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Finite-momentum Bose-Einstein condensates in optical lattices

Tesi di laurea specialistica

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The main motivation behind the work that we present in this thesis is a theory proposed in 1999 for a scalar field \([1]\). This theory takes into account higher-order derivatives in the quadratic or kinetic term of the action for a scalar field \(\Phi(x)\). Such terms reveal that the homogeneous vacuum \(\langle \Phi(x) \rangle = \text{constant}\) becomes unstable and the true vacuum is the one in which the order parameter is oscillating. In reciprocal space, a peak at a certain non-vanishing momentum is expected. Condensates with a non trivial momentum are thus generated. In the lattice model of the theory, the authors show that the generation of finite-momentum condensates is just an effect of including in the theory next-nearest-neighbor couplings; by tuning the parameters of the theory, i.e. the coupling constants in front of the higher-order derivatives of the continuum model, several phases have been found.

Starting from the proposal discussed above, we identified optical lattices to be a physical system in which such a dynamics can be observed. Ordinary optical lattices are based on the Bose-Hubbard (BH) model which takes into account nearest-neighbor-hopping \([2]\). This approximation is in general valid because next-nearest-neighbor-hopping parameters are usually at most ten times smaller than nearest-neighbor ones.
If we can tune the hopping coefficients such that the nearest neighbors are reduced to zero while keeping the higher-order neighbors still finite, we can expect that the competition between the hopping coefficients can generate instabilities and the Bose gas condenses at a non trivial momentum. In a theoretical paper, Eckardt et al. [3] proposed that it is possible to tune the hopping parameter by shaking the lattice with a sinusoidal force. The physical behavior of this system is time dependent. Due to the periodicity of the Hamiltonian, the Floquet theorem allows us to describe the system in a time independent form through an effective Hamiltonian. The hopping coefficients are multiplied by the zero order Bessel function $J_0(K_0)$, where $K_0$ is a parameter depending on shaking.

Thus, the effective hopping parameters can be tuned and can even change sign because the Bessel function has nodes. The lowest energy band of the BH model (for non-interacting particles) has a minimum at zero momentum (for the undriven system) which is the condensation momentum for the Bose gas loaded in the lattice. When the hopping coefficient changes sign, the minimum of the band moves into the edge of the first Brillouin zone. Condensates with this nontrivial momentum have been observed experimentally in time-of-flight experiments by the Pisa group, and the Mott-insulator/superfluid phase transition has been triggered by the shaking [4].

In this thesis we show that when the nearest-neighbor-hopping parameter is tuned to zero via the shaking, it becomes essential to include higher-order hopping terms in the theory, a problem that had not been investigated yet. In ordinary 1D and 2D lattices, we have found that no new phases are expected in the region where the next-nearest-neighbor-hopping terms become important. However, for 1D lattices, if we consider a toy model having the bare next-nearest-neighbor-hopping coefficients with opposite sign with respect to the nearest-neighbor ones, a phase in which the condensation momentum is tunable via the shaking emerges.
This finding has stimulated the search for a real system where such phenomenon can be observed. Because the sign of the hopping coefficients in the undriven system seems to be fixed in 1D whatever the optical potential is, we explored new possibilities for 2D square lattices. In this case, instead of using a separable potential which gives the same hopping coefficients as in the 1D case, we implemented a non-separable optical potential (as discussed in Ref. [5] in a different context). In this case, the non-separability of the potential generates hopping coefficients connecting sites along the diagonal which are zero in the separable case.

It turns out that the sign of these coefficients is just flipped in the same way that we have discussed for the toy model in 1D. When we introduce the shaking in such a way that the nearest-neighbor-hopping coefficients become less important, a new phase with a finite and tunable condensate is generated. According to our results, a very high resolution in the shaking parameter $K_0$ and the use of Feshbach resonances to reduce the interaction between the atoms are required to observe experimentally this new phase.

Finite-momentum condensates have been theoretically predicted earlier for bosons in 2D square lattices in the presence of a staggered rotation [6, 7]. In that case, a vortex-antivortex lattice forms in the finite-momentum phase. Here, the finite-momentum phase is driven by shaking, which introduces linear instead of angular momentum in the condensate. For a certain range of parameters, we find a staggered-sign superfluid phase, analogous to the one predicted in Ref. [7]. The tunable finite-momentum condensate phase, nevertheless, is peculiar to this non-separable square-lattice potential model, and did not arise under the conditions considered in Ref. [7], where the lattice potential was separable. For the case of a honeycomb geometry, where the lattice potential is unavoidably non-separable, a reminiscent of this phase has been experimentally observed for elliptical shaking [8]. The latter procedure imprints
phases to the condensate, in analogy with the rotation. Here we unveil the existence of a tunable finite-momentum condensate for linear shaking in a square lattice.

Finally, we mention that finite-momentum condensates play an important role in superconductivity and have been predicted long time ago for interacting Fermi gases. If a spin imbalance is introduced in the system such that the average number of spin up particles is different from the average number of spin down particles, the BCS superconducting state becomes unstable. In the sixties, Fulde and Ferrell (1964) and Larkin and Ovchinnikov (1965) predicted a new phase (FFLO) [9, 10]. In the FFLO phase, the order parameter is no longer homogeneous but is modulated in space; this means that Cooper pairs carrying momentum are formed. This phase has been quite elusive because of the small phase space available for it in ordinary materials. In recent years, there has been a renewed interest in this topic [11–13] due to the possibility of creating Fermi systems with population imbalance. In 2010, the first indirect measurement of this phase has been published for a 1D Fermi gas [14]. Recent progress in shaking [4, 8] or generating artificial gauge fields for the optical lattices [15] open up new possibilities to access FFLO phases for bosons.

This thesis is organized as follows: in Chap. 1 we discuss general features of Bose-Einstein condensation; in Chap. 2 we describe optical lattices and the Mott-insulator/superfluid phase transition both from the theoretical and experimental points of view; in Chap. 3 we introduce shaking in optical lattices, we present the Floquet theory and the renormalization of hopping coefficients; in Chap. 4 we study the 1D driven problem and introduce the toy model revealing the new phase; in Chap. 5 we study the 2D driven problem for non-separable optical potentials, discuss the new phases and their ground states and we predict the time-of-flight images expected to be seen in the experiments.
In this Chapter we describe the general features of the Bose-Einstein condensation (BEC) and sketch the theoretical framework behind it.

1.1 General description

Bose-Einstein condensation [16–18] is a phenomenon of particular relevance in Physics because the quantum mechanical behavior is realized on a macroscopic scale. Indeed, Bose statistics allows identical particles to occupy the same quantum state; under a certain critical temperature, most of the bosons condense in the lowest energy level. This means that a quantum state becomes macroscopically occupied and the quantum behavior is on a macroscopic scale.

Although the existence of BEC has been theoretically predicted in 1924 [16–18], the experimental realization only occurred recently, in 1995 [19, 20] (see Fig. 1.1) and has been awarded with the Nobel Prize in 2001. The reason of the huge delay between theory and experiments will be immediately clear. In the following, we will base our description on the seminal books written by Pethick and Smith [21] and Pathria [22].

If we consider a gas of free bosons with mass $m$ and density $n$, the
only temperature we can recover using dimensional analysis is

\[ T_c = C \frac{\hbar^2 n^{2/3}}{mk_B}, \]

(1.1)

where \( C \) is a numerical factor, \( k_B \) is the Boltzmann constant and \( \hbar \) is the reduced Planck constant. This temperature is just the temperature at which quantum behavior is expected to become important (classically \( \hbar \to 0 \)). If a typical temperature exists below which all the atoms are pushed into one quantum state, this should be the expression for such a temperature. We will derive the numerical prefactor later from Statistical Mechanics. In early experiments on alkali atoms, densities were of the order of \( 10^{13} \text{cm}^{-3} \), thus corresponding to temperature of the order of 100 nK. So, we are dealing with an ultracold diluted gas; this explains why BEC has been so elusive. In solids, for instance, densities are of the order of \( 10^{22} \text{cm}^{-3} \) and thus the Fermi temperature for electrons is typically \( 10^4 - 10^5 \text{K} \), much higher than the room temperature. This is the reason why the electron gas in metals requires a quantum mechanical treatment to be understood.

For years, cooling by contact has been the only way to reach low temperatures (of the order of mK); however, this is not enough to observe the Bose-Einstein condensation. The very old concept that temperature is related to movement has been the key ingredient to go beyond the
1.1 General description

mK limit and has been implemented using lasers to cool and trap atoms. Chu, Cohen-Tannoudji and Phillips were awarded with the Nobel Prize in 1997 for the development of the laser cooling technique. Due to the hyperfine structure of alkali atoms giving rise to an interaction energy $-\vec{\mu} \cdot \vec{B}$, the well-known Zeeman splitting, we can generate a trapping potential by using a quadrupolar magnetic field (created by Helmoltz coils). This leads to an anisotropic harmonic potential, which is used to trap the cloud of bosonic atoms. The cooling procedure has two major steps. The first one is known as laser cooling. In this case, the frequency of a counter-propagating laser is tuned just below the frequency of an atomic transition. The rate of absorption of photons has a Lorentzian shape, having a peak at the resonance frequency. A moving atom sees the frequencies of the photons shifted because of the Doppler effect. In its rest frame, it will absorb more photons coming from the direction opposite to its motion because they have a higher frequency and are thus close to the Lorentzian absorption peak. The atoms feel a frictional force which slows down their motion and cools them. Nevertheless, the absorption of photons is also responsible for the heating of the cloud; the two processes are in competition and, at the equilibrium, a minimum temperature is reached; it is of the order of few hundreds $\mu$K and a different approach is required to go further. The final step is known as evaporative cooling. Atoms with higher energy are removed lowering the potential barrier of the trap. This is accomplished by a radio-frequency radiation, which flips the spins of the atoms; in this way they are no more in a minimum of the energy and are expelled from the trap (recall that the trapping potential is spatially dependent; by tuning the radio-frequency, one generates holes

\footnote{At the center of the trap, where the magnetic field is almost zero (and so is the scale of energy between Zeeman states), a slowly varying magnetic field can induce transitions towards states with a magnetic dipole moment opposite in sign, for which the energy is higher. This generates loss of atoms from the condensate and thus a technique for which one superimposes a second magnetic field oscillating in time has been introduced. This is the so-called TOP trap.}
in the trap and the average temperature of the cloud decreases. With 
this last technique one can reach temperatures of few hundreds nK to 
observable BEC.

Now, we describe how Statistical Mechanics predicts BEC. Let us 
consider a 3D free gas. If we call $f^0(\epsilon)$ the Bose-Einstein distribution 
and $g(\epsilon)$ the density of states, the number of particles in the excited 
states can be written

$$N_{\text{exc}} = \frac{1}{V} \int_0^\infty d\epsilon g(\epsilon) f^0(\epsilon) = \frac{1}{\lambda_T^3} g_{3/2}(z), \quad (1.2)$$

where $V$ is the volume, $\lambda_T = h/(2\pi m kT)^{1/2}$ is the (thermal) de Broglie 
wavelength, $z = \exp(\beta \mu)$ is the fugacity and $g_{3/2}(z)$ is defined as

$$g_\alpha(z) = \frac{1}{\Gamma(\alpha)} \int_0^\infty dx \frac{x^{\alpha-1}}{z^{-1} e^x - 1}, \quad (1.3)$$

where $\Gamma(\alpha)$ is the Euler gamma function. The function $g_{3/2}(z)$ is non-
negative and bounded, i.e.

$$g_{3/2}(z) \leq g_{3/2}(1) = \zeta(3/2) \simeq 2.612, \quad (1.4)$$

where $\zeta(3/2)$ is the Riemann zeta function. Hence, the number of excited 
atoms cannot exceed $\zeta(3/2)V/\lambda_T^3$; when the total number of particles $N$ 
is larger than this value, we start populating the ground state of the 
system, i.e. under the critical temperature

$$T_c = \frac{\hbar^2}{2\pi m k_B} \left[ \frac{n}{\zeta(3/2)} \right]^{2/3}, \quad (1.5)$$

and we can thus compare this result with the argument based on dimen-
sional analysis\(^2\). One can show that below this critical temperature $z \simeq 1$ 
and the fraction of particles in the ground state $N_g$ is given by

$$\frac{N_g}{N} = 1 - \left( \frac{T}{T_c} \right)^{3/2}, \quad (1.6)$$

\(^2\)This temperature can also be seen as the critical point where $\lambda_T \approx n^{-1/3}$, i.e. 
when the thermal wavelength is of the same order as the interparticle distance, where 
quantum behavior is expected.
which indicates that the ground state becomes macroscopically populated.

Another important feature of this phase transition that can be captured is the behavior of the specific heat $C_V$ crossing the critical temperature. We do not show the detailed calculations, but we mention that the specific heat has a cusp at the critical temperature, the well known $\lambda$ point. This means that the phase transition is of second order and can be studied using the Landau mean field theory. The superfluid phase has phase coherence, indicating that the U(1) symmetry has been broken.

We close this section recalling that a 2D free gas does not undergo BEC; in this case we have to deal with $g_1(z \simeq 1) = \zeta(1)$, which is divergent. Thus, only at zero temperature the phase transition is possible.

## 1.2 Gross-Pitaevskii theory

So far we have discussed the case of a free gas of bosons. In the following, we take into account interactions between particles and we describe a classical field theory for the condensed state. We consider the following Hamiltonian for bosons subjected to an external potential $V$ and to a contact interaction $U_0$:

$$
H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V(r_i) \right] + U_0 \sum_{i<j} \delta(r_i - r_j).
$$

A contact interaction is a good approximation for low energy scattering when the gas is dilute. In reciprocal space, it becomes a constant and is just $U_0 = 4\pi\hbar^2a_s/m$, where $a_s$ is the so-called $s$-wave scattering length. We assume that, in the condensed phase, all the particles are in the same single-particle state $\phi(r)$ and thus the wave function is

$$
\Psi(r_1, \ldots, r_N) = \prod_{i=1}^{N} \frac{1}{\sqrt{N}} \phi(r_i),
$$
where the required normalization is
\[
\int \text{d} r_i |\phi_i(r)|^2 = N, \quad i = 1, \ldots, N. \tag{1.9}
\]
The density of particles is thus given by \( n(r) = |\phi(r)|^2 \) which is a correct assumption if the state is macroscopic. If we evaluate the energy of the system on such a ground state \( E = \langle \Psi | H | \Psi \rangle \) and we add the constraint that the number of particles is fixed, we obtain the following functional
\[
F[\phi, \phi^*] = E - \mu N = \int \text{d} r \left[ \frac{\hbar^2}{2m} | \nabla \phi(r) |^2 + V(r) |\phi(r)|^2 + \frac{U_0}{2} |\phi(r)|^4 - \mu |\phi(r)|^2 \right]. \tag{1.10}
\]
Thus, the condition \( \delta F/\delta \phi^* = 0 \) yields the time independent Gross-Pitaevskii equation
\[
-\frac{\hbar^2}{2m} \nabla^2 \phi(r) + V(r) \phi(r) + U_0 |\phi(r)|^2 \phi(r) = \mu \phi(r). \tag{1.11}
\]
The previous equation is a Schrödinger-like nonlinear differential equation, where the energy eigenvalue is given by the chemical potential \( \mu \) and the potential is just the sum of the external potential \( V \) and the mean field one, given by the cloud of bosons \( U_0 |\phi(r)|^2 \). Solving this equation requires some approximations.

Consider bosons trapped in a harmonic potential and a very large cloud. Calling \( R \) the spatial extent of the cloud, we can compare the kinetic energy and the onsite (repulsive) interaction: the kinetic energy is of order of \( \hbar^2/2mR^2 \) while the onsite interaction is of order of \( nU_0 \sim \hbar^2 aN/mR^3 \). The ratio is given by
\[
\frac{E_{\text{kin}}}{E_{\text{onsite}}} \sim \frac{R}{Na}. \tag{1.12}
\]
For increasing values of \( Na \), the kinetic energy becomes less important (in the experiment performed by the group of Ketterle [19], this ratio was 1/120) and this leads to the Thomas-Fermi approximation. The Gross-Pitaevskii equation in which we neglect the kinetic term is
\[
\left[ V(r) + U_0 |\phi(r)|^2 \right] \phi(r) = \mu \phi(r), \tag{1.13}
\]
and has a solution
\[
n(r) = |\phi(r)|^2 = [\mu - V(r)]/U_0.
\] (1.14)

One important result is that the total energy per particle is
\[
\frac{E}{N} = \frac{5}{7}\mu,
\] (1.15)

while the ratio between the interaction and potential energy is
\[
\frac{E_{\text{int}}}{E_{\text{pot}}} = \frac{2}{3}.
\] (1.16)

However, there are other cases in which the Thomas-Fermi approximation is not valid and the kinetic energy is crucial, for instance, to generate vortices \([5, 24]\).

So far, we have depicted the equilibrium properties of the gas. To study excitations, we need a formalism which takes into account the dynamics. This is nothing else that the time-dependent Gross-Pitaevskii equation
\[
\text{i}\hbar \partial_t \phi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \phi(r, t) + V(r)\phi(r, t) + U_0|\phi(r, t)|^2\phi(r, t).
\] (1.17)

One can thus study density excitations \(\phi \rightarrow \phi + \delta\phi\) using the ansatz
\[
\delta\phi(r, t) = \frac{e^{-i\mu t/\hbar}}{\sqrt{V}} \left[ u_k e^{i(k \cdot r - \omega t)} - v_k^* e^{-i(k \cdot r - \omega t)} \right],
\] (1.18)

and the outcome for the allowed frequencies is
\[
\hbar\omega = \pm \sqrt{\xi_k^2 - (\mu U_0)^2},
\] (1.19)

where \(\xi_k = \hbar^2 k^2/2m + nU_0\). The spectrum of excitations at small \(k^2\) is linear in momentum and thus develops a velocity of sound given by \(v = \sqrt{nU_0/m}\). A field-theoretical approach based on the Bogoliubov transformation, which has lots in common with what we have just discussed, will be developed in Chap. 5.
In this Chapter we describe optical lattices, which are lattices made by superimposing laser beams. We outline the main model, the Bose-Hubbard model for bosons, and show that a phase transition can be observed in such a system.

2.1 Optical lattices

Optical lattices are a new frontier of condensed matter physics. They are also called quantum simulators because they allow the study of “crystal-like” systems, in which the experimentalists can control all the important physical parameters: the lattice depth, the lattice spacing, the kind of particles loaded in the lattice and the interaction strength between them. This opens the possibility to study a wide range of phenomena, without facing the unavoidable problem of impurities that occurs in real crystals.

An optical lattice [2, 21] is generated by superimposing polarized electromagnetic standing waves. Consider, for instance, two laser beams polarized along the $z$ axis, propagating along the $x$ axis. The electric
2.1 Optical lattices

The electric field is then

\[ E(r, t) = E_0 \hat{z} \left[ \cos (kx - \omega t) + \cos (kx + \omega t) \right] = 2E_0 \hat{z} \cos (kx) \cos (\omega t), \] \hspace{1cm} (2.1)

where \( k \) is its wave vector and \( \omega \) its frequency. This electric field can interact with atoms possessing a non-vanishing dipole moment through the term in the atomic Hamiltonian (valid in the Born approximation)

\[ H_{\text{int}} = -\mathbf{d} \cdot \mathbf{E}. \] \hspace{1cm} (2.2)

It is worth to mention that the electric field is considered as a classical source in this context. If the frequency of the atom is large compared to the kinetic energy of the atoms, we can apply perturbation theory to evaluate the ground state shift of the energy after averaging over one period of oscillation (this is known as AC Stark effect [2]). As a consequence of the dipole selection rules, only second order perturbation theory gives a contribution to the energy shift and we find that

\[ \Delta E = -\frac{1}{2} \alpha'(\omega) \langle |\mathbf{E}(r, t)|^2 \rangle_T = -\alpha'(\omega)E_0^2 \cos^2 (kx) = V_0 \cos^2 (kx), \] \hspace{1cm} (2.3)

where \( \alpha'(\omega) \) is the real part of the polarizability, which has the approximate form

\[ \alpha'(\omega) \approx \frac{(E_e - E_g - \hbar \omega)|\langle e| \mathbf{d} \cdot \hat{z} |g\rangle|^2}{(E_e - E_g - \hbar \omega)^2 + (\hbar \Gamma_e/2)^2}. \] \hspace{1cm} (2.4)

Here, \( |g\rangle \) is the ground state, \( |e\rangle \) is the excited state contributing the most in second order perturbation theory, \( E_g \) and \( E_e \) are their corresponding energies, and \( 1/\Gamma_e \) is the lifetime of the excited state.

Thus, the effect of this shift is to generate a periodic potential, the period of which is \( \lambda/2 = \pi/k \). The atoms experience an attractive force towards the nodes or the antinodes of the potential according to the sign of \( \alpha' \), which depends on \( \omega \): \( E_e - E_g \equiv \omega_0 > \omega \) is called red detuning while \( \omega_0 < \omega \) is called blue detuning; the potential depth is under control in the experimental setup because it can be tuned by modulating \( E_0 \), i.e.
the intensity of the laser beam. A fundamental scale of energy (called recoil energy) can be defined using the wave vector of the laser beam, $E_r \equiv \hbar^2 k^2 / 2m$, which will be useful in the discussion below.

Hence, we have generated a lattice\(^1\) in which the atoms may be loaded, and we can manipulate its features on the basis of our wish. This is a very new situation, which cannot be realized in condensed matter systems. Moreover, we do not have to consider the effect of impurities or phonons because they are not present in the optical system and we can control the lattice spacing because it is related to the wavelength of the laser beam. We stress an important difference between optical lattices and ordinary crystal lattices. To generate optical lattices, wavelengths $\lambda$ of a few hundreds nanometers are used, hence the lattice spacing is three orders of magnitude larger than the one in ordinary crystals, which is of the order of the atomic size. This system represents a powerful tool to investigate new physical behaviors.

\(^1\)In the previous discussion, we presented a one dimensional optical lattice. We recall that, by using different laser beams, we can build also optical lattices in 2D and in 3D with different lattice geometries as shown in Fig. 2.1.
2.2 Bose-Hubbard model

The most general (second-quantized) Hamiltonian describing unpolarized bosons subjected to an external potential $V_{\text{ext}}(x)$ and to their mutual interaction $V(x - x')$ can be written as

$$H = \int dx \, \psi^\dagger(x) \left\{ \frac{-\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) - \mu \right\} \psi(x) +$$

$$+ \frac{1}{2} \int dx \, dx' \, \psi^\dagger(x) \psi^\dagger(x') V(x - x') \psi(x') \psi(x) . \quad (2.5)$$

One can thus use the knowledge of the symmetries of the system to do an expansion of the field $\psi(x)$ in terms of an orthonormal set of functions. We are interested in describing atoms loaded in a lattice, hence we use the Wannier functions $W_n(x - x_j)$, where $n$ is a band index and $j$ indicates a site in the lattice,

$$\psi(x) = \sum_{n,j} a_{nj} W_n(x - x_j), \quad (2.6)$$

$$W_n(x - x_j) = \frac{1}{\sqrt{V}} \sum_{k \in \text{BZ}} u_{nk}(x) e^{-i k \cdot x} . \quad (2.7)$$

The operator $a_{nj}$ annihilates a particle in the band $n$ of the site $j$. The Wannier functions are expressed in terms of Bloch wave functions $u_{nk}(x)$, thus the sum is restricted to the first Brillouin zone. At very low temperatures and sufficiently small interactions, we can neglect inter band transitions and confine the particles to the lowest band $n = 0$. From now on we drop the index $n$. It is straightforward to notice that the Wannier functions are orthonormal because they are defined through a unitary transformation of the Bloch functions, which form an orthonormal set.

The choice of Wannier functions gives the possibility of building a set of maximally localized states for a tight binding model. Indeed, the Wannier functions are given in terms of the Bloch functions, which are defined up to a (in principle momentum dependent) phase:

$$u_{nk} \rightarrow e^{i\phi_n(k)} u_{nk} . \quad (2.8)$$
This means that they are not unique and one can address the phase freedom to obtain a useful set of functions. Kohn demonstrated [25] that this freedom can be used to obtain (inside a certain band) one and only one Wannier function with the following properties: it is real, it is symmetric about the point at which it is centered, and it falls off exponentially. The only needed assumption is the inversion symmetry of the crystal potential in 1D (hence, it also applies for separable potentials in higher dimensions).

The exponential localization of the Wannier functions is an important property because they can be used in a tight-binding model like the one we are describing here. More recently [26], it has been shown that the asymptotic behavior (in 1D) is, with high accuracy,

\[ |W_n(x)| \sim |x|^{-3/4} e^{-h_n|x|}, \]  
\[ (2.9) \]

where \( h_n \) is the band decay constant. The important issue of finding an optimized set of Wannier functions has been treated by Marzari and Vanderbilt [27]. They proposed an algorithm to find optimally localized Wannier functions for composite bands, which minimizes the functional

\[ \Omega = \langle r^2 \rangle - \bar{r}^2, \]  
\[ (2.10) \]

i.e. the spread of the Wannier function.

We are now able to write explicitly our tight binding model. In the first term in the Hamiltonian (proportional to \( a_i^\dagger a_j \)), we have to consider the contributions given when \( i = j \) and when \( i \neq j \). The former is only a shift in the chemical potential if we consider a homogeneous lattice, the latter can be simplified taking into account only nearest-neighbor interactions which we denote \( \langle i, j \rangle \).

The second term in the Hamiltonian (proportional to \( a_i^\dagger a_j^\dagger a_{i'} a_{j'} \)) is largely simplified for ultracold atoms because the interaction potential is proportional to a Dirac delta function \( V(x - x') = (4\pi a_s \hbar^2 / m) \delta(x - \)
2.3 Mott-insulator/superfluid phase transition

\( x' \) (mimicking a repulsive short range interaction, i.e. between hard spheres); moreover, only on-site interactions \((i = j = i' = j')\) are allowed because the range of interactions is much smaller than the lattice spacing.

The Hamiltonian can thus be cast into the form

\[
H = - \sum_{(i,j)} (t_{ij}a_i^\dagger a_j + \text{h.c.}) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i, \tag{2.11}
\]

where

\[
t_{ij} = - \int d\mathbf{x} \, W_0^*(\mathbf{x} - \mathbf{x}_i) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V_\text{ext}(\mathbf{x}) \right\} W_0(\mathbf{x} - \mathbf{x}_j),
\]

\[
U = \frac{4\pi a_s \hbar^2}{m} \int d\mathbf{x} \, |W_0(\mathbf{x} - \mathbf{x}_i)|^4.
\]

One should notice that for a homogeneous system the coefficient \(U\) does not depend on the site \(i\) and \(t_{ij}\) is simply a number that we call \(t\). This Hamiltonian describes the celebrated Bose-Hubbard model: the hopping parameter \(t\) is the tunneling amplitude between adjacent sites, \(U\) is the onsite interaction strength, and \(\mu\) is the chemical potential.

2.3 Mott-insulator/superfluid phase transition

The physical phenomena underlying this Hamiltonian are the result of the competition between \(t\) and \(U\). Fisher et al. [28] have shown that this model gives rise to two phases, with a second order phase transition between them: the Mott-insulator/superfluid phase transition. Let us suppose that \(t\) is negligible with respect to \(U\): in this case, the Hamiltonian is diagonal in the particle number and the energy is minimized when there is the same number of particles \(n\) in each site \(j\). In this case, the energy density is

\[
\varepsilon(n) = \frac{1}{2} Un(n - 1) - \mu n. \tag{2.12}
\]
When $\mu < 0$, the energy is minimized for $n = 0$; for all values of $\mu$ in the interval $U(n-1) < \mu < Un$, there are exactly $n$ bosons per site (the range of validity of $\mu$ can be obtained by imposing that $\varepsilon(n+1) - \varepsilon(n) > 0$ and $\varepsilon(n) - \varepsilon(n-1) > 0$). If we now turn on $t > 0$, a particle can hop from a site to another one only when the cost in potential energy to remove a particle from a site and add it to a neighbor site is compensated by $t$. For small $t$, we expect that this process is highly suppressed. Thus, this phase of the system behaves like a Mott-insulator, which has a gap for the creation of particle-hole excitations and a vanishing compressibility. A finite amount of energy is required to excite the system.

When the balance between potential and hopping energy is reached, each particle is delocalized all over the lattice; its momentum is then fixed and it is the one for which the single-particle spectrum has a minimum. In this case the dilute gas is in a condensed phase or superfluid phase.

From the previous discussion, it appears that one should find a critical value $(U/t)c$ which separates the two phases. The order parameter can be easily identified with $\langle a_i \rangle$. Indeed, in the Mott-insulator phase with $N_0$ particles per site and $N_s$ sites, the ground state is (in the absence of hopping)

$$|\psi_{MI}\rangle \propto \left( \prod_{i=1}^{N_s} a_i^\dagger \right)^{N_0} |0\rangle,$$

and the expectation value $\langle a_i \rangle$ is trivially zero, while in the superfluid phase it acquires a nonvanishing value. Indeed, in the superfluid phase we know from Bogoliubov theory that $\langle a_k \rangle \propto \delta_{k,k_0}$, where $k_0$ is the condensation momentum. This means that $\langle a_i \rangle \propto \sum_k e^{-ik\cdot r_i} \langle a_k \rangle$ is nonvanishing.

Let us consider a mean field approximation of the Hamiltonian (2.11), which is useful to study the phase transition. We decouple the kinetic term

$$a_i^\dagger a_j = \langle a_i^\dagger \rangle a_j + a_i^\dagger \langle a_j \rangle - \langle a_i^\dagger \rangle \langle a_j \rangle = (a_i^\dagger + a_j)\psi - \psi^2,$$

where the (real) order parameter $\psi = \sqrt{n} = \langle a_i^\dagger \rangle = \langle a_i \rangle$ has been intro-
duced. The mean field Hamiltonian reads

\[ H_{MF} = -zt\psi \sum_j \left( a_j^\dagger + a_j \right) + \\
zt\psi^2 N_s + \frac{1}{2} U \sum_j n_j(n_j - 1) - \mu \sum_j n_j , \quad (2.15) \]

where \( z = 2d \) is the number of nearest neighbors, with \( d \) the dimension of the system.

To find the boundary between the two phases, we use the Landau theory of second order phase transitions: we have to determine when the quadratic term in \( \psi \) in the Hamiltonian (free energy) vanishes. This can be accomplished by applying second order perturbation theory, where we consider the first term as a perturbation \( \psi V = -zt(a_j^\dagger + a_j) \). The second order correction to the energy density is in this case (the Hamiltonian is diagonal with respect to the index site \( j \), so that we can drop the index \( j \) and divide the Hamiltonian by \( N_s \)),

\[ \varepsilon^{(2)}(N_0) = \psi^2 \sum_{n \neq N_0} \frac{|\langle N_0 | V | n \rangle|^2}{\varepsilon^{(0)}(N_0) - \varepsilon^{(0)}(n)} = \\
= \left( \frac{N_0}{U(N_0 - 1) - \mu} + \frac{N_0 + 1}{\mu - U N_0} \right) \psi^2 zt . \quad (2.16) \]

Note that the Hamiltonian (2.15) already contains a term proportional to \( \psi^2 \). Collecting all the quadratic terms and imposing that they must vanish, one finds the following relation between \( \bar{\mu} = \mu/zt \) and \( \bar{U} = U/zt \) [29]:

\[ \bar{\mu}_\pm = \frac{1}{2} \left( \bar{U} (2N_0 - 1) - 1 \right) \pm \frac{1}{2} \sqrt{\bar{U}^2 - 2\bar{U}(2N_0 + 1) + 1} . \quad (2.17) \]

The phase diagram is shown in Fig. 2.2. It consists of lobes with a fixed number of particles per site. The point of smallest \( \bar{U} \) for \( N_0 = 1 \) is a critical value: for smaller values of \( \bar{U} \) the system is superfluid whatever the chemical potential is; from the previous equation we obtain \( (U/t)_c \approx 5.83z \). Hence, we have found that by tuning the ratio \( U/t \) we can control
the phase transition, as we predicted on general grounds at the beginning of this section.

Figure 2.2: Phase diagram of the Bose-Hubbard model obtained from second-order perturbation theory. Each lobe has a fixed number of particles per site $N_0$.

In Refs. [28, 29], the authors found the spectrum of quasiparticle excitations using a functional formalism. We will skip most of the calculations in this section to make the discussion easier, but we will introduce the main idea, leaving the detailed calculations for later. We know that the (complex) order parameter is $\langle a_i \rangle$. Hence, we introduce an auxiliary field and use the Hubbard-Stratonovich transformation to decouple the term in the action proportional to $t_{ij}$. Then, we Taylor-expand the obtained effective action in powers of $t_{ij}$. From the terms proportional to quadratic powers of the Hubbard-Stratonovich field, we can find (after Fourier transforming) the zeros of the inverse Green function, which give the excitation spectrum. The final result is

$$\hbar \omega_k = -\mu + \frac{U}{2} (2N_0 - 1) + \frac{E_k}{2} \pm \frac{1}{2} \sqrt{E_k^2 + (4N_0 + 2)UE_k + U^2}, \quad (2.18)$$

where $E_k = -2t \sum_{j=1}^{d} \cos(k_j a)$, $a$ is the lattice spacing. From this result we can see that the Mott-insulator phase has a gap, as we should expect
for an insulator: to create a quasiparticle-quasihole pair, a finite amount of energy is required.

### 2.4 Experimental results

The investigation of the Mott-insulator/superfluid phase transition in optical lattice was theoretically discussed by Jaksch et al. [30]. Their work is based on a numerical simulation, in which they perform mean-field calculations using the Gutzwiller ansatz for the ground state wave function:

\[
|\psi_{MF}\rangle = \prod_i |\phi_i\rangle, \quad |\phi_i\rangle = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle_i .
\]  

(2.19)

They minimize the Bose-Hubbard Hamiltonian expectation value with respect to the coefficients \(f_n^{(i)}\) in the gran-canonical ensemble and compute the occupation number density \(\rho_i = \langle \hat{n}_i \rangle\) and its fluctuations \(\sigma_i^2 = (\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2)/\langle \hat{n}_i \rangle\). The evidence of the Mott-insulator phase is an integer occupation number \(\rho_i\) and fluctuations \(\sigma_i^2 \to 0\), while the presence of a superfluid phase is characterized by \(\langle a_i \rangle \neq 0\).

The first experimental evidence of the Mott-insulator/superfluid phase transition in optical lattices based on the prediction by Jaksch et al. [30] is reported in a seminal paper by Greiner et al. [31]. An ultracold gas of \(^{87}\text{Rb}\) in the \(F = 2, m_F = 2\) state with about \(10^5\) atoms is loaded in a 3D optical lattice, where depths of up to \(22E_r\) can be reached. The intensity of the laser beam was used to control the depth of the potential, i.e. the ratio \(U/t\). Indeed, the ratio \(U/t\) can be computed by approximating the Wannier function by the ground state wave function of a harmonic oscillator corresponding to each well of the optical potential.
2.4 Experimental results

One finds [2, 32]

\[ t \simeq \frac{4}{\sqrt{\pi}} \left( \frac{V_0}{E_r} \right)^{3/4} \exp \left[ -2 \left( \frac{V_0}{E_r} \right)^{1/2} \right], \quad (2.20) \]

\[ U \simeq \sqrt{\frac{8}{\pi}} k a_s \left( \frac{V_0}{E_r} \right)^{d/4}, \quad (2.21) \]

where \( d \) is the dimensionality of the system. The ratio is thus a function of the potential depth \( V_0 \) and the recoil energy \( E_r \).

The strategy to distinguish the superfluid phase from the Mott-insulator phase is to study the phase coherence of the condensate. This can be accomplished by using the time-of-flight technique, that we are going to outline below.

![Figure 2.3: Absorption images of multiple matter wave interference patterns after a time of flight of 15 ms for different potential depths \( V_0 \): (a) 0 \( E_r \), (b) 3 \( E_r \), (c) 7 \( E_r \), (d) 10 \( E_r \), (e) 13 \( E_r \), (f) 14 \( E_r \), (g) 16 \( E_r \), (h) 20 \( E_r \) [31].](image)

An initially trapped cloud of atoms is released (switching off traps and lasers) and it expands for a sufficiently long time, such that the initial extension of the cloud can be neglected with respect to the expanded cloud. We are interested in measuring the momentum distribution of the initial cloud, which yields us information on the phase coherence of the Bose gas. After a time-of-flight \( \tau \), the position of an atom with mass \( M \) and quasimomentum \( k \) will be\(^2\)

\[ x = \frac{\hbar k \tau}{M}, \]

such that we can

---

\(^2\)Recall that when all the traps are turned off, the Bloch wave function expands according to its decomposition in plane waves, where momenta from all the Brillouin zones are involved.
get information about the initial momentum distribution $n(k) \equiv \langle a_k^\dagger a_k \rangle$ from the density distribution of the atoms in the expanded cloud $n(x)$ (recorded by absorption imaging):

$$n(x) = \left( \frac{M}{\hbar \tau} \right)^3 |W_0(k)|^2 G(k),$$

where $W_0(k)$ is the Fourier transform of the lowest band Wannier function and $G(k) = \sum_{r,r'} e^{ik(r-r')} \langle a_r^\dagger a_{r'} \rangle$.

As shown in Fig. 2.3, we can see interference peaks in density corresponding to the momentum distribution of the cloud. The central peak is the one for $k = 0$ and the external peaks come from the second Brillouin zone $k + 2\pi \hat{n}/a$, where $\hat{n}$ is a unit vector. We are observing a true BEC, in which the condensed atoms occupy the lowest energy band (up to a reciprocal lattice vector shift). The intensity of peaks, which can be explained by Eq. (2.22), shows a transition at $V_0 = 10 - 13 E_r$ to a regime in which such coherence is completely lost. In Fig. 2.3 (a)-(d) the peak intensity grows because the spatial extent of the Wannier function $W_0(r)$ decreases when the potential depth increases, thus leading to an increase in its Fourier transform at high momenta. The intermediate interference peaks in (e)-(f) come from the fact that the correlation function $G(k)$ adds up constructively when $k$ is equal to a reciprocal lattice vector, even though the system is in the Mott-insulator phase. The interference pattern in (h) shows that when we are deep in the Mott-insulator phase, $G(k)$ contributes only for $r = r'$, the atoms are completely localized, and the shape that we observe comes from the Wannier function $W_0$, which is approximately a Gaussian.

The observed depth of the potential at which the transition takes place agrees with the theoretical calculations for filling fraction $N_0 = 1$, yielding $V_0 = 11.9 E_r$. In this experiment, they also found evidence of the gap in the Mott-insulator phase: they applied a potential gradient such that there is a difference in potential energy between two neighboring
2.4 Experimental results

sites. When this difference is equal to the gap energy, particles in the Mott-insulator phase can tunnel. If we restore the superfluid phase by lowering the potential depth at $V_0 = 9E_r$, then excitations in the Mott-insulator phase will cause excitations in the superfluid spectrum. These are phase fluctuations and hence a broadening of the interference peak is expected. This is observed by varying the potential gradient at a fixed potential depth and measuring the interference peak width of the restored superfluid phase when the potential depth is lowered to $V_0 = 9E_r$. In the Mott-insulator phase, we observe a wide peak in the interference pattern only for two values of the potential gradient. The first peak is interpreted as due to the gap, the second one is due to second order tunneling processes, like multiparticle tunneling.

![Figure 2.4: Interference peak width vs energy difference of neighboring sites](image)

Figure 2.4: Interference peak width vs energy difference of neighboring sites: (a) $V_0 = 10E_r$, no peaks in the spectrum, the system is still in the superfluid phase; (b) $V_0 = 13E_r$, two peaks appear in the excitation spectrum probing that the system is in the Mott-insulator phase (the peak at higher energy is due to double tunneling processes [31]).

In recent years, the Mott-insulator/superfluid phase transition has been observed also in 1D [33] and 2D [34]. In 1D, the presence of a phase transition is observed by detecting the appearance of a gap in the excitation spectrum. In this case they use a different technique with respect to Greiner et al. [31]: they modulate the potential depth with a frequency $\nu_{\text{mod}}$ and induce excitations in the spectrum from the Bragg
scattering between the atoms and the photons. In the superfluid phase
they find a continuous excitation spectrum, while in the Mott-insulator
phase they observe peaks in the interference pattern width only for fixed
frequencies (or energy transfer from the laser photons), as expected. In
2D the phase transition is observed by the time-of-flight technique.
In this Chapter, we introduce an external time periodic shaking on optical lattices and describe how we can build an effective time independent Hamiltonian using the Floquet formalism (we closely follow the calculations in Refs. [3, 35]). After introducing the details of these systems, we describe the experimental results concerning the Mott-insulator/superfluid phase transition.

3.1 Floquet theory of time periodic systems

Solving the Schrödinger equation for a time periodic Hamiltonian requires the use of the so-called Floquet formalism. This formalism is well known in Solid State physics because the discrete symmetry that one deals with is the spatial translation invariance. In our case, we are discussing time translation invariance. A time periodic Hamiltonian does not conserve energy and this is the reason why a different formalism in which time dependence is integrated out is needed. According to the Floquet theorem [36, 37], a time periodic Hamiltonian $H(t) = H(t + T)$ defined in some Hilbert space $\mathcal{H}$ has a set of Floquet modes $|u_n(t)\rangle$, which
are time periodic with period \( T \) and a set of quasienergies \( E_n \), which are solutions of the eigenvalue equation

\[
\mathcal{H}(t)|u_n(t)\rangle = E_n|u_n(t)\rangle ,
\]

(3.1)

where \( \mathcal{H}(t) \equiv H(t) - i\hbar \frac{\partial}{\partial t} \) is called the Floquet Hamiltonian. The solutions of the Schrödinger equation \( |\psi_n(t)\rangle \), called Floquet states, have thus the form

\[
|\psi_n(t)\rangle = e^{-iE_nt/\hbar}|u_n(t)\rangle ,
\]

(3.2)
as one can easily check. Let us define the frequency given by the time periodicity: \( \omega \equiv 2\pi/T \). If \( |u_n(t)\rangle \) is solution of Eq. (3.1), then \( |u'_n(t)\rangle = |u_n(t)\rangle e^{im\omega t} \), \( m \) an integer, is still a solution with quasienergy \( E'_n = E_n + m\hbar\omega \). From this we get that the Floquet states are the same,

\[
|\psi'_n(t)\rangle = |\psi_n(t)\rangle .
\]

(3.3)

This result shows that quasienergies with different index \( m \) map physically equivalent states. Hence, they have a Brillouin-zone-like structure, as in Solid State physics. We can restrict the quasienergies to the first Brillouin zone, choosing \( E_n \) to lie in the interval \([-\hbar\omega/2, \hbar\omega/2]\).

We introduce a composite Hilbert space \( \mathcal{H}' = \mathcal{H} \otimes \mathcal{H}_T \) for the Floquet Hamiltonian \( \mathcal{H} \), where \( \mathcal{H}_T \) is the Hilbert space of \( T \)-periodic functions, such that Eq. (3.1) is an eigenvalue problem in \( \mathcal{H}' \). We define the scalar product for this space by just adding a time average of the scalar product in the space \( \mathcal{H} \otimes \mathcal{H}_T \)

\[
\langle\langle \phi|\psi \rangle\rangle_T \equiv \frac{1}{T} \int_0^T dt \langle \phi|\psi \rangle ,
\]

(3.4)

where \( \phi, \psi \in \mathcal{H} \). The states \( |u_n(t), m\rangle \) form a complete set of orthonormal functions, where the completeness and orthogonality conditions read

\[
\sum_{n,m} |u_n(t), m\rangle \langle u_n(t'), m| = \delta(t - t') ,
\]

(3.5)

\[
\langle\langle u_n(t), m|u_n(t'), m' \rangle\rangle_T = \delta_{n,n'}\delta_{m,m'} .
\]

(3.6)
3.1 Floquet theory of time periodic systems

To understand the meaning of this formalism we compute the expectation value of the Hamiltonian $H(t)$ in a Floquet state $|\psi_n(t)\rangle$ which is nothing else that the averaged energy in this state \[38\]

$$
\langle H \rangle_n \equiv \frac{1}{T} \int_0^T dt \langle \psi_n(t)|H(t)|\psi_n(t)\rangle = E_n + \langle u_n|\hbar\frac{\partial}{\partial t}|u_n\rangle. \quad (3.7)
$$

The state $u_n(q,t)$ can be expanded in Fourier components with respect to the time variable $u_n(q,t) = \sum_k c_k^{(n)}(q)e^{-i\omega t}$, such that

$$
\langle H \rangle_n = \sum_{k=-\infty}^{\infty} (E_n + \hbar k\omega) \int dq |c_k^{(n)}(q)|^2. \quad (3.8)
$$

We deduce that $\langle H \rangle_n$ is the energy accumulated in each harmonic mode of the Floquet state $|\psi_n(t)\rangle$ and averaged with respect to the weight of each harmonic.

We now define a new basis in $H'$. Let $|n\rangle$ be an orthonormal basis of $H$. We perform a unitary transformation of it through the operator $\exp(-iF(t))$, where $F$ is a Hermitian time-periodic operator, while for $H_T$ we consider plane waves as basis. The basis in $H'$ is thus

$$
|n(t),m\rangle = U_{F,m}(t)|n\rangle, \quad U_{F,m}(t) \equiv e^{-iF(t)+im\omega t}. \quad (3.9)
$$

We calculate the Floquet Hamiltonian matrix elements in this basis, thus obtaining

$$
\langle\langle n(t), m|\mathcal{F}(t)|n'(t), m'\rangle\rangle_T = \delta_{m,m'} \langle n|H_{\text{eff}} + m\hbar\omega|n'\rangle \\
+ (1 - \delta_{m,m'}) \langle n|e^{i(m-m')\omega t}\mathcal{F}^{(0,0)}_{T}|n'\rangle, \quad (3.10)
$$

where we defined

$$
\mathcal{F}^{(m,m')} \equiv U_{F,m}(t)\mathcal{F}(t)U_{F,m'}(t), \quad (3.11)
$$

$$
H_{\text{eff}} \equiv \langle\langle \mathcal{F}^{(0,0)}_{T}\rangle\rangle_T. \quad (3.12)
$$

1The normalization condition required on the coefficients $c_k^{(n)}$ is $\sum_k \int dq |c_k^{(n)}(q)|^2 = 1.$
3.1 Floquet theory of time periodic systems

As discussed in Ref. [3, 35], if we assume that blocks with different $m$ satisfy the condition

$$||H_{\text{eff}}|| \ll \hbar \omega,$$

(3.13)

where $||A|| \equiv \text{Max}\{|\langle n|A|m \rangle | : n, m \}$, then the energies of each block will be separated from the energies of another block, this separation being just $\hbar \omega$; the energy levels will not mix. Even if the blocks are separated, the off diagonal terms allow coupling between the states, what that we want to neglect. According to perturbation theory\footnote{Remember that the coupling between states, in perturbation theory, is given by ratios of the matrix element connecting the states and the energy difference among them.} we assume that

$$||\langle e^{i(m'-m)\omega t}F_T^{(0,0)}\rangle|| \ll \hbar \omega.$$

(3.14)

The Floquet Hamiltonian matrix elements can then be approximated by

$$\langle \langle n(t), m|\mathcal{S}_t(t)|n'(t), m' \rangle \rangle_T \approx \delta_{m,m'} \left( \langle n|H_{\text{eff}}|n' \rangle + m \hbar \omega \delta_{n,n'} \right).$$

(3.15)

The indices $m$ and $m'$ act as labels for the basis of $\mathcal{H}_T$ and thus have to refer to the different Brillouin zones for the quasienergies. Then, within the first Brillouin zone $m = m' = 0$, the quasienergy spectrum of $H(t)$ coincides with the energy spectrum of the time-averaged Hamiltonian $H_{\text{eff}}$. Hence, we describe the physical system of interest by this Hamiltonian.

To achieve the result of computing the quasienergy spectrum of the system we need to identify a reasonable operator $F$. For this reason, we assume that the Hamiltonian $H(t)$ can be decomposed in a weakly driven part $H_<(t)$, for which $||H_<(t)|| \ll \hbar \omega$, and a strongly driven part $H_>(t)$, such that $H(t) = H_<(t) + H_>(t)$. $F$ is chosen such that

$$\hbar F(t) \equiv \int_0^t ds H_>(s).$$

(3.16)

This decomposition will be useful to satisfy the constraints (3.13), (3.14) as we will show afterwards. For arbitrary operators $A$ and $B$ the following
relations hold
\begin{align}
e^{iA} \frac{\partial}{\partial t} e^{-iA} &= -\sum_{n=0}^{\infty} \frac{i^{n+1}}{(n+1)!} [A, A']_n , \\
e^{iA}B e^{-iA} &= \sum_{n=0}^{\infty} \frac{i^n}{n!} [A, B]_n ,
\end{align}
(3.17)
(3.18)

where the multiple commutators are defined as $[A, B]_{n+1} \equiv [A, [A, B]_n]$ and $[A, B]_0 \equiv B$. For $m = m' = 0$, if we choose $A = F$ and $B = H$ we can easily compute $\hat{\mathcal{S}}_F^{(0,0)} = e^{iF(t)} (H - i\hbar \partial / \partial t) e^{-iF(t)}$

\begin{align}
\hat{\mathcal{S}}_F^{(0,0)} &= \sum_{n=0}^{\infty} \frac{i^n}{n!} \left( [F(t), H(t)]_n - \frac{\hbar}{n+1} [F(t), F'(t)]_n \right) \\
&= \sum_{n=0}^{\infty} \frac{i^n}{n!} \left( [F(t), H_{<}(t)]_n + \frac{n}{n+1} [F(t), H_{>}(t)]_n \right) .
\end{align}
(3.19)

This equation is just the starting point to write the effective Hamiltonian $H_{\text{eff}}$ with which we will describe some physical systems in a time independent picture.

### 3.2 Driven optical lattices

As an application of the theory developed in the previous paragraph, we present an example. Suppose that a particle is subjected to a periodic potential which is not static: the potential oscillates with frequency $\omega$ and has a maximum displacement $x_0$. The Hamiltonian describing such a system is

$$H = \frac{p^2}{2m} + V_0 \cos [x + x_0 \cos(\omega t)] .$$
(3.20)

As mentioned by Glück et al. [39], we can use the Kramers-Henneberger transformation to move into the reference frame of the shaked lattice. These are canonical transformations [40] and thus we introduce the generating function

$$\mathcal{F}(p', x, t) = [p' + mx_0 \omega \sin(\omega t)][x + x_0 \cos(\omega t)] ,$$
(3.21)
3.2 Driven optical lattices

leading to

\[ p = \frac{\partial F}{\partial x}, \quad x' = \frac{\partial F}{\partial p'}, \quad H'(p', x', t) = H(x, p, t) + \frac{\partial F}{\partial t}. \] (3.22)

We get

\[ p = p' + mx_0 \omega \sin(\omega t), \] (3.23)
\[ x' = x + x_0 \cos(\omega t), \] (3.24)

and for the Hamiltonian

\[ H'(p', x', t) = \frac{1}{2m} [p'^2 + m^2 x_0^2 \omega^2 \sin^2(\omega t) + 2p' mx_0 \omega \sin(\omega t)] + V_0 \cos x' + x'[mx_0 \omega^2 \cos(\omega t)] - [p' + mx_0 \omega \sin(\omega t)]x_0 \omega \sin(\omega t). \] (3.25)

Two terms cancel, yielding

\[ H'(p', x', t) = \frac{1}{2m} p'^2 + V_0 \cos x' + x'[mx_0 \omega^2 \cos(\omega t)] - \frac{1}{2} mx_0^2 \omega^2 \sin^2(\omega t). \] (3.26)

As we can see in its definition, \( x' \) is just the comoving coordinate. For \( x' \gg x_0 \), we can drop the last term, which is negligible with respect to the dipolar term \( \propto x' \), and the Hamiltonian can thus be written as

\[ H'(p', x', t) = \frac{p'^2}{2m} + V_0 \cos x' + F_\omega x' \cos(\omega t), \quad F_\omega \equiv mx_0 \omega^2. \] (3.27)

This means that the Hamiltonian in the moving frame can be approximate as the sum of two parts: the first part is just the undriven one while the second part contains the time dependence and is like a dipole.

In Quantum Mechanics, such canonical transformation is taken into account for the wave function in the following way:

\[ \psi(x, t) = e^{-iF_\omega \sin(\omega t)x/\hbar \omega} \psi'(x', t), \] (3.28)

which is the transformation used to go back to the laboratory frame.
Let us now consider a one dimensional optical lattice and a system of bosonic atoms loaded into this lattice. Assume a potential like in Eq. (2.3), $V = (V_0/2) \cos(2kx)$. If we shake the potential as $x \rightarrow x + x_0 \cos(\omega t)$ we can write the Hamiltonian in the reference frame of the moving lattice as

$$H = H_0 + H_{\text{int}} + W(t),$$  \hspace{1cm} (3.29)

where $H_0 + H_{\text{int}}$ is the undriven part and $W(t)$ is

$$W(t) = x F_\omega \cos(\omega t), \quad F_\omega = mx_0 \omega^2.$$  \hspace{1cm} (3.30)

The second-quantized version of $H_0$ has been presented in Chap. 2; expanding the field operators in terms of Wannier functions, the time dependent part of the Hamiltonian is

$$\sum_{i,j} \int dx a_i^\dagger a_j W_0^*(x - R_i) W(t) W_0(x - R_j).$$  \hspace{1cm} (3.31)

The dipolar term $W(t)$ is proportional to the position operator, which is the one involved in the integrals. As demonstrated by Kohn [25], we can take the Wannier functions to be real and symmetric with respect to the lattice point where they are centered.

When $i \neq j$ then we find

$$\int dx W_0^*(x - R_i) x W_0(x - R_j) =$$

$$\int dx W_0^* \left[ x + \frac{1}{2}(R_j - R_i) \right] x W_0 \left[ x - \frac{1}{2}(R_j - R_i) \right],$$  \hspace{1cm} (3.32)

where we shifted $x \rightarrow x + (R_i + R_j)/2$; the term coming from the shift

$$\frac{1}{2}(R_i + R_j) \int dx W_0^* \left[ x + \frac{1}{2}(R_j - R_i) \right] W_0 \left[ x - \frac{1}{2}(R_j - R_i) \right]$$  \hspace{1cm} (3.33)

vanishes when $i \neq j$ because the Wannier functions are orthogonal. Because of the symmetry properties of the Wannier functions, the product between Wannier functions in Eq. (3.32) is even, $x$ is odd, and the integral vanishes. Thus, we expect only contributions coming from $i = j$.  

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3.2 Driven optical lattices

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<td>6.15 x 10^{-3}</td>
<td>-7.16 x 10^{-4}</td>
<td>1.01 x 10^{-4}</td>
</tr>
<tr>
<td>6.0</td>
<td>-0.05077</td>
<td>1.91 x 10^{-3}</td>
<td>-1.15 x 10^{-4}</td>
<td>8.31 x 10^{-6}</td>
</tr>
<tr>
<td>8.0</td>
<td>-0.03080</td>
<td>6.35 x 10^{-4}</td>
<td>-2.08 x 10^{-5}</td>
<td>8.20 x 10^{-7}</td>
</tr>
<tr>
<td>10.0</td>
<td>-0.01918</td>
<td>2.27 x 10^{-4}</td>
<td>-4.25 x 10^{-6}</td>
<td>9.57 x 10^{-8}</td>
</tr>
</tbody>
</table>

Table 3.1: Hopping matrix elements for the lowest band of an optical lattice in units of the recoil energy $E_r$: $c_1$ refers to nearest neighbors, $c_2$ refers to next-nearest neighbors and so on [41].

When $i = j$, we use the fact that the Wannier functions are peaked at each site and they are orthonormal to obtain:

$$\int dx W_0^\ast(x - R_j) x W_0(x - R_j) \simeq a_j, \quad (3.34)$$

where $a$ is the lattice spacing and $j$ is an integer, numbering the position of the sites. One obtains

$$W(t) = K \cos(\omega t) \sum_j j a_j^\dagger a_j, \quad K = ax_0 \omega^2. \quad (3.35)$$

In sum, the effective Hamiltonian for a Bose gas in a 1D optical lattice under the action of a time dependent driven force can be written as

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{h.c.}) + \frac{U}{2} \sum_i n_i(n_i - 1) + K \cos(\omega t) \sum_j j a_j^\dagger a_j, \quad (3.36)$$

where we restricted the hopping parameters only to nearest-neighbor sites. This approximation is valid because the next-nearest-neighbor-hopping coefficients are at least two order of magnitude smaller than the nearest-neighbor ones, see Table 3.1. We used the convention $t \equiv -c_1$.

The system we have just described is in the same class of systems for which we can apply the Floquet formalism. In the previous paragraph, we presented the way to treat these systems; let us start computing $S_F^{(0,0)}$. In the following, we perform in detail the calculations mentioned
3.2 Driven optical lattices

in Ref. [35]. We choose \( H_\prec = H_0 + H_{\text{int}} \) and \( H_\succ(t) = W(t) \), obtaining for the definition of \( F \)

\[
F(t) = \frac{K}{\hbar \omega} \sin(\omega t) \sum_j j a_j^\dagger a_j,
\]

(3.37)
such that \( \hbar F'(t) = W(t) \). We can immediately conclude that \([F, H_\succ] = 0\) and \([F, H_{\text{int}}] = 0\). Then, from Eq. (3.19) we need to calculate \([F, H_0]\) only. To simplify the notation, we define the following operators

\[
Q = K \sum_j a_j^\dagger a_j,
\]

(3.38)

\[
T_\pm = \sum_{\langle i,j \rangle} a_i^\dagger a_j \pm a_j^\dagger a_i,
\]

(3.39)
such that \( F(t) = Q \sin(\omega t)/\hbar \omega \) and \( H_0 = -t T_+ \). We compute the commutator \([Q, T_\pm]\)

\[
[Q, T_\pm] = K \sum_{\nu} \sum_{\langle i,j \rangle} \nu \left[ a_i^\dagger a_\nu, a_j^\dagger a_j \pm a_j^\dagger a_i \right] = K \sum_{\nu} \sum_{\langle i,j \rangle} \nu \left( [a_i^\dagger a_\nu, a_j^\dagger a_j] + a_i^\dagger [a_i^\dagger a_\nu, a_j] \pm a_i^\dagger [a_j^\dagger a_\nu, a_j^\dagger a_i] \right)
\]

\[
= K \sum_{\nu} \sum_{\langle i,j \rangle} \nu \left( a_i^\dagger [a_\nu, a_j^\dagger a_j] a_j + a_i^\dagger [a_\nu, a_j] a_j \pm a_i^\dagger [a_\nu, a_j^\dagger] a_j^\dagger a_i \right)
\]

\[
= K \sum_{\langle i,j \rangle} \left( \delta_{i,j} [a_i^\dagger a_j - j a_i^\dagger a_j \pm j a_j^\dagger a_i \mp i a_j^\dagger a_i] \right) = K T_\mp,
\]

(3.40)

where, in the second line, we used the bosonic commutation relations \([a_i, a_j^\dagger] = \delta_{ij}\) and the following identities for operators \(A, B\) and \(C\):

\([A, BC] = [A, B]C + B[A, C]\) and \([AB, C] = A[B, C] + [A, C]B\). In the last line we have chosen \(i - j = +1\) for nearest neighbors. We are
interested in multiple commutators, then we can establish the relation
\[ [Q, T_\pm^n] = K^n T_{n \pm 1} \]. We finally obtain from Eq. (3.19)
\[
\delta_F^{(0,0)} = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{i \sin(\omega t)}{\hbar \omega} \right)^n [Q, H_0 + H_{\text{int}}]
\]
\[ = H_{\text{int}} - t \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left( \frac{i K \sin(\omega t)}{\hbar \omega} \right)^{2n} T_+ \]
\[ - t \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left( \frac{i K \sin(\omega t)}{\hbar \omega} \right)^{2n+1} T_- , \] (3.41)
where we have used the fact that \([Q, H_0 + H_{\text{int}}]_0 = H_0 + H_{\text{int}}\).

Next, we evaluate the constraints in Eqs. (3.13) and (3.14). When the two indices \(m, m'\) are both even, \((m \to 2m, m' \to 2m')\),
\[
\langle e^{i2(m' - m)\omega t} \delta_F^{(0,0)} \rangle_T = \delta_{mm'} H_{\text{int}} +
\]
\[ - t \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left( \frac{i K}{\hbar \omega} \right)^{2n} \langle \sin^{2n}(\omega t) e^{i2(m' - m)\omega t} \rangle_T T_+ \]
\[ - t \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left( \frac{i K}{\hbar \omega} \right)^{2n+1} \langle \sin^{2n+1}(\omega t) e^{i2(m' - m)\omega t} \rangle_T T_- . \]

Let us compute the first time average in the previous equation; after defining \(x = \omega t\) and \(m' - m = p\) it leads to
\[
\langle \sin^{2n}(\omega t) e^{i2(m' - m)\omega t} \rangle_T = \frac{1}{2\pi} \int_0^{2\pi} dx e^{2ipx} \left( \frac{e^{ix} - e^{-ix}}{2i} \right)^{2n}
\]
\[ = \frac{1}{2\pi} \frac{(-1)^n}{2^{2n}} \int_0^{2\pi} dx e^{2ipx} \sum_{k=0}^{2n} \frac{(2n)!}{(2n - k)! k!} (-1)^k e^{i(2n-k)x} e^{-ikx}
\]
\[ = \frac{(-1)^n}{2^{2n}} \sum_{k=0}^{2n} \frac{(2n)!}{(2n - k)! k!} (-1)^k \delta_{k,p+n} . \] (3.42)

If \(-n \leq p \leq n\), the previous expression is non-vanishing and we obtain
\[
\langle \sin^{2n}(\omega t) e^{i2p\omega t} \rangle_T = \frac{(-1)^p (2n)!}{2^{2n}(n+p)!(n-p)!} . \] (3.43)

The second time average is zero because, as in the second line of Eq. (3.42), one finds
\[
\int_0^{2\pi} dx e^{2ipx+i(2n+1-k)x-ikx} = \int_0^{2\pi} dx e^{2i(p+n-k-1/2)x} = 0 . \] (3.44)
Collecting all the terms, we find
\[
\left\langle e^{i2(m' - m)\omega t} \delta_F^{(0,0)} \right\rangle_T = \delta_{mm'}H_{\text{int}} +
-t \sum_{n=0}^{\infty} \left( \frac{iK}{\hbar\omega} \right)^{2n} \frac{(-1)^{m' - m}}{2^{2n}(n + m' - m)!(n - m' + m)!} T_+. \tag{3.45}
\]

Let us now define a new integer \( k = n - m' + m \) and change the index of summation,
\[
\left\langle e^{i2(m' - m)\omega t} \delta_F^{(0,0)} \right\rangle_T = \delta_{mm'}H_{\text{int}} +
-t \sum_{k=m-m'}^{\infty} \left( \frac{K}{\hbar\omega} \right)^{2(m'-m)+2k} \frac{(-1)^{k}}{2^{2(m'-m)+2k}(k + 2(m' - m))!k!} T_+. \tag{3.46}
\]

The condition that the matrix element is non-vanishing holds only when
\(-n \leq m' - m \leq n\), as stated before. This can be taken into account if we multiply the previous expression by a product of Heaviside step functions,
\[
\theta(m' - m + n)\theta(m - m' + n) \rightarrow \theta(k)\theta(k + 2(m' - m)). \tag{3.46}
\]

Thus, when \( m' \geq m \) we can restrict the sum over \( k \) to the interval \([0, \infty)\) and use the definition of the \( m \)th-order Bessel function
\[
J_l(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+l}}{2^{n+l}n!(l+n)!}, \tag{3.47}
\]

to get
\[
\left\langle e^{i2(m' - m)\omega t} \delta_F^{(0,0)} \right\rangle_T = -t J_{2(m'-m)} \left( \frac{K}{\hbar\omega} \right) T_+ + \delta_{m',m} H_{\text{int}}. \tag{3.48}
\]

Hence, it is sufficient to impose
\[
t, U \ll \hbar\omega \tag{3.49}
\]
to satisfy Eqs. (3.13) and (3.14). Indeed, the Bessel function \( J_l(x) \) is smaller than 1 (in modulus) for arbitrary integers \( l \) and then the previous conditions are sufficient.
3.2 Driven optical lattices

When $m' < m$, it is convenient to define a different index $k = n - m + m'$ in Eq. (3.45) and we obtain the same result as in Eq. (3.48) but with the Bessel function $J_{2(m-m')}(K/\hbar \omega)$.

A similar analysis applies for time averaged matrix elements with $2m + 1$ and $2m' + 1$ powers insted of $2m$ and $2m'$. The mixed powers yield zero matrix elements. From Eq. (3.48), putting $m = m' = 0$, we find the important result for the effective Hamiltonian

$$H_{\text{eff}} = -t_{\text{eff}} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{h.c.}) + H_{\text{int}},$$

(3.50)

where

$$t_{\text{eff}} = t J_0 \left( \frac{K}{\hbar \omega} \right).$$

(3.51)

This Hamiltonian describes the same Bose-Hubbard model that we have presented in Chap. 2. The effect of the shaking is to renormalize the hopping coefficient, by multiplying it with a Bessel function. This is a new feature because we can now modify the strength of the hopping coefficient by tuning the shaking-dependent parameter

$$K_0 = \frac{K}{\hbar \omega}.$$ 

(3.52)

![Figure 3.1: Plot of the Bessel function $J_0(x)$.](image)
3.2 Driven optical lattices

One can thus expect that we can induce the Mott-insulator/superfluid phase transition (which depends on the ratio \( U/t_{\text{eff}} \), where \( t_{\text{eff}} \) is the renormalized hopping coefficient) by tuning the shaking of the optical lattice. Indeed, the interaction strength \( U \) is not influenced by the shaking.

As shown in Fig. 3.1, the Bessel function \( J_0(x) \) has several zeros, the first one is located at \( x \simeq 2.4 \). Crossing this point, the Bessel function changes sign and so it does the hopping coefficient. The opposite process happens around the second zero and so on.

![Figure 3.2: (a) Energy bands for the undriven system; (b) First Brillouin zone of the quasienergy spectrum for the driven system.](image)

A numerical investigation of these predictions has been performed by Eckardt et al. [3]. The energy bands for a 1D undriven system with \( M = 5 \) sites and \( N = 5 \) particles have been computed as a function of the ratio \( U/t \). The bands are expected to form a continuum for \( N, M \to \infty \) and \( N/M = 1 \). As is shown in Fig. 3.2 (a) the lowest energy band splits off from the group for increasing values of \( U/t \), indicating that a gap is formed and that the system is entering the Mott-insulator phase.

For the driven system, the numerical computation of the quasienergies has been performed for \( N = M = 5 \) with \( \hbar \omega/t = 14 \). Hence, we can restrict our first Brillouin zone to the interval \([-7, 7]\). The shaking parameter has been chosen to be \( K_0 = 1.5 \) such that \( J_0(K_0) \simeq 0.5 \). According to the theory discussed previously, we expect to find the same
energy spectrum up to a rescaling of the axes, as shown in Fig. 3.2 (b). In addition, the quasienergy spectrum is richer because we have to take into account the Brillouin zone structure: the eigenvalues that dissappear in the upper part of the plot reappear in the lower one.

Nevertheless, the Brillouin zone structure generates the crossing of some energy levels because of the coupling among different Brillouin zones. They are avoided crossings and if the condition $t, U \ll \hbar \omega$ is satisfied, they are too narrow to be resolved. Before closing this section, it is important to stress that the shaking frequency must be small compared to the gap between the two lowest Bloch bands in order to avoid transitions and to obtain a valid one band description.

### 3.3 Experimental results

The experimental proof that tunneling in an optical lattice can be destroyed dynamically under the effect of shaking has been recently presented by a research group in Pisa [4, 42].

Before describing the experiment in detail, it is necessary to focus our attention on the problem of adiabaticity. When a perturbation is switched on, it is important to insure an adiabatic process in which the system (prepared in the ground state) still follows the ground state of the perturbed system. This is, for instance, the problem of loading a trapped BEC in an optical lattice and, in this case, the duration of the ramp to load the cloud of atoms must be larger than a threshold value to guarantee adiabaticity. In the system, when the shaking is turned on, we introduce two time scales. The first one is just the rate of change of the parameters $K_0$ and the second time scale is the periodicity of the Hamiltonian.

The first time scale is important because of the shape of the quasienergy spectrum. The presence of avoided crossings (as shown in Fig. 3.3) enables two processes (and the mixture of the two) to happen when $K_0$
3.3 Experimental results

Figure 3.3: Trajectories through avoided crossings: the continuous arrow indicates that the system tunnel the avoided crossing (diabatic process), the dashed arrows indicates that the system follows the upper energy level (adiabatic process) [43].

varies. The system can follow the upper level or it can tunnel through the crossing gap. The second process, called diabatic process, is the one we are interested in because, in this case, the system follows the energy eigenvalues of the undriven system (in the previous paragraph we have shown that the quasienergies map the undriven spectrum, up to level crossings). The tunneling rate depends on the rate of change of $K_0$ and on the gap amplitude. The adiabaticity we are describing has been controlled experimentally. For a BEC loaded into an optical lattice, the experimental procedure to control adiabaticity is the following: at a certain lattice depth, a linear ramp of 15ms is used to switch on the shaking from $K_0 = 0$ to $K_0 = 2.3$, then the system is held at $K_0 = 2.3$ for 200ms and back to $K_0 = 0$. At the end of this cycle, the lattice depth is ramped down to $4E_r$. What is measured is the ratio $\sigma/\sigma_0$, where $\sigma$ is the cloud width (after a time-of-flight measurement) at the end of the cycle and $\sigma_0$ is the cloud width at $K_0 = 0$. When this ratio is larger than one, excitations in the cloud generate the loss of adiabaticity. Fig. 3.3 shows that for different shaking frequencies, there is a minimum lattice depth, below which the process is not adiabatic. A detailed investigation has been performed to establish that the optimal shaking ramp is in the
range between 0 and 20 ms [43].

Figure 3.4: (a) $\sigma/\sigma_0$ vs lattice depth in 1D for linear ramping from $K_0 = 0$ to $K_0 = 2.3$ in 15 ms, holding time 200 ms at $K_0 = 2.3$. The shaking frequency $\omega/2\pi$ is 3 kHz (open triangles) and 6 kHz (solid squares). (b) $\sigma/\sigma_0$ vs driving frequency at lattice depth $V_0 = 5.7E_r$ with ramping time 10 ms and holding time 2 ms [4].

Figure 3.5: Time-of-flight image for a 1D BEC loaded into an optical lattice with $V_0 = 18E_r$. $K_0$ increases from 0 to 2.7 and then back to 0. The vertical axis converts position into condensation momentum. We start with a BEC condensing at zero momentum (side peaks come from the second Brillouin zone), then phase coherence is lost and finally it is established again with condensation momenta $\pm p_{rec}$. The symmetric part of the picture on the right comes from the ramp down to 0 [4].

The second time scale comes from the shaking frequency and is responsible for transitions between bands of the optical lattice. As we pointed out in the previous Chapter, even if the condition $\hbar \omega \gg t, U$ holds, $\hbar \omega$ must be smaller than the gap between the two lowest Bloch bands. In Fig. 3.4(b) it is shown that at the lattice depth $V_0 = 5.7E_r$, the driving frequency cannot exceed 6 kHz (while in the interval between 4
3.3 Experimental results

and 5 kHz, the breakdown of adiabaticity cannot be explained in terms of interband transitions).

Once we have understood how to take into account adiabaticity, we can thus investigate the dynamical suppression of tunneling, i.e., we can show that the Mott-insulator/superfluid phase transition can be induced dynamically by shaking the lattice. In this experiment, a BEC of $\sim 10^4$ atoms of $^{87}$Rb is loaded into an optical lattice at $V_0 = 18E_r$ with 40 sites occupied and $K_0$ is ramped from 0 to 2.7 in 113 ms and back to 0.

A time-of-flight picture taken at different times is shown in Fig. 3.5. Any inspection of the picture clearly shows that after increasing $K_0$, the phase coherence of the condensate is lost at a certain point and the cloud of atoms does not present anymore the peaked pattern. For larger values of $K_0$, the phase coherence is established again but the central peak at zero momentum is no longer present; now two side peaks are evident. This can be explained by the change of slope of the single particle spectrum due to the change of sign of the effective hopping (the Bessel function becomes negative), meaning that the condensation point is at the edges of the Brillouin zone. We will describe much more in detail this process in the next Chapter.

The last point that we want to discuss is the direct measurement of the effective hopping coefficient $t_{\text{eff}}$. After a sufficiently long time-of-flight, the expansion rate of the atomic cloud is linear in time and the slope is proportional to the hopping coefficient [44]. Hence, a direct measurement of the expansion rate can provide a direct inspection of the effective hopping coefficient. These measurements have been performed and the results are reported in Fig. 3.6. It is important to notice that it is not possible to measure the sign of the hopping coefficient because $\partial \sigma(\tau)/\partial \tau \propto |t|$.

The data show a good agreement between the theoretical prediction (dashed line) and the experimental points; moreover, the destruction of
3.3 Experimental results

Figure 3.6: Different data sets measuring the ratio $t_{\text{eff}}/t$ as a function of $K_0$. Each set of data has a fixed lattice depth and shaking frequency [42].

tunneling, in correspondence with the points where the Bessel function vanishes, seems to be clear. Nevertheless, as pointed out in Ref. [41, 44], the destruction of tunneling is not completely achieved because next-nearest-neighbor-hopping terms prevent the tunneling from vanishing. We will describe this phenomenon theoretically in the next Chapter.
In this Chapter, we show much more in detail the theoretical framework of the phase transition in 1D driven systems. We take into account next-nearest-neighbor hopping and we discuss the possibility of generating finite-momentum condensates in such systems.

4.1 Single-particle spectrum

The physical results presented in the previous Chapters are based on a description which takes into account only nearest neighbors. When the system is driven and we renormalize the hopping coefficient, by multiplying it with a Bessel function, the theory cannot be considered complete. Indeed, when the shaking parameter $K_0$ is close to the zero of the Bessel function, the effective hopping coefficient for nearest neighbors vanishes and, in principle, we should investigate if higher-order hopping terms are still present.

We will consider a 1D optical lattice for bosons; the Bose-Hubbard model for the undriven system (including next-nearest-neighbor hopping)
4.1 Single-particle spectrum

reads

\[ H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{h.c.}) + t' \sum_{\langle\langle i,j \rangle\rangle} (a_i^\dagger a_j + \text{h.c.}) + \frac{U}{2} \sum_i n_i (n_i - 1) \]

\[ = H_0 + H_{\text{int}}. \tag{4.1} \]

In the previous Chapter we have discussed what is the effect of including a sinusoidal shaking on the lattice

\[ W(t) = K \cos(\omega t) \sum_j j a_j^\dagger a_j. \tag{4.2} \]

From Eq. (3.40) it is clear that, since the difference |i − j| is equal to 2 for next-nearest neighbors, we can write the effective Hamiltonian \( H_{\text{eff}} \) of this system renormalizing the hopping amplitude as follows

\[ t \rightarrow t_{\text{eff}} = t J_0(K_0), \tag{4.3} \]

\[ t' \rightarrow t'_{\text{eff}} = t J_0(2K_0), \tag{4.4} \]

Fig. 4.1 shows that when \( t_{\text{eff}} \) is almost zero, i.e. close to the first zero of the Bessel function \( J_0(K_0) \) (\( K_0 \simeq 2.4 \)), \( t'_{\text{eff}} \) is still non-vanishing and changes sign. A similar discussion applies to the second zero. In this model we do not introduce higher-order hopping terms because \( t_{\text{eff}} \) and \( t'_{\text{eff}} \) cannot be both negligible; from Table 3.1 we see that this is a good approximation.

We analyze the single particle spectrum (i.e. in absence of interactions) of the effective Hamiltonian, and thus we write explicitly the hopping terms

\[ H_{\text{eff}}^0 = -t_{\text{eff}} \sum_i a_i^\dagger a_{i+1} + t'_{\text{eff}} \sum_i a_i^\dagger a_{i+2}. \tag{4.5} \]

To diagonalize the Hamiltonian, we expand the annihilation and creation operators in reciprocal space

\[ a_j = \frac{1}{\sqrt{N_s}} \sum_{k \in BZ} a_k e^{ikx_j}, \quad a_j^\dagger = \frac{1}{\sqrt{N_s}} \sum_{k \in BZ} a_k^\dagger e^{-ikx_j}. \tag{4.6} \]
4.1 Single-particle spectrum

Figure 4.1: Plot of the Bessel functions $J_0(x)$ and $J_0(2x)$.

where $N_s$ is the number of lattice sites and the quasimomentum $k$ is inside the first Brillouin zone. Hence, the nearest-neighbor-hopping term becomes ($a$ is the lattice spacing)

$$
\sum_j \sum_{\nu=-1,1} a_i^{\dag} a_{i+\nu} = \frac{1}{N} \sum_{j,\nu} \sum_{q,k} e^{-ikx_j+i\nu(x_j+va)} a_k^{\dag} a_q
$$

$$
= \sum_{k,\nu} e^{ik\nu a} a_k^{\dag} a_k = 2 \sum_k \cos(ka) a_k^{\dag} a_k . \quad (4.7)
$$

The next-nearest-neighbor-hopping term is analogous,

$$
\sum_i \sum_{\nu=-1,1} a_i^{\dag} a_{i+2\nu} = 2 \sum_k \cos(2ka) a_k^{\dag} a_k , \quad (4.8)
$$

hence the effective Hamiltonian is diagonal

$$
H_{\text{eff}} = \sum_k E_k a_k^{\dag} a_k , \quad (4.9)
$$

where the single particle spectrum is given by

$$
E_k = -2t_{\text{eff}} \cos(ka) + 2t_{\text{eff}}' \cos(2ka) . \quad (4.10)
$$

When $t_{\text{eff}}'$ is negligible, we recover the same spectrum as in Chap. 2. The minima of the single particle spectrum yield the momenta at which the
4.1 Single-particle spectrum

atoms condense. Let us define $y = ka$ and compute the first derivative:

$$\frac{1}{2} \frac{\partial E_k}{\partial y} = \frac{t_{\mathrm{eff}} \sin(y) - 2t'_{\mathrm{eff}} \sin(2y)}{2} = \frac{t_{\mathrm{eff}} \sin(y) - 4t'_{\mathrm{eff}} \sin(y) \cos(y)}{2} = \sin(y) [t_{\mathrm{eff}} - 4t'_{\mathrm{eff}} \cos(y)]$$

(4.11)

We find extrema at

- $y = 0, \pm \pi$
- $\cos(y) = \frac{t_{\mathrm{eff}}}{4t'_{\mathrm{eff}}}$ if and only if $|t_{\mathrm{eff}}| \leq 4 |t'_{\mathrm{eff}}|$ and $t'_{\mathrm{eff}} \neq 0$.

To find the minima, we need to compute the second derivative

$$\frac{1}{2} \frac{\partial^2 E_k}{\partial y^2} = \frac{t_{\mathrm{eff}} \cos(y) - t'_{\mathrm{eff}} [\cos^2(y) - \sin^2(y)]}{2} = \frac{t_{\mathrm{eff}} \cos(y) - 4t'_{\mathrm{eff}} [2 \cos^2(y) - 1]}{2}.$$  

(4.12)

The values if the second derivative at the extrema found before are:

- $y = 0 \rightarrow \frac{1}{2} \frac{\partial^2 E_k}{\partial y^2} = t_{\mathrm{eff}} - 4t'_{\mathrm{eff}}$
- $y = \pm \pi \rightarrow \frac{1}{2} \frac{\partial^2 E_k}{\partial y^2} = -t_{\mathrm{eff}} - 4t'_{\mathrm{eff}}$
- $\cos(y) = \frac{t_{\mathrm{eff}}}{4t'_{\mathrm{eff}}} \rightarrow \frac{1}{2} \frac{\partial^2 E_k}{\partial y^2} = \frac{t_{\mathrm{eff}}^2}{4t'_{\mathrm{eff}}} - 4t'_{\mathrm{eff}} \left( \frac{2t_{\mathrm{eff}}^2}{16t'_{\mathrm{eff}}^2} - 1 \right) = -\frac{1}{4} \frac{t_{\mathrm{eff}}^2}{t'_{\mathrm{eff}}} + 4t'_{\mathrm{eff}}$.

To understand where the minima are located as function of $K_0$ we assume that $t' = 0.1t$; this assumption has been done only to capture the qualitative behavior (the correct values are given in Table 3.1).

The effective hopping parameters are proportional to Bessel functions and we need a numerical computation to study the sign of the second derivative. For simplicity, we summarize the results concerning the first zero of the Bessel function, which is located at $K_0 = 2.405$. 

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1. For $K_0 < 2.405$, there is a global energy minimum at $ka = 0$.

2. For $K_0 > 2.405$, there is a global energy minimum at $ka = \pm \pi$.

3. For $2.136 < K_0 < 2.405$, there is a local energy minimum at $ka = \pm \pi$.

4. For $2.405 < K_0 < 2.530$, there is a local energy minimum at $ka = 0$.

5. For $2.136 < K_0 < 2.530$, there is a global maximum at $ka = \arccos(t_{\text{eff}}/4t'_{\text{eff}})$.

These results are shown in Fig. 4.2. A specular result is present at the second zero of the Bessel function.

We can thus explain in much more detail the observations of the time-of-flight experiment realized in Pisa [4, 42]. When the shaking parameter crosses $K_0 = 2.405$, the minimum of the energy changes from zero to the edge of the Brillouin zone. This clearly explains why the
central peak in the density disappears and two side peaks are now visible. A finite-momentum condensate has been generated. The minima at $k = \pm \pi/a$ are equivalent because they are separated by a reciprocal lattice vector. Nevertheless, the presence of next-nearest-neighbor interactions is responsible for creating new local minima. Indeed, in the region $2.136 < K_0 < 2.530$, the competition between nearest-neighbor hopping and next-nearest-neighbor hopping generates metastable states. These states are unstable and decay by tunneling in a very short time; this feature cannot be captured if only nearest-neighbor-hopping terms are included in the Hamiltonian.

We have seen that the competition between different hopping coefficients can create finite-momentum condensates. It would be interesting to understand how to generate condensates lying inside the Brillouin zone. This will be investigated afterwards.

The ground state wave function for a condensate of $N$ particles with momentum $k_0$ is given by

$$|G\rangle = \frac{1}{\sqrt{N!}} (a_{k_0}^\dagger)^N |0\rangle = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{N_s}} \sum_i e^{-ik_0 x_i} a_i^\dagger \right)^N |0\rangle.$$  (4.13)

A phase $\phi_i = k_0 x_i$ can be assigned to each site. When $k_0 = 0$, the phase of the condensate is the same at each site, $\phi_i = 0$. When $k_0 = \pi/a$ there is a phase difference between two adjacent sites $|\Delta\phi| = \pi$. This is a quantum phase transition, where the tuning parameter is $K_0$ and the temperature is kept at zero. This configuration is such that lattice points along the diagonal have the same (local) phase differing from the point of the adjacent diagonals by $\pi$. This is analogous to the staggered-sign superfluid which has been predicted in Ref. [6, 7] for a square lattice in presence of a staggered rotation.

We close this section by discussing what happens if we change the sign of the next-nearest-neighbor-hopping coefficient. Even though this is not a realistic case, it can help to understand how the competition
4.2 Phase boundaries

between \( t_{\text{eff}} \) and \( t'_{\text{eff}} \) can be a source of new physics. Hence, assuming that \( t' = -0.1t \), we find that in the region \( 2.136 < K_0 < 2.530 \) a new phase is generated. Indeed, the minimum of the single particle spectrum is now at

\[
ka = \arccos \left( \frac{t_{\text{eff}}(K_0)}{4t'_{\text{eff}}(K_0)} \right),
\]

where the dependence on the shaking parameter \( K_0 \) has been written explicitly. Thus, the condensate has a tunable finite momentum evolving from zero to \( \pi \), at the edge of the Brillouin zone. We stress that the two minima are no longer equivalent because they are both inside the Brillouin zone as it can be seen in Fig. 4.3.

![Figure 4.3: Single particle spectrum for \( K_0 = 2.45 \). The two inequivalent minima inside the Brillouin zone are the condensation point, corresponding to a tunable finite-momentum condensate.](image)

4.2 Phase boundaries

The superfluid phase in 1D has been discussed in the previous section. In this section, we describe in detail a method to generate the phase diagram to observe the phase transitions between the different superfluids and the Mott-insulator phases. We will generalize the calculations presented in Ref. [29, 45] in order to include next-nearest-neighbor-hopping.
4.2 Phase boundaries

terms. This method, which is applied to the Bose-Hubbard Hamiltonian with next-nearest-neighbor-hopping coefficients, is the one we mentioned in Chap. 2, and is based on the path integral approach.

The action describing the physical system is

$$S[a, a^*] = \int_0^{\beta_0} d\tau \left[ \sum_i a_i^*(\tau) \left( \hbar \frac{\partial}{\partial \tau} - \mu \right) a_i(\tau) - \sum_{ij} a_i^*(\tau) h_{ij} a_j(\tau) + H_{\text{int}} \right],$$  

(4.15)

where the hopping matrix is given by

$$h_{ij} = \sum_{\nu=-1,1} \left[ t_{\text{eff}} \delta_{j,i+\nu} - t'_{\text{eff}} \delta_{j,i+2\nu} \right].$$  

(4.16)

Let us introduce a Hubbard-Stratonovich complex field $\psi_i(\tau)$ to decouple the hopping term; this can be accomplished by multiplying the partition function by unity, which corresponds to add the following term to the action:

$$\int_0^{\beta_0} d\tau \sum_{i,j} (\psi_i^* - a_i^*) h_{ij} (\psi_j - a_j).$$  

(4.17)

The new action is thus

$$S[\psi^*, \psi, a^*, a] = S[a^*, a] + \int_0^{\beta_0} d\tau \sum_{i,j} (\psi_i^* - a_i^*) h_{ij} (\psi_j - a_j),$$  

(4.18)

where in the path integral we are integrating the fields $\psi$ and $\psi^*$. This procedure is exact because if we integrate the Hubbard-Stratonovich field, by performing the Gaussian integral, we obtain just a constant related to the inverse of the determinant of the hopping matrix. Hence, no new information has been added in the path integral. A consequence of the Hubbard-Stratonovich transformation is that the expectation value of the field $\langle \psi_i \rangle$ is proportional to the order parameter $\langle a_i \rangle$. Hence, with this method we can implement a consistent mean field theory for the phase
4.2 Phase boundaries

transition. The action reads

\[
S[\psi^*, \psi, a^*, a] = \int_0^{\beta \hbar} d\tau \left[ \sum_i a_i^* \left( \hbar \frac{\partial}{\partial \tau} - \mu \right) a_i + \sum_{i,j} \psi_i^* h_{ij} \psi_j - \sum_{i,j} h_{ij} (\psi_i^* a_j + a_i^* \psi_j) + H_{\text{int}} \right].
\]

(4.19)

If we now integrate out the atomic fields \(a(\tau)\), we are left with an effective action containing only the Hubbard-Stratonovich fields

\[
e^{-\frac{1}{\hbar} S^{\text{eff}}[\psi^*, \psi]} = \exp \left( -\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau \sum_{i,j} \psi_i^* h_{ij} \psi_j \right) \times \int D a^* D a \exp \left\{ -\frac{1}{\hbar} S^{(0)}[a^*, a] + \frac{1}{\hbar} \sum_{i,j} h_{ij} (\psi_i^* a_j + a_i^* \psi_j) \right\}
\]

(4.20)

where

\[
S^{(0)}[a^*, a] = \int_0^{\beta \hbar} d\tau \left[ \sum_i a_i^* \left( \hbar \frac{\partial}{\partial \tau} - \mu \right) a_i + H_{\text{int}} \right]
\]

(4.21)

is the action without hopping terms. Its ground state is a Mott-insulator with a fixed number of particles per site, as we have seen in Chap. 2.

To study the phase transition, we will evaluate the quadratic part of this effective action. We perform a Taylor expansion in powers of the hopping term inside the path integral. This means that we are in the limit of strong interactions and the poles of the Green’s function that we are going to find will describe the Mott-insulator phase. We find

\[
S^{(2)}[\psi^*, \psi] =
\]

\[
= -\frac{1}{2\hbar} \left\langle \left( \int_0^{\beta \hbar} d\tau \sum_{i,j} h_{ij} (\psi_i^* a_j + a_i^* \psi_j) \right)^2 \right\rangle + \int_0^{\beta \hbar} d\tau \sum_{i,j} \psi_i^* h_{ij} \psi_j
\]

\[
= -\frac{1}{2\hbar} \int_0^{\beta \hbar} d\tau d\tau' \sum_{i,j,j'} h_{ij} h_{j'j} (\psi_i^* \psi_j^* a_j a_{j'}^* + \psi_i^* \psi_j^* a_j a_{j'}^* + \psi_j^* \psi_i^* a_j a_{j'}^* + \psi_i^* \psi_j^* a_j a_{j'}^*) + \psi_j^* \psi_i^* (a_i a_{j'}^* + a_i a_{j'}^* + a_i a_{j'}^* + a_i a_{j'}^*) + \int_0^{\beta \hbar} d\tau \sum_{i,j} \psi_i^* h_{ij} \psi_j.
\]

(4.22)
4.2 Phase boundaries

The correlation functions $\langle \cdots \rangle_0$ are evaluated with respect to the action $S^{(0)}$ and then in a pure Mott-insulator with a fixed number of particles per site. Hence

$$\langle a_i a_j \rangle_0 = 0 = \langle a_i^* a_j^* \rangle_0, \quad \forall i, j \quad (4.23)$$

and

$$\langle a_i a_j^* \rangle_0 = \langle a_j^* a_i \rangle_0 = \langle a_i^* a_i \rangle_0 \delta_{ij}, \quad \forall i, j. \quad (4.24)$$

Now, let us perform a Fourier transformation in the last term of Eq. (4.22),

$$\sum_{ij} \psi_i^* h_{ij} \psi_j = \frac{1}{N_s} \sum_{ij} \sum_{kq} \sum_{\nu} e^{ikx_i - iqx_j} \left( t_{\text{eff}} \delta_{j,i+\nu} - t'_{\text{eff}} \delta_{j,i+2\nu} \right) \psi_k^* \psi_q$$

$$= \frac{1}{N_s} \sum_{i} \sum_{kq} \sum_{\nu} \psi_k^* \psi_q \left( t_{\text{eff}} e^{ikx_i - iqx_j} - t'_{\text{eff}} e^{ikx_i - iqx_j + 2\nu} \right)$$

$$= 2 \sum_{k} \psi_k^* \psi_k \left[ t_{\text{eff}} \cos(ka) - t'_{\text{eff}} \cos(2ka) \right]$$

$$= - \sum_{k} \psi_k^* \psi_k(\tau) \psi_k(\tau) E_k, \quad (4.25)$$

where $E_k = -2t_{\text{eff}} \cos(ka) + 2t'_{\text{eff}} \cos(2ka)$ is simply the single particle spectrum found in the previous section. Now, we consider the quadratic matrix:

$$\sum_{i,j,j',j''} h_{ij} h_{j'j''} \psi_i^* \psi_{j'}^* \psi_{j''} \langle a_j a_{j''} \rangle_0 = \sum_{i,j,j'} h_{ij} h_{j'j''} \psi_i^* \psi_{j'}^* \langle a_j a_{j'} \rangle_0 =$$

$$= \frac{1}{N_s} \sum_{i,j,j',j''} \sum_{kq} \sum_{\nu,\nu'} \psi_k^* \psi_q \langle a_j a_{j'} \rangle_0 \left[ t_{\text{eff}}^2 \delta_{j,i+\nu} \delta_{j',i+\nu'} + t'_{\text{eff}}^2 \delta_{j,i+\nu} \delta_{j',i+\nu'} + \delta_{j,i+2\nu} \delta_{j',i+\nu'} + \delta_{j,i+\nu} \delta_{j',i+2\nu} \right]$$

$$= \frac{1}{N_s} \sum_{i,j,j',j''} \sum_{kq} \sum_{\nu,\nu'} \psi_k^* \psi_q \langle aa^* \rangle_0 \left[ t_{\text{eff}}^2 e^{ikx_i - iqx_j} + t'_{\text{eff}}^2 e^{ikx_i - iqx_j + 2\nu} \right]$$

$$= \sum_{k} \sum_{\nu,\nu'} \psi_k^* \psi_k \langle aa^* \rangle_0 \times$$

$$\times \left[ t_{\text{eff}}^2 e^{-ika(\nu+\nu')} - 2t_{\text{eff}} t'_{\text{eff}} e^{-ika(\nu+\nu')} + t'_{\text{eff}}^2 e^{-ika(2\nu+2\nu')} \right]$$
$$= \sum_k \psi_k^* \psi_k \langle aa^* \rangle_0 \times$$
$$\times \left[ 4t_{\text{eff}}^2 \cos^2(ka) - 8t_{\text{eff}} t'_\text{eff} \cos(ka) \cos(2ka) + 4t_{\text{eff}}^2 \cos^2(2ka) \right]$$
$$= \sum_k \psi_k^* \psi_k \langle aa^* \rangle_0 E_k^2. \quad (4.26)$$

Collecting all the terms we find

$$S^{(2)}[\psi^*, \psi] = \int_0^{\beta \hbar} d\tau \left\{ -\sum_k E_k \psi_k^*(\tau) \psi_k(\tau) +$$
$$-\frac{1}{\hbar} \sum_k \int_0^{\beta \hbar} d\tau' E_k^2 \psi_k^*(\tau) \psi_k(\tau') \langle a_j(\tau) a_j^*(\tau') \rangle_0 \right\}. \quad (4.27)$$

This result is the same as the one obtained in Ref. [29], the only difference is the form of $E_k$, which now contains contributions coming from next-nearest neighbors. Hence, by performing an expansion in terms of Matsubara frequencies one obtains

$$S^{(2)}[\psi^*, \psi] = -\sum_n \sum_k |\psi_{kn}|^2 E_k \times$$
$$\times \left[ 1 + E_k \left( \frac{N_0 + 1}{-i\hbar \omega_n - \mu + N_0 U} + \frac{N_0}{i\hbar \omega_n + \mu - (N_0 - 1) U} \right) \right]$$
$$= -\hbar \sum_{k,n} \psi_{kn}^* G^{-1}(k, i\omega_n) \psi_{kn}. \quad (4.28)$$

At this point, it is important to focus on what we have found. First, we perform the analytical continuation $i\omega_n \rightarrow \omega$ and then, we identify the zeros of the inverse Green’s function (which are the poles of the Green’s function) with the energies of the quasiparticles. It is important to stress that the Green’s function just found concerns the Hubbard-Stratonovich field, which is a fictitious field. One can show that this Green’s function is related to the atomic one by the following relation [45]:

$$\langle a_{kn} a_{kn}^* \rangle = \langle \psi_{kn} \psi_{kn}^* \rangle + \frac{\hbar}{E_k}. \quad (4.29)$$

We conclude that the two Green’s functions have the same pole and the spectrum of quasiparticles for the Mott-insulator phase is

$$\hbar \omega_k = -\mu + \frac{U}{2} (2N_0 - 1) + \frac{E_k}{2} \pm \frac{1}{2} \sqrt{E_k^2 + (4N_0 + 2) U E_k + U^2}. \quad (4.30)$$
4.2 Phase boundaries

However, more information can be deduced from the quadratic part of the action. The superfluid phase is characterized by a large occupancy of the lowest energy level, for which we have excitations at the cost of zero free energy because the free energy becomes flat at the point of the transition (it changes the slope). The free energy eigenvalues are obtained after performing the analytic continuation $i \omega_n \rightarrow \omega$ and, as said before, at the point of the transition we have to consider zero energy excitations, which means $n = 0$ in the Matsubara frequencies. If we already know that the condensate has a certain momentum $k_0$, then the quantity $-\hbar G^{-1}(k_0, 0)$ plays the role of the quadratic coefficient in the Landau free energy, the zeros of which determine the boundaries of the phase transition. Thus, the boundaries between the two phases are

$$
\mu = \frac{U}{2} (2N_0 - 1) + \frac{E_{k_0}}{2} \pm \frac{1}{2} \sqrt{E_{k_0}^2 + (4N_0 + 2)UE_{k_0} + U^2}, \quad (4.31)
$$

which is just the result that we have derived in Chap. 2 (see Eq. (2.17)) using second order perturbation theory.

Analogously to the case without shaking, we can find a critical value for $U/t$ such that for smaller values of this ratio there is only a superfluid phase, whatever the chemical potential is. This corresponds to the vanishing of the energy gap

$$
\sqrt{E_{k_0}^2 + (4N_0 + 2)UE_{k_0} + U^2} = 0. \quad (4.32)
$$

Solving for $U$, one finds

$$
U_c = -(1 + 2N_0)E_{k_0} \pm \sqrt{(1 + 2N_0)^2E_{k_0}^2 - E_{k_0}^2} = |E_{k_0}| \left[ -\text{sign}(E_{k_0})(1 + 2N_0) \pm 2\sqrt{N_0^2 + N_0} \right]. \quad (4.33)
$$

For unit filling $N_0 = 1$, we obtain

$$
U_c = |E_{k_0}| \left[ -3\text{sign}(E_{k_0}) \pm 2\sqrt{2} \right]. \quad (4.34)
$$

The sign must be chosen such that $U_c > 0$ and thus we take the plus sign because $\text{sign}(E_{k_0}) = -1$, as one can see in Fig. 4.2 and Fig. 4.3.
4.2 Phase boundaries

The critical value \( (U/2t)_c \), below which only the superfluid phase is present whatever the chemical potential is, was just a constant for the ordinary phase transition discussed in Chap. 2 (see Fig. 2.2). Now, it is no longer constant because the single particle spectrum depends on the shaking parameter \( K_0 \). For \( U > U_c \) one can be in the superfluid or in the Mott-insulator phases according to what is the chemical potential (see again Fig. 2.2).

One should notice that for \( K_0 = 0 \) the critical value \( \tilde{U}_c \) is smaller than the famous value (in 1D) 5.83 because of the next-nearest-neighbor hopping contribution.

In the experiment, once we have fixed the lattice depth \( V_0 \) and the recoil energy, the onsite interaction is just constant (2.20). From Fig. 4.4 it is clear that the time-of-flight picture we have shown (see Fig. 3.5), performed at constant \( U \), shows the following sequence: we start with a BEC at zero momentum, then, increasing \( K_0 \) we cross the phase boundaries destroying phase coherence and finally, for larger values of \( K_0 \) we cross again the phase boundaries towards the finite-momentum condensate region.

\[ \frac{U_c}{t} \equiv -\frac{1}{U_c} \]

Figure 4.4: Critical value \( U_c \), for \( t' = 0.1t \). The lower part of the two lobes are region with two superfluids: (a) BEC a zero momentum for \( K_0 < 2.4 \), (b) BEC at finite momentum \( \pi/a \) for \( K_0 > 2.4 \).
4.2 Phase boundaries

The case where $t' = -0.1t$ is shown in Fig. 4.5; now, there are three regions for the three superfluid phases and thus the cusp in Fig. 4.4 has become smooth. It is clear that, to access the tunable finite-momentum BEC we need a very low value of $U$, i.e. very shallow lattices.

Figure 4.5: Critical value $\bar{U}_c \equiv (U/2t)_c$ for $t' = -0.1t$ in units where $t = 1$. The lower part of the two lobes are region with two superfluids: (a) BEC a zero momentum for $K_0 < 2.136$, (b) BEC at finite momentum $\pi/a$ for $K_0 > 2.530$, (c) BEC at tunable finite momentum for $2.136 < K_0 < 2.530$. 
In this Chapter we propose a setup for optical lattices where the tunable finite-momentum condensate can be generated and we discuss the theory in detail.

5.1 Motivation: why 2D?

In the previous Chapter we have seen that if we change the sign of the next-nearest-neighbor-hopping coefficients, the competition between nearest neighbors and next-nearest neighbors generate an instability leading to a tunable finite-momentum condensate in a certain interval of the shaking parameter $K_0$. Even if this is unrealistic in 1D because the sign of $t'$ is fixed, it is a good starting point to discuss actual setups where this phase can be generated.

In 1D, it seems that is not possible to change the sign of the next-nearest-neighbor-hopping coefficients (we investigated superlattices with two alternating well depths, i.e. a superlattice, without any result); thus, we decided to investigate 2D systems, which have more degrees of freedom that can be used to flip this sign.
Ordinary square lattice potentials, in 2D, are usually separable potentials having the form

\[ V(\mathbf{r}) = V(x) + V(y), \]  

(5.1)

where \( V(x) = V_0 \cos(2kx) \) and analogously for \( V(y) \). This potentials does not introduce new degrees of freedom; the lattice sites with \( x = \text{const.} \) or \( y = \text{const.} \) have the same hopping coefficients as in 1D, while the hopping coefficients between all the other sites are identically zero. This can be easily proved; indeed, for separable potentials the Wannier functions are just factorizable (because Bloch’s functions are) and thus \( W(\mathbf{r} - \mathbf{R}_i) = W(x - x_i)W(y - y_i) \). Let us now compute the hopping coefficient for two sites \( i \) and \( j \). From Chap. 2 we know that it must have the form

\[ t_{ij} = -\int d\mathbf{x} \; W(\mathbf{r} - \mathbf{R}_i) [H(x) + H(y)] W(\mathbf{r} - \mathbf{R}_j). \]  

(5.2)

Consider the term containing \( H(x) \); it reads

\[ -\int dx \; dy \; W(x - x_i)W(y - y_i) H(x) W(x - x_j)W(y - y_j). \]  

(5.3)

We can factorize the integral in \( y \) because the Hamiltonian is \( x \)-dependent and we use the orthogonality property of the Wannier functions to say that only sites with \( y_i = y_j \) have non zero hopping, thus proving what we stated before. Moreover, if \( y_i = y_j \) the integral becomes just the same integral computed in 1D (while the term containing \( H(y) \) vanishes because \( x_i \neq x_j \)), and we see that the same numerical values of the hopping coefficients are expected.

This argument explains why the 2D dimensional lattices we have described above are not useful to find a tunable finite-momentum condensate. If we want to keep the square geometry, only one choice is possible: to introduce a non-separable optical potential. The potential we use is\(^1\)

\[ V(\mathbf{r}) = -V_0 \left[ \sin^2(kx) + \sin^2(ky) + 2\alpha \sin(kx) \sin(ky) \right], \]  

(5.4)

\(^1\)Remember that \( \cos(2x) = 1 - 2 \sin^2(x) \), hence the sign in front of the potential is correct.
where in general $|\alpha| \leq 1$ [5]. We choose $\alpha = 1$ in the following discussion, which is the simpler case.

![Figure 5.1: (a) Non separable ($\alpha = 1$) optical potential; (b) separable ($\alpha = 0$) optical potential, in units where the wave number $k = 1$.](image)

Looking at the shape of such a potential in Fig. 5.1, one sees that it is convenient to do a rotation of the reference frame by $\pi/2$ to obtain a simple square lattice. We get new coordinates $x', y'$ and the transformation is

$$
\begin{pmatrix}
  x \\
  y
\end{pmatrix} = \frac{\sqrt{2}}{2} \begin{pmatrix}
  1 & 1 \\
  -1 & 1
\end{pmatrix} \begin{pmatrix}
  x' \\
  y'
\end{pmatrix}.
$$

The potential becomes

$$
V(r') = -V_0 \left\{ -\frac{1}{2} \cos[\sqrt{2}k(x' + y')] + \\
-\frac{1}{2} \cos[\sqrt{2}k(x' - y')] + \cos(\sqrt{2}kx') - \cos(\sqrt{2}ky') \right\},
$$

where we used the trigonometric identities

$$
\sin a \sin b = \frac{1}{2} \left[ \cos(a - b) - \cos(a + b) \right],
$$

$$
\sin^2 a = \frac{1}{2} - \frac{1}{2} \cos(2a),
$$

and we dropped a constant in the potential. From now on we will work in the rotated frame and we will call the coordinates simply $x$ and $y$. 

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5.2 Hopping coefficients

As stated at the beginning of this Chapter, non-separable potentials are candidates for realizing tunable finite-momentum condensates because new hopping terms, e.g. between sites lying along the diagonal of the elementary cell, are present. This could lead to an instability of the zero-momentum condensate, thus allowing for new phases with finite momentum. Our task is to calculate the hopping coefficient to construct a consistent Bose-Hubbard model for the system.

From Fig. 5.1 (a) we see that the barrier between two adjacent sites is higher than the one for the separable potential (b). For this reason we expect the hopping coefficients to be smaller in comparison with the ones we found for separable potentials (see Table 3.1). The largest hopping is clearly expected for shallow lattices if we consider the atoms to be in the ground state.

The hopping coefficients can be computed from the single-particle spectrum of the Bose-Hubbard model. Indeed, one finds \[ E_n(q) = \sum_\mathbf{R} t_n(\mathbf{R}) e^{i \mathbf{q} \cdot \mathbf{R}}, \] (5.9)
where \( n \) is the band index, \( q \) is the quasimomentum, and \( \mathbf{R} \) is a lattice vector. In this notation, \( t_n(\mathbf{R}) \) is the hopping coefficient between the sites separated by the lattice vector \( \mathbf{R} \) in the \( n \)-th energy band. The hopping coefficients are thus the Fourier transform of the energy bands.

To determine the energy bands, we solve numerically the Schrödinger equation. From Bloch’s theorem, we know that the eigenstates of the Hamiltonian for a periodic system have the form

\[ \psi_{q n}(\mathbf{r}) = u_n(\mathbf{r}) e^{i \mathbf{q} \cdot \mathbf{r}}, \] (5.10)
where \( u_n(\mathbf{r}) \) is a periodic function, the period of which is given by the lattice spacing. We use Fourier decomposition to obtain

\[ \psi_{q n}(\mathbf{r}) = \sum_\mathbf{m} c_{m}^{(n)} e^{i (\mathbf{q} + \frac{2\pi m}{a}) \cdot \mathbf{r}}, \] (5.11)
5.2 Hopping coefficients

where \( \mathbf{m} \) is an array of integers, the length of which depends on the dimensionality of the system. The Schrödinger equation thus reads

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi_{qn} = E_n(q) \psi_{qn} .
\] (5.12)

If we call the lattice spacing \( a = \lambda/\sqrt{2} \), where \( \lambda \) is the laser beam wavelength, we can rewrite the potential (5.6) in the following way:

\[
V(\mathbf{r}) = V_0 \left\{ \frac{1}{4} \left[ e^{i\sqrt{2}k(x+y)} + e^{-i\sqrt{2}k(x+y)} \right] + \frac{1}{4} \left[ e^{i\sqrt{2}k(x-y)} + e^{-i\sqrt{2}k(x-y)} \right] + \frac{1}{2} \left[ e^{i\sqrt{2}ky} + e^{-i\sqrt{2}ky} - e^{i\sqrt{2}kx} - e^{-i\sqrt{2}kx} \right] \right\} .
\] (5.13)

Using the orthogonality condition of plane waves, the Schrödinger equation can thus be written (the band index has been dropped for convenience of notation):

\[
T_q(h,k)c_{hk} + \frac{V_0}{4} (c_{h+1,k+1} + c_{h+1,k-1} + c_{h-1,k+1} + c_{h-1,k-1}) + \frac{V_0}{2} (c_{h,k+1} + c_{h,k-1}) - \frac{V_0}{2} (c_{h+1,k} + c_{h-1,k}) = E_c c_{hk} ,
\] (5.14)

where

\[
T_q(h,k) = \frac{1}{2} \frac{\hbar^2}{2m} \left( \frac{2\pi}{\lambda} \right)^2 \left[ (q_x + 2h)^2 + (q_y + 2k)^2 \right] .
\] (5.15)

and \( q \) has been normalized such that \(-1 \leq q_x, q_y \leq 1\). We can rewrite the Schrödinger equation in a more compact form

\[
M_{hkab} c_{ab} = E c_{hk} ,
\] (5.16)

where

\[
M_{hkab} = \delta_{ha} \delta_{kb} T_q(h,k) + \frac{V_0}{4} (\delta_{h,a+1} \delta_{k,b+1} + \delta_{h,a+1} \delta_{k,b-1} + \delta_{h,a-1} \delta_{k,b+1} + \delta_{h,a-1} \delta_{k,b-1}) + \frac{V_0}{2} (\delta_{h,a} \delta_{k,b+1} + \delta_{h,a} \delta_{k,b-1}) - \frac{V_0}{2} (\delta_{h,a+1} \delta_{k,b} + \delta_{h,a-1} \delta_{k,b}) .
\] (5.17)

The strategy is to keep a finite amount of terms, so that we diagonalize a finite linear system. If \((2l + 1)^2\) is the number of terms that we retain in
the Fourier expansion, then we have to diagonalize a \((2l + 1)^2 \times (2l + 1)^2\) matrix. One immediately sees that for \(l = 4\) we obtain an \(81 \times 81\) matrix. Its dimensionality is also the number of bands that we get at the end.

Hence, we conclude that we have to take \(l\) small to be able to solve numerically the problem, with an acceptable time of computation. Once we have found the band structure, we keep only the lowest energy eigenvalue because we are interested in the lowest band. The hopping coefficients in \(n\) dimensions are given by

\[
t(R) = \left(\frac{a}{2\pi}\right)^n \int_{1BZ} d^n q \, E(q) \, e^{-iq \cdot R}.
\] (5.18)

A lattice vector has the form \(R = h \hat{x} + k \hat{y}\) and it is indicated in short notation as \((h,k)\). For the non-separable potential that we have introduced, we expect to find non zero hopping terms also for pairs of sites identified by \((1,1)\) or \((2,1)\). The results are summarized in Tables 5.1 and 5.2.

<table>
<thead>
<tr>
<th>(V_0/E_r)</th>
<th>((1,0) \leftrightarrow t)</th>
<th>((1,1) \leftrightarrow t')</th>
<th>((2,0) \leftrightarrow t'')</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>(-2.45 \times 10^{-2})</td>
<td>(-8.89 \times 10^{-4})</td>
<td>(8.88 \times 10^{-4})</td>
</tr>
<tr>
<td>2.0</td>
<td>(-4.52 \times 10^{-3})</td>
<td>(-6.65 \times 10^{-5})</td>
<td>(2.27 \times 10^{-5})</td>
</tr>
<tr>
<td>3.0</td>
<td>(-1.06 \times 10^{-3})</td>
<td>(-5.89 \times 10^{-6})</td>
<td>(1.06 \times 10^{-6})</td>
</tr>
<tr>
<td>4.0</td>
<td>(-2.97 \times 10^{-4})</td>
<td>(-6.74 \times 10^{-7})</td>
<td>(7.86 \times 10^{-8})</td>
</tr>
</tbody>
</table>

Table 5.1: Hopping matrix elements with \(l = 5\). The discretization step of the 1BZ has been taken \(dx = 0.05\).

<table>
<thead>
<tr>
<th>(V_0/E_r)</th>
<th>((2,1))</th>
<th>((2,2))</th>
<th>((3,0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>(7.24 \times 10^{-5})</td>
<td>(-4.08 \times 10^{-6})</td>
<td>(-5.18 \times 10^{-6})</td>
</tr>
<tr>
<td>2.0</td>
<td>(7.28 \times 10^{-7})</td>
<td>(-8.67 \times 10^{-10})</td>
<td>(-1.80 \times 10^{-7})</td>
</tr>
<tr>
<td>3.0</td>
<td>(1.26 \times 10^{-8})</td>
<td>(1.82 \times 10^{-11})</td>
<td>(-1.93 \times 10^{-9})</td>
</tr>
<tr>
<td>4.0</td>
<td>(3.54 \times 10^{-10})</td>
<td>(3.25 \times 10^{-13})</td>
<td>(-2.62 \times 10^{-9})</td>
</tr>
</tbody>
</table>

Table 5.2: Hopping matrix elements with \(l = 5\). The discretization step of the 1BZ has been taken \(dx = 0.05\).
5.3 Derivation of the Hamiltonian for the driven system

The hopping coefficients in Table 5.1 have been called $-t$, $t'$ and $t''$ for a reason that will be clear later. The surprising result is that the hopping coefficients along the diagonal (1,1) have the opposite sign with respect to the nearest neighbors (1,0). Moreover the order of magnitude is the same as the (2,0) hoppings and this will be crucial for the studies in the driven system.

5.3 Derivation of the Hamiltonian for the driven system

The optical lattice discussed in the previous section does not contain shaking. In this section, we introduce the shaking in a very natural way: we extend the same kind of shaking used in 1D to our 2D lattices (but in the rotated frame). This means that we write the Hamiltonian

\[ H = H_0 + H_{\text{int}} + W(t), \]

where \( H_0 + H_{\text{int}} \) is the undriven part containing the non-separable potential and \( W(t) \) is the time periodic perturbation, given by

\[ W(t) = x F_\omega \cos(\omega t) + y F_\omega \cos(\omega t), \quad F_\omega = mx_0 \omega^2. \]

We are shaking the lattice along the \( x \) and \( y \) axes which is equivalent to shaking the system along one of the diagonals. We expect that the hopping coefficient orthogonal to this direction will not be affected by the driven force while all the other hopping coefficients should be multiplied by a Bessel function\(^2\), as seen in Chap. 2.

Writing the second quantized version of this Hamiltonian requires some assumptions. When the optical potential is not separable the

\(^2\)The choice of what kind of shaking to apply to the lattice is crucial. Indeed, if we want to see the influence of next-nearest neighbors, we need to arrange some kind of shaking that can renormalize the nearest-neighbor-hopping coefficients in the same way in the two independent lattice directions, such that they can be suppressed simultaneously. This is why we shake along the diagonal.
5.3 Derivation of the Hamiltonian for the driven system

Bloch’s functions are not factorizable and the same is true for the Wannier functions. We assume that some symmetries are still valid for the Wannier functions: they are translationally invariant, they are even with respect to the point where they are centered and real (the first two assumptions are based on symmetries of the system and the last is a reasonable conjecture supported by numerical simulations [27]). We already know how to write the undriven part, now we need to discuss the time dependent part.

There are two classes of terms: the terms proportional to the density operator \(a_i^\dagger a_r\), \(r \equiv (i, j)\) are given in analogy with the 1D case,

\[
\sum_j jn_j \longrightarrow \sum_{i,j} (i + j)n_{ij}.
\]

As in Chap. 3, terms in the shaking that are not proportional to the density operator but refer to different sites (i.e. proportional to \(a_i^\dagger a_s\)) contain an integral like (for the \(x\) part of \(W(t)\))

\[
\int dx\,dy W(x - x_r, y - y_r) x W(x - x_s, y - y_s) = \int dx\,dy W \left(x + \frac{1}{2}(x_s - x_r), y + \frac{1}{2}(y_s - y_r)\right) \times \\
\times x W \left(x - \frac{1}{2}(x_s - x_r), y - \frac{1}{2}(y_s - y_r)\right).
\]

Thus, the product of the two Wannier functions is even for \(x, y \rightarrow -x, -y\) and is multiplied by an odd function (namely \(x\)); when you perform the integral using the Fubini theorem, it vanishes. The same argument is valid for the shaking term along \(y\) and we conclude that this part of the Hamiltonian is written as

\[
W(t) = K \cos(\omega t) \sum_{i,j} (i + j)n_{ij}, \quad K = amx_0\omega^2,
\]

namely

\[
W(t) = Q \cos(\omega t), \quad Q \equiv K \sum_{i,j} (i + j)n_{ij}.
\]
5.3 Derivation of the Hamiltonian for the driven system

According to the formalism discussed in Chap. 3, we must compute the relevant commutators

\[
[Q, H_{\text{int}}] = \frac{UK}{2} \sum_{i,j,h,k} [a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk} a_{hk}^\dagger a_{hk}] (i + j). \tag{5.25}
\]

Now, we use the properties of commutators:

\[ [A, BC] = [A, B] C + B [A, C], \tag{5.26} \]
\[ [AB, C] = A [B, C] + [A, C] B, \tag{5.27} \]

to rewrite the commutator in Eq. (5.25),

\[
[Q, H_{\text{int}}] = \frac{UK}{2} \sum_{i,j,h,k} \left( [a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk}] a_{hk}^\dagger a_{hk} + a_{hk}^\dagger a_{hk} [a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk}] \right). \tag{5.28}
\]

The commutators inside the brackets are the same; we compute one of them

\[
[a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk}] = [a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk}] a_{hk}^\dagger a_{hk} + a_{hk}^\dagger a_{hk} [a_{ij}^\dagger a_{ij}, a_{hk}^\dagger a_{hk}] = \\
= \delta_{ih} \delta_{jk} \left( a_{ij}^\dagger a_{hk} - a_{hk}^\dagger a_{ij} \right) = 0. \tag{5.29}
\]

We conclude then that \([Q, H_{\text{int}}] = 0\). We define the operator

\[
T_\pm \equiv \sum_{(i, j), (r, s)} \left( a_{ij}^\dagger a_{rs} \pm a_{rs}^\dagger a_{ij} \right) \tag{5.30}
\]

and we calculate the commutator \([Q, T_\pm]\)

\[
[Q, T_\pm] = \chi \sum_{h, k} \sum_{(i, j), (r, s)} (h + k) \left( a_{hk}^\dagger a_{hk}, a_{ij}^\dagger a_{rs} \pm a_{rs}^\dagger a_{ij} \right). \tag{5.31}
\]

The commutator inside the summation has two contributions; the first one is

\[
[a_{hk}^\dagger a_{hk}, a_{ij}^\dagger a_{rs}] = [a_{hk}^\dagger a_{hk}, a_{ij}^\dagger] a_{rs} + a_{ij}^\dagger [a_{hk}^\dagger a_{hk}, a_{rs}] = \\
= \delta_{hr} \delta_{kj} a_{hk}^\dagger a_{rs} - \delta_{hr} \delta_{kj} a_{ij}^\dagger a_{hk}. \tag{5.32}
\]
5.3 Derivation of the Hamiltonian for the driven system

The second one is obtained by exchanging $rs$ with $ij$ in Eq. (5.32). Hence, we obtain

$$[Q, T_\pm] = K \sum_{h,k} \sum_{\langle (i,j),(r,s) \rangle} (h + k) \left( \delta_{hi} \delta_{kj} a_{hk}^\dagger a_{rs} - \delta_{hr} \delta_{ks} a_{ij}^\dagger a_{hk} + \right.$$

$$\left. \pm \delta_{hr} \delta_{ks} a_{hk}^\dagger a_{ij} \mp \delta_{hi} \delta_{kj} a_{rs}^\dagger a_{hk} \right)$$

$$= K \sum_{\langle (i,j),(r,s) \rangle} \left[ (i + j) a_{ij}^\dagger a_{rs} - (r + s) a_{ij}^\dagger a_{rs} + \right.$$

$$\left. \pm (r + s) a_{rs}^\dagger a_{ij} \mp (i + j) a_{rs}^\dagger a_{ij} \right]$$

$$= K \sum_{\langle (i,j),(r,s) \rangle} \left[ (i - r) + (j - s) \right] \left( a_{ij}^\dagger a_{rs} \mp a_{rs}^\dagger a_{ij} \right).$$ (5.33)

We restrict our model to the hopping coefficients given in Table 5.1. Indeed, these coefficients will be renormalized by Bessel functions and thus, when the effective nearest-neighbor hopping $t_{eff}$ vanishes, $t'$ and $t''$ have to be taken into account because they are almost of the same order of magnitude. Higher hopping terms are not important because the coefficients in Table 5.1 cannot simultaneously vanish.

It is sufficient now to fix two of the four (nearest or next-nearest) neighbors for each site because of the definition of $T_\pm$. We have to fix a certain convention in the choice of these two neighbors. Thus, calling $F = (i - r) + (j - s)$, we have $F = (\pm)1$ for nearest neighbors and $F = 0, (\pm)2$ for next-nearest neighbors. The sign depends on the convention chosen for the neighbors and it does not matter because $F$ appears in the argument of the Bessel function when we apply the Floquet formalism; the Bessel function is even and is not affected by this sign. Let us call the reference frame $xOy$: $F = 0$ is thus for the neighbors along $x = -y$ and $F = (\pm)2$ is for the neighbors along $x = y$. As expected, the hopping coefficients along the diagonal $x = -y$, orthogonal to the shaking direction, are not renormalized.

If we call the two unit vectors spanning the lattice $e_\nu$, $\nu = 1, 2$, we can
write the final Hamiltonian with the renormalized hopping coefficients

\[
H_{\text{eff}} = -t J_0(K_0) \sum_{r,\nu} a_r^\dagger a_r e^{-iK_0 (r+2e_\nu)} + t' J_0(2K_0) \sum_{r,\nu} a_r^\dagger a_{r\pm(e_1+e_2)}^+ + t'' J_0(2K_0) \sum_{r,\nu} a_r^\dagger a_{r\pm2e_\nu} .
\] (5.34)

### 5.4 Single-particle spectrum and finite-momentum condensate

In this section, we study the single-particle spectrum of the Hamiltonian (5.34). We have to perform a Fourier expansion of the first term

\[
-t J_0(K_0) \frac{1}{N_s} \sum_{k,\nu} \sum_{r,\nu} a_k^\dagger a_{q} e^{-iK_0 (r+2e_\nu)} = -2t J_0(K_0) \sum_{k} [\cos(k_1 a) + \cos(k_2 a)] a_k^\dagger a_k ,
\] (5.35)

where we defined the vector \( \mathbf{k} = k_1 \mathbf{e}_1 + k_2 \mathbf{e}_2 \). The second term is:

\[
t' J_0(2K_0) \frac{1}{N_s} \sum_{k,\nu} \sum_{r,\nu} a_k^\dagger a_{q} e^{-iK_0 (r+2e_\nu)} \left( e^{i\nu(q+e_1+e_2)} + e^{i\nu(q-e_1-e_2)} \right) =
\]

\[
= 2t' J_0(2K_0) \sum_{k} \cos[(k_1 + k_2)a] a_k^\dagger a_k .
\] (5.36)

The other two terms are trivial because they are similar to the ones that we have written. The Hamiltonian is diagonal, \( H_{\text{eff}} = \sum_{k} E_{k} a_k^\dagger a_k \) and the spectrum is given by

\[
E_{k} = -2t J_0(K_0) [\cos(k_1 a) + \cos(k_2 a)] + 2t' J_0(2K_0) \cos[(k_1 + k_2)a] +
+ 2t' \cos[(k_1 - k_2)a] + 2t'' J_0(2K_0) [\cos(2k_1 a) + \cos(2k_2 a)] .
\] (5.37)

We now define \( \varepsilon_{k} \equiv E_{k} / 2t, \quad t_1 = t' / t, \quad t_2 = t'' / t \) and we study the behavior of the spectrum along the diagonal \( k_1 = k_2 \equiv k \):

\[
\frac{\partial \varepsilon_{k}}{\partial (ka)} = 2 \sin(ka) \left[ J_0(K_0) - 2J_0(2K_0)(t_1 + 2t_2) \cos(ka) \right] .
\] (5.38)
The extrema arise for \( k = 0, \pm \pi \) and at the non-trivial value of \( k \) which solves

\[
\cos(ka) = \frac{J_0(K_0)}{2J_0(2K_0)(t_1 + 2t_2)} \equiv f(K_0) . \tag{5.39}
\]

To find the minima we investigate the second derivative

\[
\frac{\partial^2 \varepsilon_k}{\partial (ka)^2} = 2J_0(K_0) \cos(ka) - 4J_0(2K_0)(t_1 + 2t_2)(2 \cos^2(ka) - 1) . \tag{5.40}
\]

For the non trivial momentum given by Eq. (5.39), we find

\[
\frac{\partial^2 \varepsilon_k}{\partial (ka)^2} = \frac{J_0^2(K_0)}{J_0(2K_0)(t_1 + 2t_2)} - 4J_0(2K_0)(t_1 + 2t_2) \left[ \frac{1}{2} \frac{J_0^2(K_0)}{J_0(2K_0)(t_1 + 2t_2)^2} - 1 \right]
= - \frac{J_0^2(K_0)}{J_0(2K_0)(t_1 + 2t_2)} + 4J_0(2K_0)(t_1 + 2t_2)
= \frac{4J_0^2(2K_0)(t_1 + 2t_2)^2 - J_0^2(K_0)}{J_0(2K_0)(t_1 + 2t_2)} . \tag{5.41}
\]

The denominator (as a function of \( K_0 \)) is constant in sign around \( K_0 = 2.4 \) where we expect to find the non trivial minimum. Hence, the sign of the second derivative depends on the numerator. One can see that it changes sign just in the interval when \( f(K_0) \) has solutions; thus, we conclude that it is a true minimum.

Now, we discuss the case \( V_0 = 3E_r \) as an example. Using the Table 3.1 to evaluate \( t_1 \) and \( t_2 \), we can plot the minimum of the spectrum along the diagonal \( k_x = k_y = k \) as a function of the shaking parameter \( K_0 \). The momentum is plotted in Fig. 5.2, while the shape of the single-particle spectrum where the nontrivial minimum arises is shown in Fig. 5.3.
5.4 Single-particle spectrum and finite-momentum condensate

Figure 5.2: Evolution of the minimum in the single-particle spectrum in units of the lattice spacing $a$ as a function of the shaking parameter $K_0$ at $V_0 = 3E_r$ (only the positive branch is considered).

Figure 5.3: Single-particle spectrum at $V_0 = 3E_r$ for $K_0 = 2.405$ and contour plot.
5.5 Bogoliubov theory

If the optical lattice is filled with bosons at zero temperature, they will occupy the state of minimum energy. In the previous section, we have found the single-particle spectrum and its minima; we discovered that in a certain range of the shaking parameter $K_0$, two inequivalent minima arise inside the Brillouin zone. The minima are inequivalent because they are not connected by a reciprocal lattice vector. This points are the ones where a tunable finite-momentum condensate is generated; we call it tunable because we can tune the condensation momentum by changing $K_0$.

In the following, we discuss the stability of the condensate when interactions are turned on. The approach is perturbative and thus it is valid for small perturbations. Let us start with an analysis of the trivial case, when there is only one minimum at $k_0$ in the single-particle spectrum and we expect the particles to condense there.

In the superfluid phase, the many-body ground state can be approximated for sufficiently low temperatures and weak interactions by the expression

$$|G\rangle = \frac{1}{\sqrt{N!}} (a_{k_0}^\dagger)^N |0\rangle ,$$  \hspace{1cm} (5.42)

where $N$ is the number of condensed atoms with momentum $k_0$. We want to calculate the energy of the system in such a state to understand whether a small perturbation can cause an instability of the ground state with respect to the condensation momentum found for the single-particle spectrum. The Hamiltonian is

$$H = H_0 + H_{\text{int}} .$$  \hspace{1cm} (5.43)

We already know that, in momentum space, we can write $H_0 = \sum_k E_k a_k^\dagger a_k$. Hence, we have to compute the interacting part

$$H_{\text{int}} = \frac{U}{2} \sum_r a_r^\dagger a_r^\dagger a_r a_r .$$  \hspace{1cm} (5.44)
5.5 Bogoliubov theory

We insert the Fourier expansion

\[ a_r = \frac{1}{\sqrt{N_s}} \sum_k e^{-ikr} a_k, \quad (5.45) \]

into Eq. (5.44) and we obtain

\[ H_{\text{int}} = \frac{U}{2N_s} \sum_{k_1, k_2, k_3, k_4} \delta_{k_1+k_2, k_3+k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}. \quad (5.46) \]

To evaluate the ground state energy \( \langle H \rangle \), we use the following relations, valid for any integer \( M \geq 1 \),

\[ \left[ a_{k_0}^M, (a_{k_0}^\dagger)^M \right] = M! \quad \left[ a_k, (a_k^\dagger)^M \right] = M \delta_{k,k_0} (a_k^\dagger)^{M-1}. \quad (5.47) \]

First, we calculate the non-interacting part:

\[ \langle H_0 \rangle = \frac{1}{N!} \sum_k E_k \langle 0 | a_{k_0}^N a_k^\dagger a_k (a_{k_0}^\dagger)^N | 0 \rangle = \frac{N^2}{N!} \langle 0 | a_{k_0}^{N-1} (a_{k_0}^\dagger)^{N-1} | 0 \rangle = NE_{k_0}. \quad (5.48) \]

This is a trivial result because we know that the density operator \( n_{k_0} = a_{k_0}^\dagger a_{k_0} \) applied to the state \( |G\rangle \) gives as eigenvalue the number of particles \( N \) with momentum \( k_0 \). The interacting part is

\[ \langle H_{\text{int}} \rangle = \frac{U}{2N!N_s} \sum_{k_1, k_2, k_3, k_4} \delta_{k_1+k_2+k_3+k_4} \langle 0 | a_{k_0}^N a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} (a_{k_0}^\dagger)^N | 0 \rangle \]

\[ = \frac{UN^2}{2N!N_s} \sum_{k_2, k_3} \delta_{k_0+k_2+k_3+k_0} \langle 0 | a_{k_0}^{N-1} a_{k_2}^\dagger a_{k_3} (a_{k_0}^\dagger)^{N-1} | 0 \rangle \]

\[ = \frac{UN^2(N-1)^2}{2N!N_s} \langle 0 | a_{k_0}^{N-2} (a_{k_0}^\dagger)^{N-2} | 0 \rangle \]

\[ = \frac{U}{2N_s} N(N-1). \quad (5.49) \]

Collecting all the results that we found, up to first order in perturbation theory,

\[ \langle H \rangle = \langle H_0 \rangle + \langle H_{\text{int}} \rangle = NE_{k_0} + \frac{U}{2N_s} N(N-1), \quad (5.50) \]
which shows that, in this approximation of weak interactions, the condensation momentum is not affected by the interaction. This is not enough to say that the condensation momentum at the phase transition (where the interactions become of the same order as the hopping coefficients) is the one found studying the single-particle spectrum but the stability discussion we have just presented yields more support to such an assumption.

We investigate now what is the influence of a small interaction when the ground state of the single-particle spectrum has a nontrivial condensation momentum. We have found previously that the single-particle spectrum has two inequivalent minima inside the Brillouin zone and then we have to take both into account for calculating the ground state. We keep our argument general and we write the many-body ground state for condensation momenta $k_0$ and $-k_0$ (in our previous findings the momenta lie along the diagonal of the Brillouin zone):

$$|G'\rangle = \sum_{n=0}^{N} \frac{c_n}{\sqrt{n!(N-n)!}} (a_{k_0}^\dagger)^n (a_{-k_0}^\dagger)^{N-n}|0\rangle$$

$$= \sum_{n=0}^{N} c_n |n_{k_0}, (N-n)_{-k_0}\rangle.$$  \hspace{1cm} (5.51)

From now on, we drop the momentum index inside the Fock vector keeping in mind that $n$ refers to $k_0$ and $N-n$ refers to $-k_0$. Moreover, it is clear that the (complex) coefficients $c_n$ have to satisfy the normalization condition $\sum_n |c_n|^2 = 1$.

We want to find the correction to the non interacting ground state energy. We perform first order perturbation theory and minimize the energy obtained. The unperturbed ground state energy is given by $\langle H_0 \rangle = NE_{k_0}$ if $E_{k_0} = E_{-k_0}$. The first order correction requires more work. The ground state for the unperturbed Hamiltonian has a $(N+1)$-fold degeneracy. For
5.5 Bogoliubov theory

this reason, we need to diagonalize the following matrix

\[ \langle m, N-m|H_{\text{int}}|n, N-n \rangle = \frac{U}{2N_s} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2,k_3+k_4} \langle m, N-m|a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}|n, N-n \rangle \]

to obtain the first order energy correction and the zeroth order eigenstate. Let us focus our attention on \( k_3 \) and \( k_4 \). There are non-vanishing contributions only in the following cases:

- \( k_3 = k_0 \) and \( k_4 = k_0 \). Momentum conservation ensures that we must have \( k_1 = k_0 \) and \( k_2 = k_0 \) and the we get a contribution

\[ \sqrt{n(n-1)m(m-1)} \delta_{nm} = n(n-1) \delta_{nm} \]

to the sum;

- \( k_3 = -k_0 \) and \( k_4 = -k_0 \). In this case the contribution to the sum is analogous to the previous one and it becomes \((N-n)(N-n-1) \delta_{nm}\);

- \((k_3 = k_0 \) and \( k_4 = -k_0 \)) or \((k_3 = -k_0 \) and \( k_4 = k_0 \)). Let us discuss the first possibility. Momentum conservation constrains \( k_1 \) and \( k_2 \) to be \((k_1 = k_0 \) and \( k_2 = -k_0 \)) or \((k_1 = -k_0 \) and \( k_2 = k_0 \)). All these combinations give the same result \( 4n(N-n) \delta_{nm} \).

Collecting all the terms we finally obtain

\[ \langle m, N-m|H_{\text{int}}|n, N-n \rangle = \frac{U}{2N_s} \left[ n(n-1) + (N-n)(N-n-1) + 4n(N-n) \right] \delta_{mn} \]
\[ = \frac{U}{2N_s} \left[ -2n^2 + 2nN + N(N-1) \right] \delta_{mn} . \]  

(5.53)

The matrix element is in diagonal form and the eigenvalues are an upside down parabola in \( n \). This means that the minima are at the edge of the interval \( n \in [0, N] \) and that they are degenerate. This is also true for the excited states, the only case in which the degeneracy is reduced is when \( N \) is even and we consider the state corresponding to \( n = N/2 \). This

\(^3\)Remember that, according to the harmonic oscillator algebra, \( a|n\rangle = \sqrt{n}|n-1\rangle \)
is the maximum energy state in which particles are divided between the two states with momenta \( k_0 \) and \(-k_0\).

The perturbative (degenerate) ground state to zeroth order is

\[
|G'\rangle = \frac{c_1}{\sqrt{N!}} (a_{k_0}^\dagger)^N |0\rangle + \frac{c_2}{\sqrt{N!}} (a_{-k_0}^\dagger)^N |0\rangle
\]  (5.54)

and has energy

\[
\langle H \rangle = \langle H_0 \rangle + \langle H_{\text{int}} \rangle = NE_{k_0} + \frac{U}{2N_s} N(N - 1),
\]  (5.55)

showing that the ground state is a superposition of two degenerate states in which all the particles have momentum \( k_0 \) or \(-k_0\). These two states are entangled.

We study the finite-momentum condensate using the Bogoliubov theory. In Ref. [46], the authors study a system which has a degenerate finite-momentum condensate generated by a spin-orbit coupling; the generalized Bogoliubov theory presented in this work shows that the ground state which minimizes the energy is just the same that we have found using first-order perturbation theory.

They start writing the Hamiltonian as the sum of the projected Hamiltonians in the \( N + 1 \) states described by the wave function (5.51). This means that the Hamiltonian can be written as the direct sum of \( N + 1 \) contributions. They perform a Bogoliubov theory in each of these sectors and notice that, to minimize the energy (which becomes sector dependent) they have to consider only the two degenerate states that we discussed before.

The simplicity of our method can thus allow us to start the Bogoliubov theory in such a ground state \textit{ab initio}. As performed in Ref. [46], we implement the Bogoliubov theory considering each of the two states separately. In our case the two states are equivalent (all the particles with momentum \( k_0 \) or \(-k_0\)) and we choose the first case. We make the Bogoliubov substitution

\[
a_k \rightarrow \sqrt{N} \delta_{k,k_0} + a_k,
\]  (5.56)
in which we assumed that the macroscopic ground state has \(N\) particles and \(a_k\) are the fluctuations. The (gran canonical) Hamiltonian of the system reads

\[
H = \sum_k (E_k - \mu) a_k^\dagger a_k + \frac{U}{2N_s} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2,k_3+k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}, \tag{5.57}
\]

where the one particle spectrum \(E_k\) is given by Eq. (5.37)

According to the Bogoliubov theory, we keep terms which are no more than quadratic in the fluctuations. The coefficients of the terms linear in the fluctuations have to be set to zero because they would lead to a non-vanishing expectation value of the fluctuations. This gives an equation for the chemical potential

\[
\mu = E_{k_0} + UN_0, \tag{5.58}
\]

where \(N_0 = N/N_s\) is the filling factor. Up to quadratic order, we find

\[
H_{\text{Bog}} = \left( E_{k_0} - \mu + \frac{1}{2} UN_0 \right) N + \sum_k (E_k - \mu) a_k^\dagger a_k + \frac{1}{2} UN_0 \sum_k \left( a_{k_0}^\dagger a_{2k_0-k}^\dagger + 4a_k^\dagger a_{2k_0-k} + a_k a_{2k_0-k}^\dagger \right). \tag{5.59}
\]

The previous result shows that in the Bogoliubov theory we have to take into account momenta which can lie outside the first Brillouin zone. In principle this is not a problem because we can map these momenta into the equivalent ones inside the first Brillouin zone but the research of such a mapping could be avoided because we are interested in the modes with momenta close to the condensation momentum \(k_0\). For this reason, we restrict the Hamiltonian to these momenta defining \(q\) such that \(k = k_0 + q\) and \(|q| \ll |k_0|\). The previous Hamiltonian can thus be written as

\[
H_{\text{Bog}} = \left( E_{k_0} - \mu + \frac{1}{2} UN_0 \right) N + \sum_q \left( E_{k_0+q} - E_{k_0} + UN_0 \right) a_{k_0+q}^\dagger a_{k_0+q} + \frac{1}{2} UN_0 \sum_q \left( a_{k_0+q}^\dagger a_{k_0-q}^\dagger a_{k_0-q} + a_{k_0-q} a_{k_0+q} \right). \tag{5.60}
\]
which has a symmetric form. The hermiticity is not lost because we are
summing in a spherical interval around \( k_0 \), which contains momenta \( \pm q \).
In this approximation, the energy can be written as

\[
E_{k_0 + q} = E_{k_0} + \left( \frac{\partial^2 E}{\partial k_i \partial k_j} \right)_{k_0} q_i q_j + O(q^3)
\]  \tag{5.61}

Indeed, the single-particle spectrum is infinitely differentiable and thus
can be expanded in Taylor series. The first derivatives are trivially zero
because we are expanding around a minimum. The previous equation
shows that the spectrum is symmetric for \( q \rightarrow -q \) if we consider small
excitations. Hence, we can assume \( E_{k_0 + q} = E_{k_0 - q} \). The Hamiltonian
can thus be cast into the form

\[
H_{\text{Bog}} = \left( E_{k_0} - \mu + \frac{1}{2} U N_0 \right) N - \frac{1}{2} \sum_q \tilde{E}_{k_0 + q} + \\
\frac{1}{2} \sum_q \begin{pmatrix} a_{k_0 + q}^\dagger & a_{k_0 - q} \end{pmatrix} \begin{pmatrix} \tilde{E}_{k_0 + q} & U N_0 \\ U N_0 & \tilde{E}_{k_0 + q} \end{pmatrix} \begin{pmatrix} a_{k_0 + q} \\ a_{k_0 - q}^\dagger \end{pmatrix}, \tag{5.62}
\]

where \( \tilde{E}_{k_0 + q} \equiv E_{k_0 + q} - E_{k_0} + U N_0 \). In this approximation, we can now
perform the Bogoliubov transformation

\[
\begin{pmatrix} b_{k_0 + q} \\ b_{k_0 - q}^\dagger \end{pmatrix} = \begin{pmatrix} u_q & v_q \\ v_q & u_q \end{pmatrix} \begin{pmatrix} a_{k_0 + q} \\ a_{k_0 - q}^\dagger \end{pmatrix}. \tag{5.63}
\]

We assume, for simplicity, that the matrix elements of the Bogoliubov
transformation are real and even with respect to the inversion \( q \rightarrow -q \).
Moreover, they must satisfy the relation \( u_q^2 - v_q^2 = 1 \) to have a canonical
transformation, which is a requirement of unitarity.

Requiring that only the non diagonal terms must vanish, we obtain
the following equations

\[
U N_0 (u_q^2 + v_q^2) - 2 \tilde{E}_{k_0 + q} u_q v_q = 0 \tag{5.64}
\]

\[
\tilde{E}_{k_0 + q} (u_q^2 + v_q^2) - 2 U N_0 u_q v_q = \hbar \omega_{k_0 + q}, \tag{5.65}
\]
the solution of which is

\[ \hbar \omega_{k_0+q} = \sqrt{E_{k_0+q}^2 - U^2 N_0^2}, \]  
(5.66)

\[ \nu_k^2 = \frac{1}{2} \left( \frac{E_{k_0+q}}{\hbar \omega_{k_0+q}} - 1 \right). \]  
(5.67)

The Hamiltonian thus becomes

\[ H_{\text{Bog}} = \left( E_{k_0} - \mu + \frac{1}{2} U N_0 \right) N + \]
\[ \frac{1}{2} \sum_q \left( \hbar \omega_{k_0+q} - E_{k_0+q} \right) + \sum_q \hbar \omega_{k_0+q} b_{k_0+q}^\dagger b_{k_0+q}. \]  
(5.68)

Now that we have found the spectrum of excitations \( \hbar \omega_{k_0+q} \), we can observe that it is linear in the momentum \( q \) and we can calculate the velocity of sound along specific directions. We can approximate the spectrum as

\[ \hbar \omega_{k_0+q} = \sqrt{E_{k_0} + q - E_{k_0} + 2 U N_0 \sqrt{E_{k_0} + q}} \]
\[ \approx \sqrt{2 U N_0 \frac{\partial^2 E}{\partial k_i \partial k_j} q_i q_j}, \]  
(5.69)

which shows that the spectrum is indeed linear. If we fix a direction \( i \), we get the excitation spectrum along that direction

\[ \hbar \omega_{k_0+q}^{(i)} \approx \left( 2 U N_0 \frac{\partial^2 E}{\partial k_i^2} \right)^{1/2} |q_i|. \]  
(5.70)

### 5.6 Phase diagram

The formalism to determine the phase diagram of the system has been developed in Chap. 4 for the 1D case. The 2D case is analogous; hence we can write the final expression for the phase boundaries,

\[ \bar{\mu}_\pm = \frac{\bar{U}}{2} (2 N_0 - 1) + \frac{\bar{\varepsilon}_{k_0}}{2} \pm \frac{1}{2} \sqrt{\bar{\varepsilon}_{k_0}^2 + 2(2 N_0 + 1) \bar{U} \bar{\varepsilon}_{k_0} + \bar{U}^2}, \]  
(5.71)

where \( \bar{\mu} = \mu / 2t, \bar{U} = U / 2t \) and \( \bar{\varepsilon}_{k_0} = E_{k_0} / 2t \) and \( k_0 \) is the condensation momentum (which depends on \( K_0 \)). Recall that \( \bar{\varepsilon}_{k_0} \) depends on the next-nearest-neighbor-hopping coefficients \( t' \) and \( t'' \), which are renormalized by the Bessel functions. We plot the phase diagram in Fig. 5.4.
Figure 5.4: Phase boundaries for $V_0 = 3E_r$ where $\bar{\mu} \equiv \mu/2t$ and $\bar{U} \equiv U/2t$: (a) lobe with $N_0 = 1$, (b) zoom of the region of shaking for which the finite-momentum condensate is generated; lobes with $N_0 = 1, 2$ for increasing $\bar{\mu}$ are shown.
5.6 Phase diagram

For $K_0 = 0$, one can see that the lobe ($N_0 = 1$) is just the one we encountered in Chap. 2. The only difference is the normalization of the axes. Here, we considered for instance $\bar{U} = U/2t$ while in Chap. 2 it was $\bar{U} = U/zt$ with $z = 2d$ and $d$ the number of dimensions. Replacing $d = 2$ we have $\bar{U} = U/4t$, which explains why the axis has a rescaling twice as large as the one seen in Chap. 2.

As done before, we can establish a critical value of $U$

$$U_c = |E_{k_0}| \left[ -3 \text{sign}(E_{k_0}) \pm 2\sqrt{2} \right]. \quad (5.72)$$

For $U < U_c$, the Bose gas is in the superfluid phase, independently of the value of the chemical potential.

![Graph](image)

Figure 5.5: Critical value $U_c = (U/2t)_c$ at $V_0 = 3E_r$ as a function of the shaking parameter $K_0$; in the inset, the region $2.4016 \leq K_0 \leq 2.4081$ where the tunable finite-momentum condensate is generated.

Bosons loaded in optical lattices have a fixed on-site interaction parameter $U$, which depends only on the lattice depth and on the laser wavelength. The expression for $U$ in 2D systems is

$$U = \sqrt{\frac{8}{\pi} k a_s E_r \left( \frac{V_0}{E_r} \right)^{1/2}}, \quad k \equiv 2\pi/\lambda \quad (5.73)$$

The previous equation is quite accurate for deep lattices and separable potentials. It is not applicable for the case treated here but we can
nevertheless use it to have an order of magnitude of $U$. In our system, once you have fixed the setup, the parameters entering the formula must be rescaled. If $V_0$ is the laser intensity and $\lambda$ its wavelength, then our system can be thought as a sinusoidal potential with potential depth $2V_0$ generated by a laser with wavelength $\sqrt{2}\lambda$.

Using a laser with wavelength 852 nm for $^{23}\text{Na}$ and $^{87}\text{Rb}$ with $a_s = 19a_0$ and $a_s = 106a_0$, respectively, where $a_0 = 0.053$ nm is the Bohr radius, we find

$$U = 0.021 \text{ (Sodium)},$$

$$U = 0.115 \text{ (Rubidium)}.$$  \hfill (5.74)

To compare these results with Fig. 5.5 we need to divide these numbers by $2t$. We already know that $t$ is of the order of $10^{-3} - 10^{-4}$ and this is enough to state that the typical values of $U$ are too large to probe the tunable-momentum superfluid with ordinary experimental setups. However, we can reduce the s-wave scattering length with Feshbach resonances which are available for both the Rubidium isotopes and also for other alkali atoms [47], thus reducing $U$ further. This fact opens the possibility to measure the tunable-momentum condensate in the immediate future. The group of Hemmerich in Hamburg is envisaging such a possibility.

<table>
<thead>
<tr>
<th>$V_0/E_r$</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>No finite-momentum condensate</td>
</tr>
<tr>
<td>2.0</td>
<td>$2.40051 &lt; K_0 &lt; 2.40906$</td>
</tr>
<tr>
<td>3.0</td>
<td>$2.40155 &lt; K_0 &lt; 2.40806$</td>
</tr>
<tr>
<td>4.0</td>
<td>$2.40277 &lt; K_0 &lt; 2.40686$</td>
</tr>
</tbody>
</table>

Table 5.3: Range of the shaking parameter $K_0$ for which the finite-momentum condensate is achieved as a function of the lattice depth $V_0$.

In Table 5.3 we list the range of $K_0$ for which the tunable finite-momentum condensate is generated. For $V_0 = 1.0 E_r$ the minimum of the spectrum is no longer inside the Brillouin zone. This is due to the
5.7 Time-of-flight predictions

fact that the slope of the function \( f(K_0) \) (see Eq. (5.39)) changes sign. We expect that in between these two regimes there is a range of values for \( V_0 \) such that \( f(K_0) \) is enough flat around \( K_0 = 2.4 \), to enlarge the range in \( K_0 \) for the generation of the tunable finite-momentum condensate. The table suggests that we should search for an optimized value of \( K_0 \) around \( V_0 = 2 E_r \). One can immediately see from Eq. (5.39) that to enlarge the region we need the quantity \((t_1 + 2t_2) = (t' + 2t'')/t\) to be as large as possible. Our numerical simulations yield the results shown in Table 5.4.

<table>
<thead>
<tr>
<th>( V_0/E_r )</th>
<th>Range</th>
<th>((t' + 2t'')/t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.8</td>
<td>2.40150 &lt; ( K_0 ) &lt; 2.40810</td>
<td>(-3.54 \times 10^{-3})</td>
</tr>
<tr>
<td>1.9</td>
<td>2.40092 &lt; ( K_0 ) &lt; 2.40867</td>
<td>(-4.23 \times 10^{-3})</td>
</tr>
<tr>
<td>2.0</td>
<td>2.40051 &lt; ( K_0 ) &lt; 2.40906</td>
<td>(-4.64 \times 10^{-3})</td>
</tr>
<tr>
<td>2.1</td>
<td>2.40035 &lt; ( K_0 ) &lt; 2.40921</td>
<td>(-4.85 \times 10^{-3})</td>
</tr>
<tr>
<td>2.2</td>
<td>2.40029 &lt; ( K_0 ) &lt; 2.40927</td>
<td>(-4.91 \times 10^{-3})</td>
</tr>
<tr>
<td>2.3</td>
<td>2.40034 &lt; ( K_0 ) &lt; 2.40922</td>
<td>(-4.86 \times 10^{-3})</td>
</tr>
</tbody>
</table>

Table 5.4: Band structure calculation has been performed with \( l = 4 \). The discretization step of the 1BZ has been taken to be \( dx = 0.1 \).

From Table 5.4 we see that the largest interval for the shaking parameter is achieved when \( V_0 = 2.2 E_r \). Nevertheless, it is clear that we do not get a significant improvement by adjusting the value of \( V_0 \). The results that we have shown are the best that one can obtain with the potential and the shaking that we have been using.

5.7 Time-of-flight predictions

As discussed in Chap. 2, the way to determine the phase coherence of the condensate is a time-of-flight experiment. The cloud is released after all the lasers are switched off and the density distribution of the cloud is measured by imaging. The density distribution is mapped into the momentum distribution \( \mathbf{k} = (m/\hbar \tau) \mathbf{x} \). For this reason we are interested
5.7 Time-of-flight predictions

in the evaluation of the density distribution

\[ n(k) = \langle \psi^\dagger(k) \psi(k) \rangle. \quad (5.76) \]

The field operator is decomposed in terms of Wannier functions in our tight-binding model \( \psi(r) = \sum_R W(r-R) a_R \). We perform a Fourier expansion:

\[ \psi(k) = \frac{1}{\sqrt{N_s}} \sum_r e^{-ikr} \psi(r) = \frac{1}{\sqrt{N_s}} W(k) \sum_R e^{-ikR} a_R, \quad (5.77) \]

and the density becomes

\[ n(k) = \frac{1}{N_s} |W(k)|^2 \sum_{R,R'} e^{-ik(R'-R)} \langle a_R^\dagger a_{R'} \rangle. \quad (5.78) \]

To calculate the matrix element \( \langle a_R^\dagger a_{R'} \rangle \) in the 2-fold degenerate ground state, we write

\[ |\psi\rangle = \sum_{\sigma=\pm} \frac{c_{\sigma}}{\sqrt{N!}} (a_{\sigma k_0}^\dagger)^N |0\rangle = \sum_{\sigma=\pm} \frac{c_{\sigma}}{\sqrt{N!}} \left( \frac{1}{\sqrt{N_s}} \sum_R e^{i\sigma k_0 \cdot R} a_R^\dagger \right)^N |0\rangle. \quad (5.79) \]

We will show that this state can be approximated by a coherent state. Let us define the following coherent state

\[ |\psi_c\rangle = \sum_{\sigma=\pm} c_{\sigma} \prod_R e^{-N_0/2} \exp \left( \sqrt{N_0} e^{i\theta_R^\sigma} a_R^\dagger \right) |\psi^+\rangle + c_- |\psi^-\rangle, \quad (5.80) \]

where \( N_0 \) is the filling factor and \( \theta_R^\sigma = \sigma k_0 \cdot R \). We will describe the meaning of the filling factor in the definition of the coherent state later.

From the Taylor expansion of the exponential we obtain

\[ |\psi_c\rangle = e^{-N/2} \sum_{\sigma=\pm} c_{\sigma} \prod_R \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \left( \sqrt{N_0} e^{i\theta_R^\sigma} a_R^\dagger \right)^{\nu} |0\rangle. \quad (5.81) \]

This coherent state is a superposition of states containing an arbitrary large number of particles at each site \( R \). In the thermodynamic limit
\[ N, N_s \to \infty \text{ but } N/N_s = N_0 \text{ fixed and we can approximate this state with one having the set } \{ \nu_R \} \text{ satisfying } \sum_R \nu_R = N, \text{ such that we can exchange the sum and the product, thus finding} \]

\[ |\psi_c \rangle = e^{-N/2} \sum_{\sigma = \pm} c_\sigma \sum_{\{ \nu_R \}} \prod_{R} \frac{1}{\nu_R!} \left( \sqrt{N_0} e^{i \theta_R a_R^\dagger} \right)^{\nu_R} |0\rangle, \quad (5.82) \]

This is nothing but the multinomial expansion

\[ (x_1 + x_2 + \cdots + x_m)^N = \sum_{k_1 + \cdots + k_m = N} \frac{N!}{k_1! \cdots k_m!} x_1^{k_1} \cdots x_m^{k_m}. \quad (5.83) \]

from which we can write the coherent state in the form

\[ |\psi_c \rangle = \frac{e^{-N/2}}{N!} N^{N/2} \sum_{\sigma = \pm} c_\sigma \left( \frac{1}{\sqrt{N_s}} \sum_{R} e^{i \theta_R} a_R^\dagger \right)^N |0\rangle. \quad (5.84) \]

Now, we can compare this state with the original ground state (5.79). Making use of the Stirling formula

\[ \ln N! \simeq N \ln N - N \implies N! \simeq N^N e^{-N}, \quad (5.85) \]

we find

\[ \frac{e^{-N/2}}{N!} N^{N/2} \simeq \frac{1}{\sqrt{N!}}, \quad (5.86) \]

and then \[ |\psi_c \rangle \simeq |\psi \rangle, \] which proves that we can approximate the original ground state with a coherent state. This is an important result because it allows us to compute the matrix element \( \langle a_R^\dagger a_{R'} \rangle \) in an easy way. Indeed, coherent states are eigenstates of the annihilation operator. Let us consider, for instance, the harmonic oscillator. It is straightforward to show that

\[ a \exp(\lambda a^\dagger)|0\rangle = \lambda \exp(\lambda a^\dagger)|0\rangle. \quad (5.87) \]

Hence, to calculate the expectation value \( \langle \psi_c | a_R^\dagger a_{R'} | \psi_c \rangle \), we may use Eq. (5.80) and notice that the coherent states are normalized, such that \( \langle \psi_c^\sigma | \psi_c^\sigma \rangle = 1 \). We then find

\[
\frac{1}{N_0} \langle \psi_c | a_R^\dagger a_{R'} | \psi_c \rangle = |c_+|^2 e^{i (\theta_R^+ - \theta_R^-)} + |c_-|^2 e^{i (\theta_R^+ - \theta_R^-)} + \\
+ c_+^* c_- e^{i (\theta_R^- - \theta_R^+)} \langle \psi_c^+ | \psi_c^- \rangle + c_-^* c_+ e^{i (\theta_R^- - \theta_R^+)} \langle \psi_c^- | \psi_c^+ \rangle. \quad (5.88)
\]
Now, we need to compute the scalar product $\langle \psi_c^+ | \psi_c^- \rangle$, which is given by

\[
\langle \psi_c^+ | \psi_c^- \rangle = e^{-N} \left[ \prod_r \sum_n \frac{1}{n!} \left( \sqrt{N_0} e^{-i \theta_r} \right)^n \right] \times \left[ \prod_{r'} \sum_m \frac{1}{m!} \left( \sqrt{N_0} e^{i \theta_{r'}} \right)^m |m_{r'}\rangle \right].
\]

\[
= e^{-N} \sum_n \frac{N_0^n}{(n!)^2} \exp \left(-2i n k_0 \cdot \sum_r r \right)
\]

\[
= e^{-N} \sum_n \frac{N_0^n}{(n!)^2} \leq e^{-N} \sum_n \frac{N_0^n}{(n!)^2} = e^{-N+N_0} \simeq 0 ,
\]

(5.89)

where in the last steps we used the fact that $\sum_r r = 0$ because the lattice (even if large) is finite and that $N \gg 1, N_0$. This almost exact orthogonality condition is quite important because we started with two degenerate orthogonal ground states and the coherent states that we are using instead of them cannot lose this symmetry.

If we put $R = R'$, we see that we find $\langle \psi_c | a_R^\dagger a_R | \psi_c \rangle = N_0$, the average number of particles per site is thus taken to be equal to $N_0$ and this explains the definition of the coherent state we have given: we assumed a uniform average density per site for the bosonic superfluid.

Now, replacing in Eq. (5.88)

\[
\theta_{R'}^+ - \theta_R^+ = k_0 \cdot (R' - R) ,
\]

\[
\theta_{R'}^- - \theta_R^- = -k_0 \cdot (R' - R) ,
\]

(5.90)

we obtain

\[
n(k) = \frac{N_0}{N_s} |W(k)|^2 \sum_{R,R'} \left[ |c_+|^2 e^{-i(k-k_0) \cdot (R'-R)} + |c_-|^2 e^{-i(k+k_0) \cdot (R'-R)} \right].
\]

(5.91)

It is easy to compute the sum; indeed the first term becomes

\[
\sum_{R,R'} e^{-i(k-k_0) \cdot (R'-R)} = \left( \sum_{R} e^{i(k-k_0) \cdot R} \right) \left( \sum_{R'} e^{-i(k-k_0) \cdot R'} \right) = N_s^2 \delta_{k,k_0} .
\]

(5.92)
Hence, the final expression for the momentum distribution is

\[ n(k) = N |W(k)|^2 \left( |c_+|^2 \delta_{k,k_0} + |c_-|^2 \delta_{k,-k_0} \right). \]  

(5.93)

Figure 5.6: Time of flight image for the finite-momentum superfluid phase. The momentum is in units of \( \pi/a \). We assumed a condensate with momentum \( k_0 \equiv (\pm 1/2, \pm 1/2) \) and the density has been divided by \( |W(k)|^2 \) such that all the peaks have the same height. The peak broadness has been represented using Gaussians.

The two coefficients \( c_+ \) and \( c_- \) are random numbers. This means that in a real experiment the height of the peaks depends on the momentum dependence of the Wannier function and on the ratio between these coefficients. There is no dependence on their relative phase. In any case, a single time-of-flight experiment cannot detect both peaks at \((k_0\) and \(-k_0\)) the same time. Indeed, when the image is recorded, and the first atom is measured having one of the two momenta, then the wave function collapses on that state, showing only one peak. It can be convenient to prepare an experiment made of several arrays of 2D systems, in which the finite-momentum condensate is generated. Then, one can release the trap and detect the result of all these identical 2D systems. In this way, the randomness of the coefficients is partially suppressed (to be realistic,
we cannot consider an infinite number of copies of the 2D system, so we say 'partially') and we can study the effect of the non separability of the optical potential on the Wannier functions in reciprocal space.

We close this section by mentioning a recent work [8] in which a condensate at finite-momentum has been found for a 2D triangular lattice. In this case, the non separability of the potential is part of the geometry of the lattice. They study the phases arising after shaking the lattice in an elliptical way and only nearest-neighbors are taken into account. In our model, the finite-momentum condensate is a consequence of the next-nearest-neighbor competition solely.
CONCLUSIONS

In this thesis, we have explored some possibilities to generate finite-momentum condensates in optical lattices. We have seen that lattices under shaking undergo a phenomenon known as dynamical localization: tunneling is suppressed at a certain value of an external parameter related to the shaking. This opens the possibility to investigate the role of next-nearest-neighbor hopping in the generation of condensates. We have seen in 1D that condensates with momentum at the edge of the Brillouin zone are generated and this result has been confirmed experimentally.

To look for nontrivial condensation points lying inside the first Brillouin zone we have studied non-separable optical potentials in 2D. Applying a shaking along the diagonal of the condensate, we have seen that in a small region of the shaking parameter where the nearest-neighbor tunneling is suppressed, two kinds of next-nearest-neighbor-hopping coefficients still rule the dynamics of the condensate. In this region, we have found an intermediate phase with condensation point varying continuously from the center to the edge of the Brillouin zone as we tune the shaking parameter. There are two minima in the single-particle spectrum and they are symmetric with respect to the center of the Brillouin zone.

We have studied the ground state of this phase and we have found
that small interactions between particles force the ground state to be a superposition of two possible Fock states: one where the particles are all condensing in one minimum and the other where all the particles are condensing in the second minimum. In the absence of interactions, all the states with \( n \) and \( N - n \) particles form the ground state, the interactions reduce the degeneracy to only two states.

We have pointed out that condensates with tunable momentum are generated in other systems due to different reasons. One is a Bose gas with spin-orbit interaction (no lattice) and the other one is a triangular optical lattice with elliptical shaking. In our case, the generation of the non trivial condensate is given by the competition between higher-order hopping terms when the nearest-neighbor hopping is suppressed.

Finally, we noticed that the tunable-momentum condensate can be measured experimentally if the on-site interaction is reduced significantly. This can be achieved with present state-of-the-art experimental techniques, and we hope that our results can stimulate further experiments in this direction.
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