter-tube coupling can be neglected and the system of Fig. 3.1 can be mapped to a single 1D tube immersed in a Fermi gas. The Fermi gas has two important effects: it introduces screening of the boson-boson interactions and it behaves as a dissipative bath that introduces quantum dissipation. Assuming that a periodic potential is applied longitudinally to the tube(s), which drives a transition from the superfluid to a Mott insulating phase, we study the modification of the phase diagram due to these effects.

the kinetic energy. However, strictly speaking the bosons will mediate effective fermion-fermion interactions, which, at sufficiently low temperature, lead to a pairing instability of the Fermi gas. Since the gas contains a single species of fermions, such a paring instability takes place in a high angular momentum wave (most likely, p-wave) and at relatively low temperatures compared to the Fermi energy $\mu_F$. Given that present cooling techniques in optical lattices cannot reach temperatures below a few percent of $\mu_F$, we can safely neglect this possibility. Other possible instabilities such as a charge density wave occur at particular values of the lattice filling and/or lattice parameters and we will also neglect them in what follows.

3.2.3 Low-energy effective theory

In order to deal with the effective boson model in Eq. (3.17), we shall use the method of bosonization [26, 123]. Thus, we first integrate the high-energy density and phase fluctuations of the bosons, and introduce two collective fields, $\theta(x)$, and $\phi(x)$ describing the phase fluctuations in each 1D system. In terms of these fields, the Bose field and density operators read:

$$\Psi_B(x) \simeq A \rho_0^{1/2} e^{i\theta(x)},$$

$$\rho_B(x) = \Psi_B^\dagger(x)\Psi_B(x) \simeq \rho_0 + \frac{1}{\pi} \partial_x \phi(x) + \rho_0 \sum_{m>0} B_m \cos 2m(\phi(x) + k_F x),$$

where $A$ is a constant.
3.2 Basic model

where $\rho_0 = N_B/(ML)$ is the linear density of bosons in each of the $M$ 1D systems of length $L$ of the lattice and $k_B^2 = \pi \rho_0$. The amplitudes $A$ and $B_m$ depend on the microscopic details of the model and cannot be obtained using bosonization. Using the above expressions and retaining only the most relevant operators in the renormalization-group sense yields [26]:

\[
S_B[\phi] = S_0[\phi] + S_u[\phi],
\]

\[
S_0[\phi] = \frac{1}{2\pi K} \int dx \left[ \frac{1}{v} (\partial_x \phi)^2 + v (\partial_x \phi)^2 \right],
\]

\[
S_u[\phi] = -\frac{g_u}{\pi a_0^2} \int d\tau dx \cos (2p\phi(x, \tau) + x\delta_p),
\]

where we have introduced the following notation: $v$ is the sound velocity of the 1D Bose gas whereas $vK = v_B^2 = \hbar k_B^2/m_B$ and $K/v$ is proportional to the system compressibility; $a_0 \approx \hbar v/\mu_B$ is a short-distance cut-off [26].

The bare dimensionless coupling of the term describing the periodic potential in the bosonization language is $g_u = \tilde{U}_B/|B\rho_0a_0^2|/2\hbar v$. The cosine term with $p=1$ describes the effect of the potential in the case of integer filling of the lattice, $\delta_p=1 = 2(k_L - k_B^2)$ being a measure of the incommensurability of the system. However, near half filling, we must consider the $p=2$ term with $\delta_p=2 = 2k_L - 4k_B^2$ as a measure of the incommensurability. In the half-filled case, the above effective Hamiltonian describes the transition from a Tomonaga-Luttinger liquid (TLL) to a fractional Mott insulating state which is also known as a charge density wave (CDW). The stability of the CDW state requires smaller values of the Luttinger parameter $K$ than those that are achievable in the Lieb-Liniger model [83, 124] describing bosons interacting via a short range potential in a 1D wave-guide [9], for which the minimum value of $K$ is one [26]. Smaller values of $K$ are accessible when either the bosons possess a dipolar moment [26, 125–127] or in the so-called super-Tonks regime [21, 26, 89–92] .

The above action, Eq. (3.20), provides an effective description of the low-temperature properties of the boson system which includes (through the renormalization of the potential $U_B \rightarrow \tilde{U}_B$) the effect of the Fermi gas at the mean-field level. The dynamical effect of the fermions on the bosons is taken into account, to leading order in $g_{BF}$, by the last term in Eq. (3.17). However, since the dynamics of the (heavier) bosons described by Eq. (3.21) is much slower than the lighter fermions, some further simplifications of Eq. (3.15) are possible. First, we note (see Appendix B.2) that, at $T = 0$, the fermion density correlation function introduced above, $\chi_F(x, x', \tau)$ can be written as follows:

\[
\chi_F(x - x', \tau) = \int_0^{+\infty} \frac{d\omega}{\pi} e^{-\omega|\tau|} \text{Im} \chi^R_F(x - x', \omega),
\]

where $\chi^R_F(x - x', \omega)$ is the retarded version of the same correlation function. We have also assumed, consistently with what was stated above, that the
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures

effect of the periodic potential can be neglected as far as the calculation of $\chi_F(x - x', \omega) \simeq \chi_F(x - x', \omega)$. The above expression allows us to treat separately the high frequency density fluctuations from the low-frequency fluctuations of the fermionic gas. This can be done by introducing the following response functions:

$$\chi_F^R(x, \tau) = \int_0^{+\infty} \frac{d\omega}{\pi} g(\omega)e^{-\omega|\tau|} \text{Im}\chi_F^R(x, \omega), \quad (3.24)$$

$$\chi_F^G(x, \tau) = \int_0^{+\infty} \frac{d\omega}{\pi} g_c(\omega)e^{-\omega|\tau|} \text{Im}\chi_F^G(x, \omega), \quad (3.25)$$

where $g(\omega)$ is a frequency cut-off function, which can be chosen in various ways as the result will be largely independent of this function; $g_c(\omega) = 1 - g(\omega)$. Below we use $g(\omega) = e^{-\omega\tau_c}$, where $\tau_c \ll \max\{\frac{\hbar}{\mu_F}, \frac{\hbar}{\mu_B}\}$. The cut-off frequency $\simeq \frac{\hbar}{\tau_c}$ is chosen such that the high-frequency density fluctuations of the Fermi gas can adapt instantaneously to the (slow) dynamics of the boson density fluctuations described by $\rho_B(x, \tau)$ (cf. Eq. (3.19)). Thus,

$$\int dx d\tau dx' d\tau' \rho_B(x, \tau) \chi_F^R(x - x', \tau - \tau') \rho_B(x', \tau')$$

$$= \int dx dx' d\tau d\tau' \rho_B(x, \tau + \frac{t}{2}) \chi_F^G(x - x', t) \rho_B(x, \tau - \frac{t}{2})$$

$$\simeq \int dx dx' d\tau \rho_B(x, \tau) \chi_F^G(x - x', \omega = 0) \rho_B(x', \tau)$$

$$= \int dx dx' d\tau \rho_B(x, \tau) \chi_F(x - x', \omega = 0) \rho_B(x', \tau)$$

$$- \int dx dx' d\tau \rho_B(x, \tau) \chi_F^G(x - x', \omega = 0) \rho_B(x', \tau), \quad (3.26)$$

where $\chi_F^G(x - x', \omega = 0) = \int dt \chi_F^G(x - x', t)$ and similar definitions for $\chi_F^R(x - x', \omega = 0)$ and $\chi_F(x - x', \omega = 0)$. Therefore, the effective action describing the interactions between the bosons mediated by the fermi gas takes the form:

$$S_{\text{eff}, BF} = \frac{g_{BF}^2}{2\hbar} \int dx dx' d\tau \rho_B(x, \tau) \chi_F(x - x', \omega = 0) \rho_B(x', \tau)$$

$$+ \frac{g_{BF}^2}{2\hbar} \int dx dx' d\tau d\tau' \rho_B(x, \tau) \Gamma(x - x', \tau - \tau') \rho_B(x', \tau'), \quad (3.28)$$

where the dissipative kernel $\Gamma(x, x', \tau)$ is defined as:

$$\Gamma(x - x', \tau) = \chi_F^G(x, \tau) - \chi_F^G(x - x', \omega = 0)\delta(\tau). \quad (3.29)$$

Note that, by definition, $\int d\tau \Gamma(x - x', \tau) = 0$. This kernel can be evaluated as follows. Since we assume the Fermi component of the mixture to be a
3.2 Basic model

Fermi liquid, we note that for the latter $-\text{Im} \chi^R_F(x-x',\omega) \propto \omega$ for $\omega \ll |\mu_F|$ [93]. In the present system, the small $\omega$ limit of this function is obtained explicitly in Appendix B.2 at $T = 0$. It can be written as

$$\text{Im} \chi_F(x-x',\omega \ll \hbar/\tau_c) = -D(x-x')\omega. \quad (3.30)$$

where $D(x)$ is a positive function of $x$ which is computed in Appendix B.2. Introducing this expression into Eq. (3.24), yields:

$$\Gamma(x-x',\tau) = -\frac{D(x-x')}{(|\tau| + \tau_c)^2} \quad (3.31)$$

at $T = 0$. Introducing the above expression into Eq. (3.28), we arrive at:

$$S_{\text{eff,BF}} = \frac{g_{BF}^2}{2\hbar} \int dx dx' d\tau \rho_B(x,\tau) \chi_F(x-x',\omega = 0) \rho_B(x',\tau) - \frac{g_{BF}^2}{2\hbar} \int dx dx' d\tau d\tau' \rho_B(x,\tau) \frac{D(x-x')}{(|\tau - \tau'| + \tau_c)^2} \rho_B(x',\tau'). \quad (3.32)$$

The results of the model calculation described in Appendix B.2 for the functions $D(q)/\hbar = -\text{Im} \chi^R_F(q,\omega)$ (for $\omega \ll \hbar/\tau_c$ and the static response function $\chi^R_F(q,\omega = 0)$ are displayed in Figs. 3.4 and 3.3. It can be seen that both functions are rather smooth (i.e. non-singular) functions of the longitudinal wavevector $q$. This assumption will prove important below. Furthermore, for certain values of the lattice filling, which determines the Fermi energy $\epsilon_F$, see Appendix B.2, $D(q)$ can be made negligible or zero for wide ranges of the wavevector $q$. This opens the possibility of tuning the strength of the dissipative effects by simply changing the fermion density. Note, however, that by strongly reducing the fermion density, the stability of the mixture may be jeopardized [119].

Thus we see that the boson interaction mediated by the Fermi gas consists, at low frequencies, of an instantaneous part (which stems for high frequency density fluctuations of the Fermi gas) and a dissipative part, which takes the form of a retarded $\sim 1/\tau_c$ interaction. The latter stems from the excitation by the motion of the bosons of real low-energy particle-hole pairs, which in a Fermi liquid yield the linear-$\omega$ behavior of the density response function (i.e. Landau damping). As discussed above, the instantaneous part of the interaction can related to the static density response of the Fermi gas and leads to a renormalization of the sound velocity $v$ and Luttinger parameter $K$ describing the low-temperature properties of 1D boson system. The renormalized parameters obey:

$$\frac{v(g_{BF})}{K(g_{BF})} = \frac{v(g_{BF} = 0)}{K(g_{BF} = 0)} + 2 \frac{g_{BF}^2}{\hbar} \chi_F(q = 0,\omega = 0), \quad (3.33)$$
Figure 3.3: The static response function $\chi^R(q, \omega = 0)/A$ of the fermions for different values of the Fermi energy $\epsilon_F = 2.0, 1.5, 1.0, 0.5, -0.5$ in units where $\hbar^2/2m = 1$ and $W = 1$. See Appendix B.2 for details of the calculation.

Furthermore, since the fermion-induced interaction is a density-density interaction (cf. first term in Eq. (3.32)), we have that [26]:

$$v(g_{BF})K(g_{BF}) = v(g_{BF} = 0)K(g_{BF} = 0).$$

(3.34)

These equations describe, to lowest order in $g_{BF}$, the screening of the boson-boson interaction by the fermion gas, which leads to corrections to the parameters $K$ and $v$ in Eq. (3.21), which depend only on the boson-boson interaction.

Using the bosonization formula (3.19), we obtain the representation of the dissipative action in terms of the density field $\phi(x, \tau)$:

$$\tilde{S}_D = S_D^f + S_D^b$$

(3.35)

$$S_{Db}^f = -\frac{g_{fD}}{\pi^2} \int dx d\tau d\tau' \frac{\partial_x \phi(x, \tau) \partial_x \phi(x, \tau')}{(|\tau - \tau'| + \tau_c)^2},$$

(3.36)

$$S_{Du}^b = -\frac{g_{bD}}{a_0} \int dx d\tau d\tau' \frac{\cos 2[\phi(x, \tau) - \phi(x, \tau')]}{|\tau - \tau'| + \tau_c^2}. $$

(3.37)

In the derivation of the above perturbations to the Gaussian action, Eq. (3.21), we have retained only terms whose integrands are not oscillatory and are the leading terms in a gradient expansion. However, in the case of a half-filled lattice, the following term:

$$S_{Du}^b = -\frac{g_{aD}}{a_0} \int dx d\tau d\tau' \frac{\cos 2[\phi(x, \tau) + \phi(x, \tau')]}{|\tau - \tau'| + \tau_c}.$$
3.3 Renormalization Group Analysis

must be also taken into account. This dissipative umklapp interaction arises from the periodicity of the boson system, for which which at half-filling $4k_F^B = \frac{\pi}{\tau_c}$ is a reciprocal lattice wave number. In this regard, we must recall that, in a periodic system, the (lattice) momentum along the $x$ direction is conserved modulo a reciprocal lattice wave number. Note that this term will be also generated by the renormalization group flow from product of the $S_u$ (cf. Eq. (3.22)) and $S_D^b$ (cf. (3.37)).

Furthermore, the bare dimensionless couplings are:

$$\bar{g}_D(0) = g_{BF}^2 D(q = 0),$$ (3.39)
$$g_{bD}(0) = 2g_{BF}^2 B_1^2 \rho a_0 D(q = 2k_F^B),$$ (3.40)
$$g_{uD}(0) = 2g_{BF}^2 B_1^2 \rho^2 a_0 D(q = 2k_F^B).$$ (3.41)

In the above expressions we have made explicit the dependence of the couplings of the cut-off scale, $a_0$ through the parameter $\ell = \log \frac{a_0(\ell)}{a_0}$, that is $a_0(\ell) = e^\ell a_0$ and thus $\ell = 0$ corresponds to the scale of the bare cut-off $a_0 \approx v\tau_c$, being $\tau_c$ the short-time cut-off introduced earlier.

3.3 Renormalization Group Analysis

Physically, the renormalization group (RG) flow of a system describes its behavior as it is cooled down towards the absolute zero. The effect of temperature can be mimicked by decreasing the short wavelength cutoff $\sim \frac{1}{a_0}$ introduced to properly define the low-temperature effective model of the
last section. As the absolute temperature decreases, the ground state is approached, and the couplings that define the effective low-energy theory of equations (3.21), (3.22), (3.36) (3.37), etc. (i.e., \(K, v, g_u, g_{bD}, \ldots\)), must change accordingly in order to account for the reduction of the available excited states. Thus, the quantum phases of the system can be studied by analyzing the asymptotic behavior of the ‘flow’ of these couplings in the limit where the cut-off tends to zero, that is, as the absolute temperature vanishes. In the perturbative approach to RG, the flow is described by a set of differential equations, whose solutions we study in this section.

Simple power-counting arguments show that \(S_f \sim \int dq dq' |q||\phi(q, q')|^2\) is an irrelevant perturbation in the renormalization-group sense. This is true provided \(D(q = 0)\) is not singular, which is indeed the case (see Fig. 3.4 and Appendix B.2). Indeed, this term alone leads to a momentum dependent broadening of the long-wave length phonon excitations of the gapless phase of the model in Eq. (3.21)). Therefore, in order to study the low-temperature properties of the model, it is justified to drop \(S_f\), and therefore we shall next focus our attention on the second term in Eq. (3.35) and consider the effective model described by \(S = S_B + S_{bD}\), where \(S_B\) is given by Eq. (3.21) and \(S_{bD}\) given by Eq. (3.37). In the half-filled case, we also have to take into account \(S_u\) given by Eq. (3.38). The resulting action contains only marginal and (potentially) relevant perturbations in the RG sense, which we shall analyze in this section. In what follows we shall consider the cases of integer and half-integer lattice filling separately. The details of the perturbative derivation of the RG equations are given in the Appendix B.3.

3.3.1 Integer Lattice filling

To \(O(g_{bD}, g_u^2)\) the flow equations in this case read:

\[
\frac{dg_u}{d\ell} = (2 - K)g_u, \tag{3.42}
\]

\[
\frac{dg_{bD}}{d\ell} = (1 - 2K)g_{bD}, \tag{3.43}
\]

\[
\frac{dK}{d\ell} = -(g_u^2 + 2\pi g_{bD})K^2, \tag{3.44}
\]

\[
\frac{dv}{d\ell} = -2\pi g_{bD}Kv. \tag{3.45}
\]

We neglect terms of \(O(g_{bD}^2)\) or higher because \(g_{bD}(0) \propto g_{BF}^2\), that is, \(g_{bD}\) is already second order in the Bose-Fermi coupling, which is assumed to be small. For \(g_{bD} = 0\), the equations reduce to those of a 1D Boson system in a commensurate potential first derived by Haldane [37–39] (see also [26]); for \(g_u = 0\), the equations reduce to those derived in Ref. [128].

The above equations show that near the SF to MI quantum critical point (corresponding to \(K^* = 2, g_u = 0, g_{bD} = 0\)) the dissipative interaction is a
highly irrelevant operator because $1 - 2K \approx -3$. Thus, the most important effect of the Fermi component of the mixture is to introduce a renormalization of the periodic potential and the screening of the interactions, which leads to the renormalization of the Luttinger parameter $K$ and the sound velocity $v$ given by Eq. (3.33).

From the analysis of the RG equations, which imply that the dissipation is an irrelevant operator in the RG sense, we conclude that dissipative effects are weak in the MI phase where $g_u$ grows as the energy cut-off $\hbar c/e^{\tau}$ ($\sim$ the absolute temperature) decreases. Thus, the dissipative term can be treated using perturbation theory, and leads to a small (when compared to the excitation energy) broadening of the phonon excitations in the superfluid TLL phase. As for the excitations of the MI phase, which corresponds to a ‘particle’ (i.e. excess by one bosons) or a ‘hole’ (i.e. absence of bosons) propagating against the Mott-insulating background, the dissipative part of the interaction with the Fermi gas similarly introduces damping on their motion, which translates into the broadening of the excitation energy dispersion. Such increased broadening could be measured by lattice modulation spectroscopy [73, 91, 129].

### 3.3.2 Half-Integer Lattice filling

In this case, and given that the initial conditions are the same for the $S^b_D$ and $S^u_D$ we note that they can be combined into a single term $S_D[\phi] = S^b_D[\phi] + S^u_D[\phi]$, which can be written as:

$$S_D[\phi] = \frac{g_D}{2a_0} \int dx d\tau d\tau' \frac{[\cos 2\phi(x, \tau) - \cos 2\phi(x, \tau')]^2}{(|\tau - \tau'| + \tau_c)^2},$$  

(3.46)

where $g_D(0) = \frac{1}{2} [g_{bD}(0) + g_{uD}(0)]$. The RG flow equations for this system then read:

$$\frac{dg_u}{d\ell} = (2 - 4K)g_u + \pi g_D,$$  

(3.47)

$$\frac{dg_D}{d\ell} = (1 - 2K + 4g_u)g_D,$$  

(3.48)

$$\frac{dK}{d\ell} = -(4g_u^2 + 2\pi g_{bD})K^2,$$  

(3.49)

$$\frac{dv_n}{d\ell} = -2\pi g_D K v.$$  

(3.50)

These RG equations describe the flow in the vicinity of a quantum critical point located at $K^* = \frac{1}{2}$, $g^*_u = g^*_D = 0$. Integrating them numerically, we obtain the phase diagram depicted in Fig. 3.5. Thus, we find that, for a relatively weak boson-fermion coupling $|g_{BF}|/\mu_B \sim 10^{-2}$, the part of the phase diagram occupied by the SF Tomonaga-Luttinger liquid phase (TLL) shrinks considerably. The latter phase is identified by the RG flows for which
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures

Figure 3.5: Phase diagram for the Tomonaga-Luttinger liquid (TLL) to Charge Density Wave (CDW) transition in the presence of a Fermi gas for $g_D \approx 2.5 \times 10^{-4}$, which corresponds to $|g_{BF}|/\mu_B \sim 10^{-2}$ ($\mu_B$ being the chemical potential of the bosons). $K$ is the Luttinger parameter of the bosons in the mixture (cf. Eq. (3.33)) and $g_u \propto U_B^{||} + O(g_{BF})$, where $U_B^{||}$ is the external periodic potential. The shaded area is the TLL phase. The diagonal dashed line represents the TLL-CDW phase boundary in the absence of fermions. The curves in the diagram represent RG flows for the $K$ and $g_u$ couplings for a set of initial conditions lying on the quarter circle on the right. The flow proceeds from right to left as $K$ always decreases according to Eq. (3.49).

both $g_u$ and $g_D \to 0$ as the phonon cut-off $\hbar a_0 e^\ell$ is reduced to zero (i.e. for $\ell \to +\infty$), that is, as the absolute temperature is decreased. On the other hand, the CDW phase is identified with those flows for which $g_u \sim 1$ at a certain value of $\ell^*$. However, it is also worth noticing that we have observed numerically (see Fig. 3.6) that, especially close to the phase boundary (red curve in Fig. 3.5), $g_u(\ell^*)/g_D(\ell^*) \sim 1$, even if $g_u$ becomes of order one first in all cases studied. This means that, even if the low-energy physics of this phase is dominated by the potential term $\propto g_u$, the dissipative effects are by no means negligible. It is interesting that this happens independently of how small the bare $g_u(0)$ is, and even in the limit $g_u(0) \to 0^+$. This is because, ultimately, the RG flow of $g_u(\ell)$ is controlled by the first term in Eq. (3.47), which leads to a much faster growth, although for small $g_u(0)$, the initial flow may be controlled by the second term in Eq. (3.47).

The RG flow equations indicate that the quantum phase transition occurs at $K = 1/2$, where the dissipation and periodic potential simultaneously become relevant, and the system is driven from a superfluid to a CDW Mott-insulating states. To study the interplay between the dissipation and interaction around the critical point, we adopt a variational self-consistent harmonic approximation (SCHA) by choosing a trial effective action of the
3.3 Renormalization Group Analysis

### Figure 3.6: Runaway renormalization-group (RG) flow of the couplings $g_u$, representing the periodic potential, and $g_D$, representing the effect of the fermion-induced dissipation for $K \lesssim \frac{1}{2}$. We found that even for relatively small initial potential $g_u(0)$ the RG flow of $g_u(\ell)$ eventually overcomes the flow of $g_D(\ell)$ and becomes $g_u(\ell) \sim 1$ first. This means that the system localizes and becomes a Mott insulator. However, as this plot illustrates, the effect of $g_D$, i.e. the renormalized dissipative coupling, is not negligible.

From:

$$S_v[\phi] = \int \frac{dq d\omega}{(2\pi)^2} G^{-1}_v(q, \omega) \phi^*(q, \omega) \phi(q, \omega)$$

(3.51)

where we have defined the Green’s function $G_v(q, \omega) = \left[ \frac{1}{2\pi K} \left( \frac{\omega^2}{v_s} + v_s q^2 \right) \right] + \frac{\eta}{a_0 |\omega| + \Delta a_0 \tau_c}^{-1}$ with the dimensionless self-consistent parameters $\eta$ and $\Delta$ that can be determined by the minimization of the variational free-energy. A variational estimate $F_{var}$ of the true free-energy $F$ can be obtained from Feynman’s variational principle [40]:

$$F \leq F_{var} = F_v + \beta^{-1}(S - S_v)$$

(3.52)

Therefore, optimizing $\delta F_{var}[G_v] / \delta G_v = 0$, the parameters $\eta$ and $\Delta$ are found by solving the self-consistent equation above (Eq. ((B.95))), so that (see appendix B.4 for further details):

$$\eta = \frac{8g_u}{(2\pi)^2} \alpha(\eta, \Delta)^{4K}$$

(3.53)

$$\Delta = \frac{8(g_u + g_D)}{(2\pi)^2} \alpha(\eta, \Delta)^{4K}$$

(3.54)

where we have defined $\alpha(\eta, \Delta) = \left[ \frac{2K\pi + 2\sqrt{K}\pi \Delta}{4} \right]$. Overall, the gap is largely enhanced for $K < \frac{1}{2}$ as shown in Fig. 3.7. This is because the dissipation...
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Figure 3.7: Mott gap $\Delta$ in the presence and absence of fermion-induced dissipation as obtained from the self-consistent harmonic approximation (SCHA, see Sec. 3.3.2 for details). It can be seen that the dissipation greatly enhances the Mott gap by suppressing the quantum fluctuations of the bosons in the CDW Mott insulating state. Note that the SCHA erroneous yields a discontinuous phase transition at the critical point $K^* = \frac{1}{2}$. This is a well known artifact of this approximation [40].

plays a similar role to friction, which hinders the motion of the particles and thus helps to stabilize the CDW Mott-insulating state. Note, however, that the SCHA erroneously yields a discontinuous transition for $K = \frac{1}{2}$. This is a well known artifact of this approximation [40].

3.4 Commensurate - Incommensurate transition in the Presence of Dissipation

3.4.1 Integer filling

In this case, as for the TLL to MI transition, the effect of dissipation is rather weak. A way of understanding this is to stop the RG flow when $g_0(\ell) \sim 1$ and consider the sine-Gordon model at the Luther-Emery point where it maps to a 1D relativistic model of massive (Dirac) fermions [40, 123]. Diagonalization of this model yields two bands separated by a gap: a filled ‘valence’ band and an empty ‘conduction’ band [40, 123]. Tuning the chemical for the bosons amounts to introducing particles in the conduction band or holes in the valence band [123]. For small particle (hole) density, the system can be described as a Tonks-Girardeau gas [88] characterized by Luttinger
3.5 Conclusions

parameter $K \approx 1$. The dissipation being an irrelevant for $K > K^* = \frac{1}{2}$, its effect on such a dilute liquid of particles (holes) is negligible as far as the ground state properties are concerned (although it will lead to a small linewidth of the excitations, which is due to collisions between the bosons and the fermions). Thus, in particular, the exponents characterizing the commensurate to incommensurate (C-IC) transition are thus expected to remain unchanged and, therefore, the density of particles (or holes) \[26, 123\] will grow as $\sqrt{\mu - \mu_c}$, where $\mu_c \sim \Delta$, where $\Delta$ is the MI gap.

3.4.2 Half-integer filling

For half-integer filling the situation is very different, as it was already pointed out in our discussion of the previous section. We can realize this by considering again the case where we take $g_D$ infinitesimally small but $g_u \sim 1$. Applying the same reasoning used in the previous section, the sine-Gordon model $S_b[\phi] + S_u[\phi]$ in this case maps to a system of Dirac fermions describing the (fractionally charged) soliton and anti-soliton excitations of the CDW state (configurations of the form 10101011010101, for the solitons, and 101010101011, for the anti-solitons). A dilute gas of such excitations can be described as a Luttinger gas with a parameter $K \approx \frac{1}{4} < K^* = \frac{1}{2}$. Thus, the dissipative term $S_D[\phi]$ from Eq. (3.46) is a strongly relevant perturbation, which, as discussed in Ref. [128], leads to the localization of the system in a new phase, which we term dissipative insulator (DI). In this phase, the boson density, $\langle \rho_B(x) \rangle$ exhibits long-range order [128] with a characteristic wave number equal to $4\pi \rho_0$.

However, it is worth mentioning that, as Fig. 3.6 demonstrates, assuming that $g_D$ is infinitesimal when $g_u \sim 1$ is not representative of the RG flow described in the previous section. Indeed, we numerically found that even in the case $g_u(0)\to 0, g_D(\ell^*) \lesssim g_u(\ell^*) \sim 1$ (see Fig. 3.6) in other words, the dissipation, although diverging less strongly than the periodic potential, is not a small perturbation on the CDW state. Thus, we expect that the dissipative term needs to be treated on equal footing with the potential term $\propto g_u$. The universality class of the commensurate to incommensurate transition is therefore expected to be different from the case of integer filling.

3.5 Conclusions

In conclusion, we have studied a model for a mixed dimensional Bose-Fermi mixture in an optical lattice, where the bosons are confined to one dimension whereas the fermions are free to hop in three dimensions (albeit with renormalized dispersion). We have argued that this system is a realization of a 1D interacting Bose gas coupled to a dissipative bath of the Ohmic type. In addition, the fermions also screen the boson-boson interactions. For integer filling we have found that, as it was also observed in mean-field studies of
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures

Figure 3.8: Schematic phase diagram of a 1D Boson system embedded in a Fermi Gas.

3D dimensional optical lattices [108], the dominant effect of the fermions on the bosons is the screening of their interactions. Provided the so-called self-trapping effect can be subtracted or compensated, the screening of the boson interactions leads to an enhancement of the superfluid properties as the bosons become polarons with reduced effective interactions. In this case, dissipation effects only contribute to an increase in the linewidth of the excitations in both the super-fluid and Mott-insulating phases, which could be detected by means of lattice modulation spectroscopy [73, 91, 129].

On the other hand, the effect of the fermion-induced dissipation is much more severe on the system close to a superfluid to CDW Mott-insulator transition, which happens at half-integer filling. In this case, the dissipative effects strongly hinder the motion of the bosons and help to stabilize the CDW phase (cf. Fig. 3.5) and to enhance the CDW gap (cf. Fig. 3.7). This effect will lead to a dramatic suppression of the superfluid phase, which will be observed as a reduction (relative to the pure boson case) of the potential depth required for the bosons to localize in the CDW phase. The enhancement of the gap can be also probed using lattice modulation spectroscopy.

We have also studied the commensurate-incommensurate transition and argued that in the case of integer lattice filling, the fermion-induced dissipation is an irrelevant perturbation and therefore, the universality class should not be altered. However, in the case of half-integer filling the dissipation is relevant (but less than the external potential) and therefore we expect the universality class will be modified. This subject requires further
study, but it has not been pursued here. The conclusions of this chapter are summarized in the schematic phase diagram of Fig. 3.8.
Chapter 3. Superfluid to insulator transition in mixed dimensionality

Bose-Fermi mixtures
Appendices
A Phase equilibria

A.1 Mean-field approximation

In this appendix, we provide the intermediate steps necessary to obtain the mean-field Hamiltonian, Eq. (2.16). First of all, let us evaluate the expectation value of the fermion density operator in a tube \( \hat{\rho}_{FR} (x) \). By substituting the expression (2.6) into (2.11) and using that, for a non-interacting Fermi gas, \( \langle \hat{f}_{k} \hat{f}_{k} \rangle = \delta_{kk'} n_{k} \), with \( n_{k} \) being the Fermi-Dirac distribution function, we obtain:

\[
\langle \hat{\rho}_{FR} (x) \rangle = \frac{1}{L} \sum_{k} n_{k} \int d\mathbf{r}_{\perp} |\varphi_{R}(\mathbf{r}_{\perp})|^{2} |\phi_{k_{\perp}}(\mathbf{r}_{\perp})|^{2} \, . \tag{A.1}
\]

Furthermore, we can assume that the fermions occupy only the lowest Bloch band of the square lattice, thus the Bloch wave function \( \phi_{k_{\perp}}(\mathbf{r}_{\perp}) \) can be developed in terms of Wannier functions \( w_{R}(\mathbf{r}_{\perp}) \) localized at the \( R \)-th tube:

\[
\phi_{k_{\perp}}(\mathbf{r}_{\perp}) = \frac{1}{\sqrt{N}} \sum_{R} e^{ik_{\perp} \cdot \mathbf{R}} w_{R}(\mathbf{r}_{\perp}) \, . \tag{A.2}
\]

where \( N = N_{y} N_{z} \). Therefore, Eq. (A.1) reads:

\[
\langle \hat{\rho}_{FR} (x) \rangle = \frac{1}{L} \sum_{k} n_{k} \frac{1}{N} \sum_{R,R''} \int d\mathbf{r}_{\perp} e^{ik_{\perp} \cdot (R'' - R')} w_{R}^{*}(\mathbf{r}_{\perp}) w_{R''}(\mathbf{r}_{\perp}) |\varphi_{R}(\mathbf{r}_{\perp})|^{2} \, . \tag{A.3}
\]

\[
\simeq \frac{N_{F}}{L} \frac{1}{N} \int d\mathbf{r}_{\perp} |w_{R}(\mathbf{r}_{\perp})|^{2} |\varphi_{R}(\mathbf{r}_{\perp})|^{2} = \rho_{F}^{0} A \, , \tag{A.4}
\]

where \( N_{F} = \sum_{k} n_{k} \), \( \rho_{F}^{0} \) is the 1D density of fermions (2.15), and

\[
A = N \int d\mathbf{r}_{\perp} |\varphi_{R}(\mathbf{r}_{\perp})|^{2} |\phi_{k_{\perp}}(\mathbf{r}_{\perp})|^{2} \simeq \frac{1}{N} \int d\mathbf{r}_{\perp} |w_{R}(\mathbf{r}_{\perp})|^{2} |\varphi_{R}(\mathbf{r}_{\perp})|^{2} \, . \tag{A.5}
\]

In this derivation, we have used the fact that the boson Wannier orbital \( \varphi_{R}(\mathbf{r}_{\perp}) \) is strongly localized around \( \mathbf{r}_{\perp} = \mathbf{R} \), thus we have neglected the contributions of the terms \( \mathbf{R}' \) and \( \mathbf{R}'' \) different from \( \mathbf{R} \), because the corresponding wavefunction overlaps are negligible. Note also that the constant \( A \) (A.5) does not depend on the tube index \( R \). Furthermore, we can approximate \( \varphi_{R}(\mathbf{r}_{\perp}) \simeq e^{-|\mathbf{r}_{\perp} - \mathbf{R}|^{2}/2\ell_{B}^{2}/(\sqrt{\pi} \ell_{B})} \) and therefore \( w_{R}(\mathbf{r}_{\perp}) \simeq \ldots \).
Appendices

\[ e^{-|\mathbf{r}_\perp - \mathbf{R}|^2/2\ell^2_F}/(\sqrt{\pi} \ell_F) \] with \( \ell_B < \ell_F \ll d \), therefore the constant \( A \) is given by:

\[ A \simeq \frac{1}{\pi (\ell_F^2 + \ell_B^2)} \quad (A.6) \]

Taking into account that the mean-field averages of the boson and fermion densities are given by the expressions \((2.13)\), in order to obtain the final expression of the Hamiltonian, Eq. \((2.16)\), we need to deal with

\[ \sum_R \int dx \langle \hat{\rho}_{BR}(x) \rangle \hat{\rho}_{FR}(x) \]

\[ = \rho_B^0 \sum_R \sum_k \int d\mathbf{r}_\perp |\varphi_R(\mathbf{r}_\perp)|^2 |\phi_{k\perp}(\mathbf{r}_\perp)|^2 \hat{f}_{k\perp} \hat{f}_{k\perp} \quad (A.7) \]

\[ \simeq \rho_B^0 A \sum_k \hat{f}_{k\perp} \hat{f}_{k\perp} \quad (A.8) \]

\[ \simeq \rho_B^0 A \sum_k \hat{f}_{k\perp} \hat{f}_{k\perp} \quad (A.9) \]

**A.2 Character of the transitions for which the Fermi density changes**

In this appendix we want to carry on an expansion for small fermion density so that to be able to establish the nature of the phase transitions where the number of Fermi surfaces changes from zero to one, such as the phase transition between a pure boson and a mixed phase. This is done in the same spirit to the expansion for small boson density conducted at the end of Sec. 2.3.1 that has allowed us to establish that the transitions between pure fermion and any phase with a finite density of bosons can only be first order.

The starting point is the mean-field Hamiltonian derived in Eq. \((2.16)\), with the difference that now, to simplify the analysis, we will assume that the fermion dispersion appearing in Eq. \((2.18)\) is quadratic, \( \varepsilon(\mathbf{k}) = k^2/2m_F \), where \( \mathbf{k} = k_x \) if fermions, like bosons, move strictly in 1D, whereas \( \mathbf{k} = (k_x, k_y, k_z) \) if we instead consider the mixed-dimensional case where fermions are free to move in all three dimensions, while bosons still move strictly in 1D. Note that assuming a quadratic isotropic dispersion for the fermions is expected to be a good approximation in the small fermion density regime that we are going to consider here, even if the true dispersion in the mixed-dimensional case is anisotropic: In fact, when fermions start to mix with bosons, they must necessarily occupy the lowest band energy levels, for which the dispersion can be approximated as quadratic. The anisotropy can be rescaled out when evaluating the fermion density \( \rho_F^0 \) as a function of the Fermi wavevector \( k_F \), and yields to an overall prefactor relative to the isotropic result.

Considering the mean-field Hamiltonian derived in Eq. \((2.16)\), the following step is to average over the fermion operator density in the fermion
Hamiltonian (2.18), obtaining the Fermi-Dirac distribution function at zero temperature, \( \langle \hat{f}_{k} \hat{f}_{k} \rangle = n_{k} = \theta(k_{F} - k) \). The free energy density we obtain this way will have a different dependence on the Fermi density depending on how fermions move in 1D or 3D.

Let us start considering the case where fermions move in 1D, so that the lineal Fermi density defined in Eq. (2.15) is \( \rho_{F}^{0} = N_{F}/NL = k_{F}/\pi \) and the free energy potential \( g = \langle \hat{H}_{mf} \rangle / LN \) reads as:

\[
g = \frac{\pi^{2}}{6m_{F}}(\rho_{F}^{0})^{3} - (\mu_{F} - g_{BF} A \rho_{B}^{0}) \rho_{F}^{0} + \frac{(\rho_{B}^{0})^{3}}{2m_{B}} e(\gamma) - \mu_{1D}^{1D} \rho_{F}^{0} . \tag{A.10}
\]

Note that now the free energy potential \( g = g(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}, \rho_{F}^{0}) \) depends on both the boson and fermion densities as well as on the chemical potentials. This means that minimizing \( g \) with respect to the fermion density,

\[
f(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}) = \min_{\rho_{F}^{0}} g(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}, \rho_{F}^{0}) , \tag{A.11}
\]

we retrieve the free energy potential \( f(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}) \) considered in Eq. (2.19), which global minimum with respect to the boson density gives the true thermodynamic grand-canonical free energy density (2.22).

However, if we instead minimize \( g = g(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}, \rho_{F}^{0}) \) with respect to the boson density,

\[
h(\mu_{1D}^{1D}, \mu_{F}, \rho_{F}^{0}) = \min_{\rho_{B}^{0}} g(\mu_{1D}^{1D}, \mu_{F}, \rho_{B}^{0}, \rho_{F}^{0}) , \tag{A.12}
\]

so that to eliminate \( \rho_{B}^{0} \) in favor of \( \rho_{F}^{0} \), \( \mu_{F} \) and \( \mu_{1D}^{1D} \), then the free energy potential \( h(\mu_{1D}^{1D}, \mu_{F}, \rho_{F}^{0}) \) thus obtained can be used to study the phase transitions where the number of Fermi surfaces changes from zero to one, by expanding for small values of \( \rho_{F}^{0} \). Because the dimensionless function \( e(\gamma) \) coming from the Bethe ansatz is determined numerically, this plan of deriving the free energy potential \( h(\mu_{1D}^{1D}, \mu_{F}, \rho_{F}^{0}) \) is not a trivial one. However, we can carry on this procedure in two opposite limits, corresponding to high \((\gamma = m_{B} g_{BB}^{1D} / \rho_{B}^{0} \ll 1)\) and low \((\gamma \gg 1)\) density, respectively:

\[
e(\gamma) \simeq \begin{cases} 
\gamma & \gamma \ll 1 \\
\gamma & \gamma \gg 1 
\end{cases} . \tag{A.13}
\]

Note that the last limit results in a contribution to the free energy potential \( h \) of \( \pi^{2}(\rho_{F}^{0})^{3}/6m_{B} \), which is identical to the kinetic energy of a free 1D Fermi gas. This is the result of fermionization in the Tonks-Girardeau limit [26].

Evaluating (A.12) by solving \( \partial g / \partial \rho_{B}^{0} = 0 \) for \( \rho_{B}^{0} \), in both cases of high and low boson density, we obtain a series in terms of the Fermi density of cubic form:

\[
h = h_{0} + h_{2}\rho_{F}^{0} + h_{4}(\rho_{F}^{0})^{2} + h_{6}(\rho_{F}^{0})^{3} + \cdots . \tag{A.14}
\]
For high boson density the coefficients, for \( \mu_B^{1D} > A g_{BF} \rho_F^0 \), which requires \( \mu_B^{1D} \) and \( g_{BF} \) to have the same sign, are given by

\[
\begin{align*}
    h_2 &= \frac{A g_{BF}}{g_{BB}^{1D}} \mu_B^{1D} - \mu_F \quad \text{(A.15)} \\
    h_4 &= -\frac{A^2 g_{BF}^2}{2 g_{BB}^{1D}} \quad \text{(A.16)} \\
    h_6 &= \frac{\pi^2}{6 m_F} . \quad \text{(A.17)}
\end{align*}
\]

In the low boson density limit, instead, we obtain (also for \( \mu_B^{1D} > A g_{BF} \rho_F^0 \)) that the coefficients of the expansion (A.14) are now given by

\[
\begin{align*}
    h_2 &= \frac{A g_{BF}}{\pi} \sqrt{2m_B \mu_B^{1D}} - \mu_F \quad \text{(A.18)} \\
    h_4 &= -\frac{A^2 g_{BF}^2 \sqrt{m_B}}{2 \pi \sqrt{2 \mu_B^{1D}}} \quad \text{(A.19)} \\
    h_6 &= \frac{\pi^2}{6 m_F} - \frac{A^3 g_{BF}^3 \sqrt{m_B}}{12 \sqrt{2 \pi \mu_B^{1D^{3/2}}}} . \quad \text{(A.20)}
\end{align*}
\]

In this last case, note that, for \( m_F \ll m_B \), as we have assumed in the main text, the coefficient of the cubic term is expected to be positive and large. In both cases, while \( h_6 > 0 \), the coefficient of the square term is always negative, \( h_4 < 0 \), implying that the transition cannot be continuous, rather it is first order. For small fermion density, the transition has place for \( h_2 > 0 \) and \( h_4 = -2 \sqrt{h_2 h_6} \), implying that, for large values of the coefficient \( h_6 \), \( h_2 \to 0 \) and the transition is weakly first order, as we have indeed observed numerically in many cases.

The \( \rho_F^0 \) expansion just carried on thus allows us to understand the nature of the transition between the pure Bose gas and mixed phases and deduce that it has to be first order in the strictly 1D limit. We can merge this result with the one obtained in Sec. 2.3.1, where we were expanding for small boson density (Tonks-Girardeau limit), and found that the transition between the pure Fermi gas and the mixed phases is also first order. We can thus conclude that in the 1D limit the transitions between the pure boson/fermion phases and the mixed phase, must be all first order.

For comparison purposes, we can now consider the case of mixed dimensionality, i.e., where fermions move in 3D. Now, the 3D Fermi density is given by \( N_F / \Omega = \rho_F^0 d^{-2} = k_F^3 / 6 \pi^2 \), where the volume is \( \Omega = N d^2 L \), \( d \) is the spacing between the tubes (cf. Fig 3.8), and \( \rho_F^0 \) the lineal fermion density. Thus the kinetic energy contribution to the free energy potential
A.2 Character of the transitions for which the Fermi density changes

\( g = \langle \hat{H}^{mf} \rangle / LN \) now scales differently than in the 1D limit:

\[
g = \frac{d^2 (6\pi^2 d^2 \mu_F^0)^{5/3}}{20\pi^2 m_F} - (\mu_F - g_{BF} \rho_B^0) \rho_F^0 + \frac{(\rho_B^0)^3}{2m_B} c(\gamma) - \mu_B^1 \rho_B^0. \tag{A.21}
\]

As before, we eliminate the boson density \( \rho_B^0 \) from the potential \( g \) by making use of (A.12) and then we expand for small values of the Fermi density \( \rho_F^0 \). In this case we obtain:

\[
h = h_0 + h_2 \rho_F^0 + h_{10/3} (\rho_F^0)^{5/3} + \cdots, \tag{A.22}
\]

where the coefficient \( h_2 \) is given by the expressions (A.15) for the high boson density, while by (A.18) for the low boson density limit. The coefficient \( h_{10/3} \) is in both cases instead given by:

\[
h_{10/3} = \frac{d^{-4/3} (6\pi^2)^{5/3}}{20\pi^2 m_F}. \tag{A.23}
\]

We can thus see that, while the coefficient \( h_2 \) can change sign depending on the values of the system parameters, the coefficient of the next order term, which scales like \((\rho_F^0)^{5/3}\) rather than quadratically, is always positive \( h_{10/3} > 0 \). This means that the position of the closest minimum to \( \rho_F^0 = 0 \) is entirely controlled by the sign of \( h_2 \), that is, the transition between the pure boson and mixed phases must be continuous. By contrast, as we have argued in Sec. 2.3.1, the transition between the pure fermion and the mixed phase is independent on the dimensionality where fermions live and is always first order.

The main conclusion of the simple exercise carried on in this appendix is that the different nature of the phase transitions where the number of Fermi surfaces changes from zero to one between the strictly 1D case and the mixed-dimensional case is a consequence of the different scaling of the fermion kinetic energy in 1D and in 3D. Note that this result is also applicable to the transitions between the pure fermion and mixed phases, as bosons in 1D at low density behave as a free Fermi gas by virtue of fermionization.
B Superfluid to insulator transition in mixed dimensionality Bose-Fermi mixtures

B.1 Relating \( \chi^R_F(x, \omega) \) to \( \chi_F(x, \tau) \)

In this appendix we will derive the identity that we used in the main text to relate the retarded density correlation function to its imaginary time version at zero temperature. We shall first recall that the retarded correlation function is defined as:

\[
\chi^R_F(x, t) = -\frac{i}{\hbar} \vartheta(t) \langle [\delta \rho_F(x, t) \delta \rho_F(0, 0)] \rangle_F, \tag{B.1}
\]

where \( \delta \rho_F(x, t) = \int d\mathbf{r}_\perp |w_0(\mathbf{r}_\perp)|^2 \delta \rho_F(x, \mathbf{r}_\perp, t), \delta \rho_F(x, t) = e^{iH_F t/\hbar} \delta \rho_F(x) e^{-iH_F t/\hbar}, \)

and \( \delta \rho_F(\mathbf{r}) = \rho_F(\mathbf{r}) - \rho^0_F(\mathbf{r}). \)

However, the imaginary time correlation is defined by the expectation value

\[
\chi_F(x, \tau) = -\frac{1}{\hbar} \langle \delta \rho_F(x, \tau) \delta \rho_F(0, 0) \rangle_F, \tag{B.2}
\]

where \( \delta \rho_F(x, \tau) = e^{H_F \tau/\hbar} \delta \rho_F(x) e^{-H_F \tau/\hbar}. \) By taking the Fourier transform of the spectral representation of Eq. (B.1) and comparing it to the spectral representation of

\[
\chi^R_F(x, i\omega_n) = \int_0^{\beta/2} d\tau \chi_F(x, \tau) e^{i\omega_n \tau}, \tag{B.3}
\]

we arrive at the following relation:

\[
\chi_F(x, i\omega_n) = \int d\omega \frac{\text{Im} \chi^R_F(x, \omega)}{\omega - i\omega_n} = \int_0^{+\infty} d\omega \frac{\text{Im} \chi^R_F(x, \omega)}{\omega - i\omega_n} + \frac{\text{Im} \chi^R_F(x, \omega)}{\omega + i\omega_n}, \tag{B.4}
\]

where, in the deriving the last expression, we have used that \( \text{Im} \chi_F(x, -\omega) = -\text{Im} \chi_F(x, -\omega). \)

Hence, introducing the last expression in Eq. (B.3), taking \( \beta \to +\infty, \) and performing the integral over \( \omega_n \) with the help of Jordan’s lemma, we arrive at the desired result:

\[
\chi_F(x, \tau) = \int_0^{+\infty} d\omega \frac{e^{-\omega |\tau|}}{\pi} \text{Im} \chi^R_F(x, \omega). \tag{B.5}
\]
B.2 Fermion bath response function

Let us consider the Fourier transform of the density response of the Fermi gas at zero temperature, which, as we neglect the interactions induced by the bosons on the fermions, is just the Lindhard function. Recalling that the Matsubara version of the latter is defined as 

\[ \chi_F(x, r_\perp, r'_\perp, \tau) = -\frac{1}{\beta} \langle \delta \rho_F(x, r_\perp, \tau) \delta \rho_F(0, r'_\perp, 0) \rangle_F, \]

where \( \delta \rho_F(x, r_\perp) = \rho_F(x, r_\perp) - \rho^0(x, r_\perp) \),

being \( \rho_F(x, r_\perp) = \sum_{k,k',k_\perp} \varphi_{k,k_\perp}^*(x, r_\perp) \varphi_{k,k_\perp}(x, r_\perp) f_{k,k_\perp} f_{k',k_\perp} \) the density operator and \( \rho^0(x, r_\perp) = \langle \rho_F(x, r_\perp) \rangle_F \), the equilibrium density. We shall assume that the single particle orbitals of the fermions are given by

\[ \varphi_{k,k_\perp}(x, r_\perp) = \varphi_k(x) \varphi_{k_\perp}(r_\perp) = \frac{1}{\sqrt{LM}} \sum_R e^{i(kx + k_\perp \cdot R)} w^F_0(r_\perp - R), \]

where \( L \) is the (normalization) length in 1D and \( M \) is the number of lattice sites labelled by \( R = (n, m)b_0 \) (\( b_0 \) is the lattice parameter), and \( w^F_0(r_\perp) \) is Wannier orbital for the fermions. In the above expression we have assumed that the strength of the longitudinal potential in 1D is weak so that the Bloch orbitals \( \varphi_k(x) \approx \frac{e^{ikx}}{\sqrt{L}} \). Thus, we arrive at the following expression:

\[ \chi_F(q, r_\perp, r'_\perp, \omega) = \int d\tau e^{i(\omega \tau - qx)} \chi_F(x, r_\perp, r'_\perp, \tau) \]

\[ = \sum_{k,k',k_\perp} \frac{n_{k,k_\perp} - n_{k+q,k_\perp'}}{i \hbar \omega - \epsilon(k + q, k_\perp') + \epsilon(k, k_\perp)} A_{k,k_\perp}(r_\perp, r'_\perp), \]

(B.7)

where the function \( A_{k,k_\perp}(r_\perp, r'_\perp) = \varphi_{k_\perp}(r_\perp) \varphi_{k_\perp'}(r'_\perp) \varphi_{k_\perp}(r_\perp) \varphi_{k_\perp'}(r'_\perp) \).

The single-particle dispersion of the fermions is

\[ \epsilon(k, k_\perp) = \epsilon_\parallel(k) + \epsilon(k_\perp) \]

\[ = \frac{\hbar^2 k^2}{2m^*_F} - 2t_\perp (\cos k_y b_0 + \cos k_z b_0) \]

(B.8)

where we have assumed that the longitudinal dispersion is approximated by a quadratic dispersion characterized by an effective mass \( m^*_F \approx m_F \) and transverse motion is described by a tight-binding dispersion characterized by a transverse hopping \( t_\perp \).

Indeed, the response function in which we are interested is not the Lindhard function, Eq. (B.7), but the following integral of it:

\[ \chi_F(q, \omega_n) = \int d\mathbf{r}_\perp d\mathbf{r}'_\perp F_0(\mathbf{r}_\perp, \mathbf{r}'_\perp) \chi(q, \mathbf{r}_\perp, \mathbf{r}'_\perp, \omega_n), \]

(B.9)

where \( F_0(\mathbf{r}_\perp, \mathbf{r}'_\perp) = |w_0(\mathbf{r}_\perp)w_0(\mathbf{r}'_\perp)|^2 \), where \( w_0(\mathbf{r}) \) are the Wannier orbitals for the bosons in the lowest Bloch band. Thus, in order to compute
Eq. (B.9), we need to consider the following integral:

$$
\int dr_\perp dr'_\perp F_0(r_\perp, r'_\perp) A_{k_\perp, k'_\perp}(r_\perp - r'_\perp)
= \left| \int dr_\perp \varphi_{k_\perp}^*(r_\perp)|w_0(r_\perp)|^2 \varphi_{k'_\perp}(r_\perp) \right|^2
= \frac{1}{M} \sum_{\mathbf{R}, \mathbf{R'}} e^{i(k_\perp \cdot \mathbf{R} - k'_\perp \cdot \mathbf{R'})} \int dr_\perp |w_0(r_\perp)|^2 |w_0^F(r_\perp - \mathbf{R})|^2
\approx \frac{1}{M} \int dr_\perp |w_0(r_\perp)|^2 |w_0^F(r_\perp)|^2 = \frac{A}{M^2},
$$

(B.10)  

(B.11)  

(B.12)

where we have approximated $w_0(r_\perp) \approx e^{-|r_\perp|^2/(2\ell_B^2)}$ and $w_0^F(r_\perp) \approx e^{-|r_\perp|^2/(2\ell_F^2)}$ and assumed that $\ell_B \ll \ell_F$, so that we can neglect overlap between the Wannier orbitals for $\mathbf{R} \neq \mathbf{R'}$. In the above expression,

$$
A = \int dr_\perp |w_0(r_\perp)|^2 \left| w_0^F(r_\perp) \right|^2 = \frac{1}{\pi^2(\ell_F^2 + \ell_B^2)^2}.
$$

(B.13)

Hence,

$$
\chi_F(q, i\omega_n) \approx \frac{A}{M^2 L} \sum_{k, k_\perp, k'_\perp} \frac{n_{k, k_\perp} - n_{k+q, k'_\perp}}{i\hbar \omega_n - \epsilon(k + q, k'_\perp) + \epsilon(k, k_\perp)}.
$$

(B.14)

Next, we take the thermodynamic limit, transform the sums over $k, k_\perp, k'_\perp$ into integrals, and introduce the density of states of the 2D (square) lattice of tubes [130],

$$
\rho(\varepsilon) = \frac{2}{\pi^2 W} K \left[ \sqrt{1 - \left( \frac{\varepsilon}{W} \right)^2} \right]^2 \theta(W^2 - \varepsilon^2).
$$

(B.15)

where $K(z)$ denotes the complete elliptic integral of the first kind and $W = 4t_\perp$. Thus, the retarded response function (obtained from $\chi_F(q, i\omega_n)$ by means of analytic continuation where $i\omega_n \rightarrow \omega^+ = \omega + i0^+$) can be rewritten
as follows

\[
\chi^R_F(q, \omega_n) = A \int_{-W}^{+W} d\varepsilon d\varepsilon' \rho(\varepsilon)\rho(\varepsilon') \int \frac{dk}{2\pi} \frac{n_{k,\varepsilon} - n_{k+q,\varepsilon'}}{\hbar(\omega^+ + \varepsilon - \varepsilon' - \epsilon_\parallel(k + q) + \epsilon_\parallel(k)}
\]

\[
= A \int_{-W}^{+W} d\varepsilon d\varepsilon' \rho(\varepsilon)\rho(\varepsilon') \times \int \frac{dk}{2\pi} n_{k,\varepsilon} \left[ \frac{1}{\hbar\omega^+ + \varepsilon - \varepsilon' - \epsilon_\parallel(k + q) + \epsilon_\parallel(k)} \right.
\]

\[
+ \frac{1}{-\hbar\omega^+ + \varepsilon - \varepsilon' + \epsilon_\parallel(k + q) - \epsilon_\parallel(k)} \left. \right] = A \int_{-W}^{+W} d\varepsilon d\varepsilon' \rho(\varepsilon)\rho(\varepsilon') \int \frac{dk}{2\pi} n_{k,\varepsilon} \times \left[ \frac{1}{\hbar\omega^+ + \varepsilon - \varepsilon' - \epsilon_\parallel(k + q) + \epsilon_\parallel(k)} + (\omega^+ \rightarrow -\omega^+) \right]
\]

At zero temperature \(n_{k,\varepsilon} = \theta(\epsilon_F - \varepsilon - \epsilon_\parallel(k))\), where \(\epsilon_F = \mu_F(T = 0)\) is the Fermi energy (note that \(\epsilon_F > -W\) otherwise there will be no fermions in the mixture).

Let us first consider (minus) the imaginary part of \(\chi^R_F(q, \omega)\):

\[
\text{Im} \left[ -\chi^R_F(q, \omega) \right] = A \frac{1}{2} \int_{-W}^{+W} d\varepsilon \int \frac{dk}{2\pi} \theta \left( \epsilon_F - \epsilon - \frac{\hbar^2 k^2}{2m_F^*} \right)
\]

\[
\times \rho(\varepsilon) \left[ \rho \left( \hbar\omega + \varepsilon - \frac{\hbar^2 q^2}{2m_F^*} - \frac{\hbar^2 q k}{m_F^*} \right) - \rho \left( \hbar\omega - \varepsilon + \frac{\hbar^2 q^2}{2m_F^*} + \frac{\hbar^2 q k}{m_F^*} \right) \right],
\]

where we have set \(\epsilon_\parallel(k + q) - \epsilon_\parallel(k) = \frac{\hbar^2 q^2}{2m_F^*} + \frac{\hbar^2 q k}{m_F^*}\). The above expression can be used to obtain the (imaginary part of the) response for arbitrary \(\omega\). However, we are only interested in the regime of small \(\omega\), for which we can expand \(\rho(\hbar\omega \pm E(k, q, \varepsilon)) = \rho(E(k, q, \varepsilon)) \pm \rho'(E(k, q, \varepsilon))\hbar\omega + \cdots\) (where \(E(k, q, \varepsilon) = \varepsilon - \frac{\hbar^2}{2m_F^*}(q^2 + 2kq)\)) and therefore, to lowest order in \(\omega\),

\[
\text{Im} \left[ -\chi^R_F(q, \omega) \right] \simeq A \hbar\omega \int_{-W}^{+W} d\varepsilon \int \frac{dk}{2\pi} \rho(\varepsilon)\rho' \left( \varepsilon - \frac{\hbar^2}{2m_F^*}(q^2 + 2kq) \right) \theta \left( \epsilon_F - \varepsilon - \frac{\hbar^2 k^2}{2m_F^*} \right).
\]

In order to perform the integration over \(k\), we define from the constraints imposed by the Heaviside step function in Eq. (B.19), \(k_F(\varepsilon) = \sqrt{\frac{2m_F^*}{\hbar^2}(\epsilon_F - \varepsilon)}\).
B.2 Fermion bath response function

for $\varepsilon < \epsilon_F$, and note that

$$
\int_{-k_F(\epsilon)}^{+k_F(\epsilon)} dk \partial_k \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 + 2kq) \right)
$$

(B.20)

$$
= -\frac{m^*_F}{\hbar^2 q} \int_{-k_F(\epsilon)}^{+k_F(\epsilon)} dk \partial_k \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 + 2kq) \right)
$$

(B.21)

$$
= -\frac{m^*_F}{\hbar^2 q} \left[ \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 + 2k_F(\epsilon)q) \right) - \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 - 2k_F(\epsilon)q) \right) \right]
$$

(B.22)

Thus, the expression is simplified and only the integration over $\varepsilon$ only remains:

$$
\text{Im}[-\chi^R(q, \omega)] \approx A \hbar \omega \left\{ -\frac{m^*_F}{\hbar^2} \int_{-W}^{+W} d\varepsilon \frac{1}{k_F(\varepsilon)} \partial(\varepsilon_F - \varepsilon) \rho(\varepsilon) \right\}
$$

$$
\times \left[ \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 + 2k_F(\epsilon)q) \right) - \rho \left( \varepsilon - \frac{\hbar^2}{2m^*_F} (q^2 - 2k_F(\epsilon)q) \right) \right]
$$

(B.23)

This expression can be numerically evaluated. However, for $q \to 0$, further analytical progress is possible by noting that $\rho(\varepsilon)\rho'(\varepsilon) = \frac{1}{2} d[\rho(\varepsilon)]^2/d\varepsilon$, and hence,

$$
\text{Im}[-\chi^R_F(q \to 0, \omega)] \approx A \hbar \omega \int_{-W}^{\text{min}\{+W,\epsilon_F\}} d\varepsilon \frac{\rho(\varepsilon)}{k_F(\varepsilon)} \frac{d[\rho(\varepsilon)]^2}{d\varepsilon}.
$$

(B.24)

From which, upon integration by parts, we obtain:

$$
\text{Im}[-\chi^R_F(q \to 0, \omega)] \approx A \hbar \omega \int_{-W}^{\text{min}\{+W,\epsilon_F\}} d\varepsilon \frac{\rho(\varepsilon)}{k_F(\varepsilon)} \frac{d[\rho(\varepsilon)]^2}{d\varepsilon}
$$

(B.25)

$$
= A \hbar \omega \frac{m^*_F}{\hbar^2} \int_{-W}^{\text{min}\{+W,\epsilon_F\}} d\varepsilon \frac{[\rho(\varepsilon)]^2}{k_F(\varepsilon)}.
$$

(B.26)

Hence, by direct numerical evaluation of the above expression we see that it is in general not singular, which implies that the $q \sim 0$ term (denoted $S_D^f$ in Eq. (3.36)), can be neglected. In general, using Eq. (B.23) to evaluate $\text{Im}[-\chi(q, \omega)]$ for finite $q$, we find it is also a nonsingular function of $q$ the retention of $q = 2k_F^2$. Evaluating the integrals in equations (B.23) and (B.26) numerically, Fig. (3.4) has been obtained.
On the other hand, the real part of the response function is given by:

\[
\text{Re}[\chi^R_F(q, \omega)] = A \int_{-\infty}^{\infty} d\varepsilon d\varepsilon' \rho(\varepsilon) \rho(\varepsilon')
\]

\[
\frac{dk}{2\pi} n_{k,\varepsilon} P \left[ \frac{1}{\hbar \omega + \varepsilon - \varepsilon' - \epsilon_{\parallel}(k + q) + \epsilon_{\parallel}(k)} + (\omega \to -\omega) \right]
\]

\[
= A \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon \rho(\varepsilon) \frac{dk}{2\pi} \theta(\varepsilon_F - \varepsilon - \frac{\hbar^2 k^2}{2m_F^*})
\times \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon' P \left[ \frac{\rho(\varepsilon')}{\hbar \omega + \varepsilon - \varepsilon' - \epsilon_{\parallel}(k + q) + \epsilon_{\parallel}(k)} + (\omega \to -\omega) \right]
\]

\[
= A \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon \rho(\varepsilon) \int_{-k_F(\varepsilon)}^{k_F(\varepsilon)} \frac{dk}{2\pi} \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon' P \left[ \frac{\rho(\varepsilon')}{E - \varepsilon'} + (\omega \to -\omega) \right]
\]

(\text{B.27})

where we have defined \(E = \hbar \omega + \varepsilon - \epsilon_{\parallel}(k + q) + \epsilon_{\parallel}(k)\). Furthermore, by using the well-known Kramers-Kronig relations that connect the real and imaginary part of any complex function which is analytic in the upper half plane:

\[
\text{Re}[G^R(\mathbf{R} = 0, \varepsilon)] = -P \int_{-\infty}^{\infty} \frac{d\varepsilon'}{\pi} \text{Im}[G^R(\mathbf{R} = 0, \varepsilon')] \quad (\text{B.28})
\]

we have that:

\[
P \int d\varepsilon \frac{\rho(\varepsilon')}{E - \varepsilon'} = P \int d\varepsilon' \frac{(-1/\pi)\text{Im}[G^R(\mathbf{R} = 0, \varepsilon)]}{E - \varepsilon'} = \text{Re}[G^R(\mathbf{R} = 0, E)]
\]

(\text{B.29})

Then, we can rewrite equation (\text{B.27}), so that:

\[
\text{Re}[\chi^R_F(q, \omega)] = A \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon \rho(\varepsilon) \int_{-k_F(\varepsilon)}^{k_F(\varepsilon)} \frac{dk}{2\pi} \left[ (\text{Re}[G^R(\mathbf{R} = 0, E)]) + (\omega \to -\omega) \right]
\]

\[
= \frac{A}{2\pi} \int_{-W}^{\text{min}[W,\varepsilon]} d\varepsilon \rho(\varepsilon) \int_{-k_F(\varepsilon)}^{+k_F(\varepsilon)} dk \left[ g \left( \hbar \omega + \varepsilon - \frac{\hbar^2 q^2}{2m_F^*} - \frac{\hbar^2 k q}{m_F^*} \right) 
\right.
\]

\[
+ g \left( -\hbar \omega + \varepsilon - \frac{\hbar^2 q^2}{2m_F^*} - \frac{\hbar^2 k q}{m_F^*} \right) \quad (\text{B.30})
\]

where \(g(\varepsilon) = -\text{Re}[G^R(\mathbf{R} = 0, \varepsilon)]\) is the Hilbert transform of the density of states in a 2D square lattice modeled by a tight-binding approximation [130]:

\[
g(\varepsilon) = P \int d\varepsilon' \frac{\rho(\varepsilon')}{\varepsilon' - \varepsilon} = \begin{cases} 
-\frac{2}{\pi} \mathcal{K} \left( \frac{\varepsilon}{W} \right) & \text{for } |\varepsilon| \geq W, \\
-\frac{\text{sgn}(\varepsilon)}{\pi W} \mathcal{K} \left( \frac{\varepsilon}{W} \right) & \text{for } |\varepsilon| < W,
\end{cases}
\]

(\text{B.31})
In particular, the static limit \( \omega = 0 \) reads:

\[
\chi_s(q) = \text{Re} \left[ \chi^R_F(q, \omega = 0) \right] = \frac{A}{\pi} \int_{-W}^{\min \{W, \epsilon_F \}} \! \! d\varepsilon \rho(\varepsilon) \int_{-k_F(\varepsilon)}^{+k_F(\varepsilon)} \! \! dk \, g \left( \varepsilon - \frac{\hbar^2 q^2}{2m^*_F} - \frac{\hbar^2 k q}{m^*_F} \right)
\]

(B.32)

Therefore, it is possible to perform the calculation of the previous expression.

At low frequencies (\( \hbar \omega \ll \mu_B < \epsilon_F \)) we are going to approximate the response function of the Fermi gas by the two first terms in the series about \( \omega = 0 \), that is, we shall write:

\[
\chi^R_F(q, \omega) \simeq \chi_s(q) - i \hbar D(q), \quad (B.33)
\]

where \( D(q) = \hbar \text{Im} \left[ -\chi^R_F(q) \right] \).

Next we shall employ the following spectral properties of relating the retarded response function to its analytical continuation to imaginary frequencies:

\[
\chi(q, \omega_n) = -\int \frac{d\omega}{\pi} \frac{\text{Im} \chi^R(q, \omega)}{i\omega_n - \omega}. \quad (B.34)
\]

In particular, the static limit \( \omega_n = 0 \) corresponds to:

\[
\chi_s(q) = \chi(q, 0) = \int \frac{d\omega}{\pi} \frac{\text{Im} \chi^R(q, \omega)}{\omega}. \quad (B.35)
\]

Adding and subtracting the static part,

\[
\chi(q, \omega_n) = \chi_s(q) - \int \frac{d\omega}{\pi} \frac{\text{Im} \chi^R(q, \omega)}{\omega} \left[ \frac{1}{i\omega_n - \omega} + \frac{1}{\omega} \right] \nonumber
\]

\[
= \chi_s(q) - \int \frac{d\omega}{\pi} \frac{\text{Im} \chi^R(q, \omega)}{\omega} \left[ \frac{i\omega_n}{i\omega_n - \omega} \right]. \quad (B.36)
\]

and recalling that

\[
\chi(q, \tau) = \int \frac{d\omega_n}{2\pi} e^{-i\omega_n \tau} \chi(q, \omega_n)
\]

\[
= \chi_s(q) \delta(\tau) - \int \frac{d\omega}{2\pi} \frac{\text{Im} \chi^R(q, \omega)}{\omega} \int_{-\infty}^{+\infty} \frac{d\omega_n}{\pi} \left[ \frac{i\omega_n e^{-i\omega_n \tau}}{i\omega_n - \omega} \right] \nonumber
\]

\[
= \chi_s(q) \delta(\tau) - \int_{0}^{+\infty} \frac{d\omega}{\pi} \frac{\text{Im} \chi^R(q, \omega)}{\omega} \nonumber
\]

\[
\times \int_{-\infty}^{+\infty} \frac{d\omega_n}{2\pi} \left[ \frac{i\omega_n}{i\omega_n - \omega} + \frac{i\omega_n}{i\omega_n + \omega} \right] e^{-i\omega_n \tau}. \quad (B.37)
\]
Thus, upon performing the above integral over $\omega_n$ using Cauchy’s theorem, the following expression is obtained:

$$
\chi(q, \tau) = \chi_s(q)\delta(\tau) + \int_0^{+\infty} d\omega \frac{e^{-\omega|\tau|}}{\tau} \operatorname{Im} \chi_R^{PF}(q, \omega).
$$

(B.38)

Hence, introducing Eq. (B.33) in the expression above,

$$
\chi(q, \tau) \simeq \chi_s(q)\delta(\tau) - \frac{D(q)}{\hbar\omega\pi(|\tau| + \tau_c)^2}
$$

(B.39)

The first term describes the short time behavior, which is dominated by the screening, whereas the second term describes the long time behavior, which is dominated by dissipation.

B.3 RG analysis at half-filling

In order to obtain the RG flow equations, we consider the functional integral representation of the partition function:

$$
Z(\tau_c) = \int [d\phi] e^{-S[\phi]},
$$

(B.40)

where

$$
S[\phi] = S_0[\phi] + S_{\text{int}}[\phi],
$$

(B.41)

$S_0[\phi]$ being the Gaussian part of the action (the first term in Eq. (3.21)). When writing Eq. (B.40), we have made explicit the dependence of the partition function on the short-distance cut-off $a_0 \simeq \nu\tau_c$. Note, however, that (up to a multiplicative constant), the partition function is independent of the cut-off, and we will base our subsequent analysis on this fact. For a general perturbation $S_{\text{int}}[\phi]$ we cannot compute the partition function exactly. Thus, we resort to a perturbative expansion of $Z[(1 + \delta\ell)\tau_c]$ (where $\delta\ell \ll 1$) in powers of $S_{\text{int}}$:

$$
Z[(1 + \delta\ell)\tau_c] = Z_0[(1 + \delta\ell)\tau_c] \bigg\{ 1 - \langle S_{\text{int}}[\phi] \rangle + \frac{1}{2} \langle S_{\text{int}}^2[\phi] \rangle + \cdots \bigg\}
$$

(B.42)

To deal with this expansion it is convenient to define the normal ordered vertex operators:

$$
:\! e^{2p\phi(x)} : = \frac{1}{a_0^{p^2K}} e^{2p\phi(x)}
$$

(B.43)

where $x = (v\tau, x)$ the limit $a_0 \to 0$ is implicitly understood. Then, when inserted in an expectation value, we have the following operator product
expansions (OPE):

\[ e^{2ip\phi(r)} :: e^{-2ip\phi(r')} :: = \frac{1}{|r - r'|^{2p^2K}} : [1 + 2i(p(r - r')\nabla\phi(R) - 2p^2[(r - r')\nabla\phi(R)]^2 + ...] : \]

(B.44)

\[ : e^{2ip\phi(r)} :: e^{2ip\phi(r')} ::= a_0^{2p^2K} : e^{4ip\phi(R)} : + ... \]

(B.45)

where \( r = (v\tau, x) \), \( R = (r - r')/2 \) \( \nabla = ((1/v)(\partial\tau, \partial x)) \) and \( a_0 = v\tau_c \) is a short-distance cut-off. Hence,

\[ : \cos 2\phi(r) :: \cos 2\phi(r') : = \frac{1}{4} \left( : e^{2ip\phi(r)} + e^{-2ip\phi(r)} :: e^{2ip\phi(r)} + e^{-2ip\phi(r)} : \right) \]

\[ = \frac{1}{|r - r'|^{2p^2K}} : [1 - 2[(r - r')\nabla\phi(R)]^2 - 2[(r - r')\nabla\phi(R)]^2 + ...] : \]

\[ + \frac{a_0^{2p^2K}}{4} \left( : e^{4ip\phi(R)} : + : e^{-4ip\phi(R)} : \right) \]

\[ = \frac{1}{2|r - r'|^{2p^2K}} : [1 - 2[(r - r')\nabla\phi(R)]^2 + ...] : + \frac{a_0^{2p^2K}}{2} : \cos 4\phi(R) : + ... \]

(B.46)

Next, let us consider the partition function at the scale \((1 + \delta l) a_0\), where \( \delta l > 0 \) and \( \delta l \ll 1 \):

\[ Z[(1 + \delta l) a_0] = Z_0[(1 + \delta l) a_0] \left\{ 1 - \langle S_{int} \rangle + \frac{1}{2!} \langle S_{int}^2 \rangle + \ldots \right\} \]

(B.47)

where

\[ S_{int}[\phi] = S_u[\phi] + S_D[\phi] \]

(B.48)

\[ S_u[\phi] = -\frac{g_u}{\pi a_0^2} \int dxd\tau \cos 4\phi(r) \]

\[ S_D[\phi] = -\frac{g_D}{a_0} \int_{|r-r'|>a_0} dr'd\tau' \delta(x-x') \frac{\cos 2\phi(r) \cos 2\phi(r')}{|r-r'|^2} \]

We first, need to normal order these perturbations:

\[ S_u[\phi] = -\frac{g_u}{\pi a_0^2} \int dxd\tau : \cos 4\phi(r) : \]

\[ S_D[\phi] = -\frac{g_D}{a_0} \int_{|r-r'|>a_0} dr'd\tau' \frac{\delta(x-x')}{|r-r'|^2} : \cos 2\phi(r) :: \cos 2\phi(r') : \]

(B.49)
B.3.1 First order terms

Now, let us consider the first order term $\langle S_{int} \rangle = \langle S_u \rangle + \langle S_D \rangle$:

$$-\langle S_u \rangle = + \frac{g_u(l + \delta l)}{\pi[(1 + \delta l)a_0]^{1 - 2K}} \int dr \langle \cos 4\phi(r) \rangle$$  \hspace{1cm} (B.50)

When compared with the same operator at the scale $a_0$, we find that:

$$g_u(l + \delta l) = g_u(l) = g_u(l)[1 - (2 - 4K)\delta l], \hspace{1cm} (B.51)$$

which immediately leads to the differential equation:

$$\frac{dg_u(l)}{dl} = (2 - 4K)g_u(l) \hspace{1cm} (B.52)$$

Next, we take up:

$$-\langle S_D \rangle = + \frac{g_D(l + \delta l)}{\pi[(1 + \delta l)a_0]^{1 - 2K}} \int_{|r - r'| > a_0(1 + \delta l)} dr dr' \frac{\delta(x - x')}{|r - r'|^2} \langle \cos 2\phi(r) \rangle \langle \cos 2\phi(r') \rangle$$  \hspace{1cm} (B.53)

To bring this expression to a form which can be compared with the same expression at the cut-off scale $a_0$, we first split the integral on $r$ and $r'$ as follows:

$$\int_{|r - r'| > a_0(1 + \delta l)} dr dr' = \int_{|r - r'| > a_0} dr dr' - \int_{a_0(1 + \delta l) > |r - r'| > a_0} dr dr' \hspace{1cm} (B.54)$$

Thus, from the first term in the right hand-side of the above equation, we have that:

$$+ \frac{g_D(l + \delta l)}{\pi[(1 + \delta l)a_0]^{1 - 2K}} \int_{|r - r'| > a_0} dr dr' \frac{\delta(x - x')}{|r - r'|^2} \langle \cos 2\phi(r) \rangle \langle \cos 2\phi(r') \rangle$$  \hspace{1cm} (B.55)

Hence, following the same procedure as before:

$$\frac{g_D(l + \delta l)}{[(1 + \delta l)]^{1 - 2K} = g_D(l) \implies \frac{dg_D(l)}{dl} = (1 - 2K)g_D(l), \hspace{1cm} (B.56)$$
Next, we take up the other contribution by using Eq. (B.46):

\[
- g_D(l + \delta l) \int_{a_0(l+\delta l)>|r-r'|>a_0} drdr' \frac{\delta(x-x')}{|r-r'|^2} \cos 2\phi(r) \cos 2\phi(r') \\
= - g_D(l + \delta l) \int_{a_0(l+\delta l)>|r-r'|>a_0} drdr' \frac{\delta(x-x')}{|r-r'|^{1+2K}} \langle 1 - 2[(r-r')\nabla\phi(R)]^2 + \ldots \rangle \\
= - g_D(l + \delta l) \int_{a_0(l+\delta l)>|r-r'|>a_0} drdr' \frac{\delta(x-x')}{|r-r'|^{2+2K}} \langle 4\phi(R) \rangle
\]

Now, if one considers the following integral with \( u = r - r' = (ur, x) \):

\[
- g_D(l) \int_{a_0(l+\delta l)>|u|>a_0} du \frac{\delta(ux)}{|u|^2} = \left[ \int_{a_0}^{a_0(l+\delta l)} du \frac{1}{u^{1-4K}} \right] \frac{1}{a_0^{1-4K}} = \frac{\delta l}{a_0^{2-4K}}
\]

Hence, the second term in Eq. (B.57) yields:

\[
- g_D(l) \delta l \int dr : \cos 4\phi(r) \\
= \frac{\delta l}{a_0^{2-4K}} \int dr : \cos 4\phi(r) \tag{B.59}
\]

Therefore, the equation for \( g_u(l) \) (Eq. (B.52)) (the umklapp) must be modified to:

\[
\frac{g_u(l + \delta l)}{[(1 + \delta l)]^{2-4K}} - \pi g_D(l) \delta l = g_u(l) \\
g_u(l + \delta l) = [1 + (2 - 4K)\delta l]g_u(l) + \pi g_D(l) \delta l \\
\frac{dg_u(l)}{dl} = (2 - 4K)g_u(l) - \pi g_D(l) \\
\]

Finally, it is necessary to consider the first term in Eq. (B.57). To this end, we need to consider the following integral with:

\[
- g_D(l) \delta l \int_{a_0(l+\delta l)>|u|>a_0} du \frac{\delta(ux)}{|u|^2u^{2K}} \\
= \left[ \int_{a_0}^{a_0(l+\delta l)} du \frac{1}{u^{2K}} \right] \frac{1}{a_0^{1-4K}} \\
= \left[ \int_{a_0}^{a_0(l+\delta l)} d\left( \frac{u}{a_0} \right) \left( \frac{a_0}{u} \right)^{2K} \right] = \delta l \tag{B.61}
\]

Thus, we find a term of the following form:

\[
\frac{2g_D(l)}{v(l)} \delta l \int dx d\tau \langle (\partial_\tau \phi)^2 \rangle \\
\tag{B.62}
\]
Note that this term has the same form of the $\frac{1}{2\pi K v}(\partial_r \phi)^2$ operator in the Gaussian action, $S_0[\phi]$. When re-exponentiated, we find that, upon comparing with the same action at the cut-off scale as:

$$\frac{1}{2\pi K (l + \delta l) v(l + \delta l)} - \frac{2 g_D(l)}{v(l)} \delta l = \frac{1}{2\pi K (l) v(l)}$$

Hence,

$$\frac{1}{K (l + \delta l) v(l + \delta l)} = \frac{1}{2\pi K (l) v(l)} + 4\pi \frac{g_D(l)}{v(l)} \delta l \implies \frac{d}{dl} \left( \frac{1}{K v} \right) = \frac{4\pi g_D}{v}$$

Furthermore, the coefficient of $\int dx \tau (\partial_r \phi)^2$ is renormalized:

$$\frac{v(l + \delta l)}{K (l + \delta l)} = \frac{v(l)}{K(l)} \implies \frac{d}{dl} \left( \frac{v}{K} \right) = 0$$

From these equations we can extract the RG flow equations for $k$ and $v$:

$$\frac{1}{K} \frac{dv}{dl} + v \frac{d}{dl} \left( \frac{1}{K} \right) = 0$$

$$\frac{1}{K v^2} \frac{dv}{dl} + \frac{1}{v} \frac{d}{dl} \left( \frac{1}{K} \right) = \frac{4\pi g_D}{v} \implies \frac{1}{K} \frac{dv}{dl} + v \frac{d}{dl} \left( \frac{1}{K} \right) = 4\pi g_D v$$

Thus, adding Eq. (B.66) and Eq. (B.67):

$$2 \frac{d}{dl} \left( \frac{1}{K} \right) = 4\pi g_D \implies \frac{d}{dl} \left( \frac{1}{K} \right) = 2\pi g_D.$$  

**B.3.2 Second order terms**

After considering the first order contributions, we need to take up the second order:

$$\frac{1}{2!} \langle S_{2\text{int}}^2 \rangle = \frac{1}{2!} \langle S_{a[\phi]}^2 \rangle + ...$$

We do not consider terms of order $g_u g_D$ or $g_D^2$ because $g_D \propto g_{BF}^2$ is already a second order and $g_u \ll 1$ is considered small. Thus, taking:

$$\frac{1}{2!} \langle S_{a[\phi]}^2 \rangle = \frac{1}{2} \left( \frac{g_u (l + \delta l)}{\pi [(1 + \delta l) a_0]^2 - 4K} \right)^2 \int_{|r - r'| > a_0(1 + \delta l)} dr dr' \langle : \cos 4\phi(r) : \cos 4\phi(r') : \rangle$$
B.3 RG analysis at half-filling

Again, we need to split the integral as before, which leads us to consider:

\[- \frac{1}{2} \left( \frac{g_u(l)}{\pi a_0^2 - 4K} \right)^2 \int_{a_0(1+\delta l) > |r-r'| > a_0} \frac{1}{2} d\mathbf{r} d\mathbf{r}' \langle \left( 1 - 8 |(\mathbf{r} - \mathbf{r}') \nabla \phi(\mathbf{R})|^2 + \ldots \right) \rangle \]
\times \frac{4}{|r-r'|^{8K-4 - 2^2}} \int d\mathbf{R} \langle |\nabla \mathbf{R} \phi(\mathbf{R})|^2 \rangle \int_{a_0(1+\delta l) > |r-r'| > a_0} \frac{(a_0)}{||\mathbf{u}||}^{8K-4} \cos^2 \phi + \ldots \]
\[= \frac{2}{\pi} g_u^2 \delta l \int d\mathbf{r} \langle \left( \nabla \phi(\mathbf{r}) \right)^2 \rangle + \ldots \]

(B.71)

Thus, we need to revise our previously derived equations for the renormalization of the Gaussian action parameters:

\[\frac{1}{2\pi K(l + \delta l)} v(l + \delta l) - 2 \frac{gD(l)}{v(l)} \delta l - 2 \frac{g_u^2(l)}{\pi v(l)} \delta l = \frac{1}{2\pi K(l)} \frac{v(l)}{v(l)} \]

(B.72)

\[\frac{v(l + \delta l)}{2\pi K(l + \delta l)} - \frac{2v(l)g_u^2(l)}{\pi} \delta l = v(l) \]

(B.73)

Hence,

\[\frac{d}{dl} \left( \frac{1}{Kv} \right) = \frac{4\pi gD}{v} + \frac{4\pi g_u^2}{v} \]

(B.74)

\[\frac{d}{dl} \left( \frac{v}{K} \right) = 4\pi g_u^2 \]

(B.75)

\[\frac{1}{v} \frac{d}{dl} \left( \frac{1}{K} \right) - \frac{1}{Kv^2} \frac{dv}{dl} = \frac{4\pi}{v} \left[ gD + \frac{g_u^2}{\pi} \right] \]

(B.76)

\[v \frac{d}{dl} \left( \frac{1}{K} \right) + \frac{1}{Kv} \frac{dv}{dl} = 4\pi g_u^2 \]

(B.77)

And from these equations we can obtain the RG flow equations for both K and v:

\[\frac{d}{dl} \left( \frac{1}{K} \right) - \frac{1}{Kv^2} \frac{dv}{dl} = \frac{4\pi}{v} \left[ gD + \frac{g_u^2}{\pi} \right] \]

(B.78)

\[\frac{d}{dl} v = -2\pi gD K v \]

(B.79)

Finally, in the analysis of the second order contributions, we need to consider the term:

\[O(g_u g_D) = \frac{2g_u(l + \delta l)}{\pi a_0(1+\delta l) [a_0(1+\delta l)]^{-2K}} g_D(l + \delta l) \]

\times \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \delta(x_1 - x_2) \frac{\delta}{|\mathbf{r}_1 - \mathbf{r}_2|^2} \langle \cos 4\phi(\mathbf{r}_1) \cos 4\phi(\mathbf{r}_2) \cos 4\phi(\mathbf{r}_3) \rangle \]

(B.80)

where the star (*) under the integral means that: |\mathbf{r}_1 - \mathbf{r}_2| > a_0(1 + \delta l), |\mathbf{r}_1 - \mathbf{r}_3| > a_0(1 + \delta l), and |\mathbf{r}_2 - \mathbf{r}_3| > a_0(1 + \delta l). Let us consider the
contraction resulting from the OPE when $r_1 \to r_2$ (or equivalently $r_1 \to r_3$):

$$: \cos 4\phi(r_1) :: \cos 4\phi(r_2) := \frac{1}{2|r-r'|^{4K}} : \cos 2\phi(R) : +... \quad (B.81)$$

Hence, as the above factor of 2 is cancelled by the two possible contractions $r_1 \to r_2$ and $r_2 \to r_3$:

$$O(g_u g_D) = -\frac{2g_u(l + \delta l)}{\pi |a_0(1 + \delta l)|^{4-2K}} \frac{g_D(l + \delta l)}{|a_0(1 + \delta l)|^{1-2K}} \int_{a_0(1+\delta l)>|\rho|>a_0} d\rho \frac{1}{|\rho|^{4K}}$$

$$\times \int_d R d\mathbf{r}_3 \frac{\delta(X - x_3)}{|R - \mathbf{r}_3|^2} (\cos 4\phi(R) \cos 4\phi(r_3) : +...$$

$$= -\frac{4g_u(l)g_D(l)}{\pi |a_0(1 + \delta l)|^{1-2K}} \delta l \int d\mathbf{r} d\mathbf{r}' \delta(x - x') \frac{\cos 2\phi(r) :: \cos 2\phi(r') :}{|\mathbf{r} - \mathbf{r}'|^2}$$

(B.82)

Therefore, we obtain the following differential equation:

$$\frac{g_D(l + \delta l)}{|a_0(1 + \delta l)|^{1-2K}} - \frac{4g_u(l)g_D(l)\delta l}{|a_0(1 + \delta l)|^{1-2K}} = \frac{g_D(l)}{a_0^{1-2K}} \implies \frac{g_D}{\delta l} = (1 - 2K)g_D + 4g_D g_u \quad (B.83)$$

This completes the derivation of the RG equations, and putting all equations together yields:

$$\frac{dv}{dl} = -4\pi g_D K v \quad (B.84)$$

$$\frac{dK}{dl} = -(4g_u^2 + 2\pi g_D)K^2 \quad (B.85)$$

$$\frac{dg_u}{dl} = (2 - 4K)g_u + \pi g_D \quad (B.86)$$

$$\frac{dg_D}{dl} = (1 - 2K)g_D + 4g_D g_u \quad (B.87)$$

Focusing on (RG1, RG2, RG3), we can introduce the following set of variables:

$$K = \frac{1}{2}(1 + x) \implies \dot{x} = -2(y^2 + z^2) \quad (B.88)$$

$$g_u = y \implies \dot{y} = -2xy + 2z^2 \quad (B.89)$$

$$g_D = \frac{2}{\pi} z^2 \implies \dot{z} = -\frac{1}{2}(x + y)z \quad (B.90)$$

Thus, these are the equations that represent the RG flow (see Fig. (3.5)):

$$\dot{x} = -2(y^2 + z^2) \quad (B.91)$$

$$\dot{y} = -2xy + 2z^2 \quad (B.92)$$

$$\dot{z} = -\frac{1}{2}(x + y)z \quad (B.93)$$
B.4 SCHA

In this appendix, we provide the details of the Self-Consistent Harmonic Approximation (SCHA) that we employed in Chapter 3 to estimate the effect of quantum dissipation on the CDW gap. To this end, we need to find a variation estimate of the free energy by performing the average with a trial effective action such as in Eq. (3.51) by using $S_0$ (Eq. (3.21)), $S_u$ (Eq. (3.22)) with $p = 2$ for half-lattice filling, $S_{Du}^b$ (Eq. (3.37)) and $S_u^b$ (Eq. (3.38)). Thus, the variational free energy $F_{\text{var}}$ that follows from Eq. (3.52) will be:

$$F_{\text{var}}[G] = -\frac{T}{2} \int \frac{dq d\omega}{(2\pi)^2} \ln G(q, \omega)$$

$$+ T \left[ \frac{1}{2\pi K} \left( \frac{\omega^2}{v_s} + v_s q^2 \right) \right] G(q, \omega)$$

$$- T \frac{g_a}{a_0 \tau_0} \int dx d\tau \left[ 8 \int \frac{dq d\omega}{(2\pi)^2} G(q, \omega) \right]$$

$$- T \frac{g_D}{a_0} \left[ \int dx \int_{|\tau - \tau'| > \tau_0} d\tau d\tau' \frac{-4 \int \frac{dq d\omega}{(2\pi)^2} [1 - \cos \omega (\tau - \tau')] G(q, \omega)}{|\tau - \tau'|^2} \right]$$

$$- \langle S_v \rangle$$

(B.94)

Therefore, optimizing $\frac{\delta F_{\text{var}}[G]}{\delta G} = 0$ yields:

$$\delta F_{\text{var}}[G]/\delta G = \frac{T}{2} \int \frac{dq d\omega}{(2\pi)^2} \frac{1}{G(q, \omega)}$$

$$+ T \left[ \frac{1}{2\pi K} \left( \frac{\omega^2}{v_s} + v_s q^2 \right) \right] + T \frac{8g_a}{(2\pi)^2 a_0 \tau_0} \alpha(\eta, \Delta)^4K$$

$$+ T \frac{4g_D}{(2\pi)^2 a_0} \left[ \alpha(\eta, \Delta)^2K + \alpha(\eta, \Delta)^4K \right] = 0 \quad (B.95)$$

where we have defined $\alpha(\eta, \Delta) = \left[ \frac{\eta K + 2\sqrt{K \pi \Delta}}{4} \right]$. And in summary, by only keeping the $\tau$-independent terms in the integrals in Eq. (B.94) we have found the parameters $\eta$ and $\Delta$ solving the self-consistent equation above (Eq. (B.95)), so that:

$$\eta = \frac{8g_a}{(2\pi)^2} \alpha(\eta, \Delta)^4K \quad (B.96)$$

$$\Delta = \frac{8(g_a + g_D)}{(2\pi)^2} \alpha(\eta, \Delta)^4K \quad (B.97)$$
Bibliography


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