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# Analytic Study of Ultracold, Synthetically Spin–Orbit Coupled, Weakly Interacting, Two-Component Bose Gases Residing on Bravais Lattices

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# *Abstract*

In this Master's thesis, the behavior of ultracold, synthetically spin-orbit coupled, weakly interacting, two-component Bose gases residing on Bravais lattices, is explored analytically. In particular, utilizing a mean field approach, general expressions for the chemical potentials are deduced for the superfluid phase, and non-diagonal expressions for the Hamiltonian are subsequently provided. An application of these expressions is presented for the case of a pure condensate residing on a square lattice, yielding an analytically derived phase diagram that coincides with numerical results found in the literature. Finally, future continuations of this work are suggested.

# *Sammendrag*

I denne masteroppgava presenteres en analytisk studie av oppførselen til ultrakalde, syntetisk spinn-bane-koplede, svakt vekselvirkende, to-komponents Bose-gasser bundet til Bravais-gitre. Spesielt utledes generelle uttrykk for de kjemiske potensialene under en middelfeltstilmnærming gyldig for superfluidfasen, og ikke-diagonale uttrykk for Hamilton-funksjonen presenteres deretter. Disse uttrykkene anvendes til å utlede et fasediagram analytisk for et system bestående av et reint kondensat bundet til et kvadratisk gitter; diagrammet samsvarer med numeriske resultat funnet i litteraturen. Avslutningsvis foreslås videreføringer av arbeidet.

# Preface

وَجَعَلْنَا اللَّيْلَ وَالنَّهَارَ آيَاتٍ ۖ فَمَحَوْنَا آيَةَ اللَّيْلِ وَجَعَلْنَا آيَةَ النَّهَارِ مُبْصِرَةً لِّتَبْتَغُوا  
فَضْلًا مِّن رَّبِّكُمْ وَلِتَعْلَمُوا عَدَدَ السِّنِينَ وَالْحِسَابَ ۚ وَكُلُّ شَيْءٍ فَضْلَنَّهُ نَفْصِيلاً ﴿١٢﴾

*Suggested by my friend Abdulrahman Alhasan.*

By and large entirely rewritten over the course of two summer months, the process of this thesis has been demanding, but experiential. What I anticipated would be a short phone call with my supervisor on a Sunday morning, evolved into a five hour long discussion, at the end of which the majority of the calculations in my 130 pages long thesis had been deemed erroneous, one week before the deadline. A few errors in the preliminary material—some rather subtle—had pervaded the remainder, and what initially appeared to be a moderately challenging exercise for a Master’s thesis, proved instead to be beyond the scope of expertise. Rewriting this thesis in light of the former has, however, lead to the discovery of results to be presented in Ch. 3 and 4 that the reader hopefully finds as interesting as I do myself. The weather and temperatures this summer has either way been unbearably bad by every definition save the one used by meteorologists on television; I have saved the longer bike trips for cooler days.

I would like to thank my supervisor Professor Asle Sudbø for his guidance throughout this past year, and his excellent availability. He has displayed outstanding interest for, and knowledge about, the subject. I am also very grateful for all the invaluable help that has been offered by fellow Master’s degree student Stian Thomas Heimdal Hartman, with which I have had several rewarding discussions; as well as the equally invaluable aid by Sigve Solli, who shared all the code he had written for his Master’s thesis—from which the analysis presented in this thesis draws many elements—and who kindly gave me feedback on my project work after it was submitted for evaluation in December 2017. Furthermore, I would like to thank Steinar Brattøy Gundersen, for his technical assistance with computing and programming during this past year, as well as aiding me in running a number of quite resource-intensive numerical simulations; Morten Andreas Klausen Elvekrok, who kindly aided me as well in running these simulations; the student organization Norsk Start, the volunteers and attendees of which are all amazing people; and finally, my family and other friends, for aid and support throughout this period.

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# CHAPTER 1

## *Introduction*

### 1.1 Theoretical and Experimental Exploration of Bose–Einstein Condensation

In certain bosonic systems, when cooled to below a critical, typically near absolute zero temperature, a macroscopic number of bosons enter a single quantum state to form a Bose–Einstein condensate (BEC), a coherent matter wave that may exhibit exotic large-scale quantum behavior, such as superfluidity and superconductivity [1, 2]. The behavior of identical particles in this context was first explored theoretically by S. N. Bose in 1924 [3], for the special case of non-interacting photons. In particular, he derived the Planck distribution employing the then still quite novel *Lichtquantenhypothese* that had been explored before him by, among others, M. Planck in 1900 [4], in relation to his empirically derived law that came to be known as Planck’s law; and A. Einstein in 1905 [5], in relation to the photoelectric effect, for which A. Einstein was awarded the 1921 Nobel Prize in Physics [6]. The work of S. N. Bose was subsequently generalized to non-interacting massive particles by A. Einstein in 1924 [7], and the phenomenon of Bose–Einstein condensation was first predicted and explored theoretically shortly after, in his paper from 1925 [8] .

In terms of experimental realization, one of the earliest applications of the theory of Bose–Einstein condensation was in the description of superfluid  $^4\text{He}$ ,<sup>1</sup> discovered experimentally in 1938 by P. Kapitza [9] and by J. F. Allen *et al.* [10]. The same year, F. London proposed to model the system as a condensed Bose gas [11], and the theory was further developed and refined to account for interactions, in particular between the condensate and

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<sup>1</sup>Though the constituent particles of  $^4\text{He}$  are fermionic, their collective spin is integral; for this reason,  $^4\text{He}$  obeys bosonic statistics.



the excited states, by L. D. Landau in 1941 [12]—theory for which he would later be awarded the 1962 Nobel Prize in Physics [13]. He proposed that below a critical fluid velocity in viscous capillary flow, spontaneous excitations would become energetically unfavorable, eliminating this dissipative mechanism and allowing for frictionless flow [14, Ch. 6]. In the 1950s, condensed matter theory was developed to describe superconduction: In particular, the celebrated Ginzburg–Landau theory, which was developed in 1950 by V. L. Ginzburg, applying Landau theory of phase transition to describe type-I superconductors; and the also very much celebrated BCS theory devised in 1957 by J. Bardeen, L. N. Cooper and J. R. Schrieffer, to provide a broader theoretical description of what are now known as conventional superconductors, crucially attributing the phenomenon of superconductivity to energetically favorable pairing of conduction electrons—Cooper pairs—resulting from electron–phonon interactions [15, 16]. For these theoretical advances, J. Bardeen, L. N. Cooper and J. R. Schrieffer, and V. Ginzburg, were awarded the Nobel Prize in Physics in 1972 and 2003, respectively [17, 18].

These early applications concerned systems with *strong* interactions, which suffered some important limitations [19]. In particular, the relative occupancy of the zero-momentum state of experimentally engineered superfluid  $^4\text{He}$ , one of the then most central systems of study concerning Bose–Einstein condensation, was typically at around 0.1 *or less*, as the interactions caused non-zero momentum states to persist even at zero temperature [15]. An interest was thus sparked for engineering systems of *weakly* interacting Bose gases, potentially with higher condensate fractions. Due to technological limitations, however, experimental engineering and exploration of such gases proved to be generally infeasible prior to the advent of laser cooling and evaporative cooling techniques in the 1980s and 1990s. Combining quantum mechanics and special relativity, one laser cooling technique ingeniously exploits the Doppler shift and discrete atomic transitions to transfer momentum from photons to moving atoms *only if* the frequency, and thereby the energy, of light that the atom ‘perceives’ matches the gap between atomic energy levels. Alkali metal have proved to be particularly interesting in this respect, carrying internal energy levels apt for low-temperature cooling, as well as being suited for cooling using accessible laser technology [20].

The use of these techniques in order to produce a Bose–Einstein condensate in a weakly interacting Bose gas, was pioneered in 1995 by a group

lead by E. A. Cornell and C. E. Wieman, using a dilute<sup>2</sup> atomic gas of  $^{87}\text{Rb}$  cooled to below a mere 170 nanokelvin; at 20 nanokelvin, their condensate comprised 2000 atoms of rubidium, and it persisted for more than 15 seconds [19, 21]. Shortly after their work was published, another paper by C. C. Bradley *et al.* reported independently achieving Bose–Einstein condensation in a dilute gas of  $^7\text{Li}$  atoms [22]. A mere three months after the first publication, a third group, headed by W. Ketterle [23], reported independently achieving Bose–Einstein condensation in a dilute gas of yet another alkali metal,  $^{23}\text{Na}$ , engineering a sample large enough to further explore the behavior of the condensate: For instance, the coherent properties of the BEC were explored by studying interference patterns produced by two condensates that were allowed to mutually expand into one another; and droplets of the BEC were made to fall under gravity, appropriately and amusingly described as a “material laser beam” in a press release by the Nobel Institute [24]. E. A. Cornell, C. E. Wieman and W. Ketterle were awarded the 2001 Nobel Prize in Physics for the work of their groups [24, 25, 26].

## 1.2 Engineering and Exploring Bose–Einstein Condensation on a Lattice

In recent years, in particular the past two decades, a considerable interest for Bose–Einstein condensates trapped in various lattice geometries has been sparked, and with it, a rapidly growing body of research. Such a system bears several alluring features: Of particular interest is the conspicuous resemblance of this system to that of electrons on a crystal lattice, as well as easily realizable methods for tuning system parameters [27, 28]. As such, they have become invaluable tools in theoretical and experimental research, and are used to explore, among other things, the Bose–Hubbard model, Mott insulators, and—of particular interest for this thesis—the effects of spin–orbit coupling (SOC) on particles trapped in lattices.

One routine procedure by which atomic gases are cooled and trapped, is by first applying laser cooling to lower the temperature into a range below

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<sup>2</sup>The motivation for using *dilute* gases is that at very low temperatures, various gases form solids or liquids; the diluted nature of the gases in question enables them to instead form Bose–Einstein condensates for extended periods at these temperatures.

which this method is no longer viable, before the cold atomic gas is transferred to a conservative magnetic or optical trap, and cooled further using decreasing trap depths to cool the sample evaporatively [27]; this was the procedure employed in the dilute alkali gas experiments of Ref. [19] and [22], whereas another trapping method combining both magnetic and optical forces was employed by the group of W. Ketterle [23]. There is a multitude of techniques available to trap particles at low temperatures: For ions, one may make use of Coulomb interactions; for neutral atoms, however, one may, at sufficiently low temperatures, make use of weaker methods. These include *radiation-pressure trapping*, which, though often used to prepare the system for dipole trapping, is itself not suitable for the lowest of temperatures due to strong optical interactions; *magnetic trapping*, which exploits dipole momenta to trap particles at exceptionally low temperatures, but carry crucial limitations to its applicability due to its inherent reliance on the internal atomic state, as well as to its trapping geometry; and *optical trapping*, which enables trapping at very low temperatures employing couplings between dipole momenta and far-detuned light, neither relying on internal atomic states such as magnetic traps, nor being limited in applicability by optical interactions to the same extent as radiation-pressure traps [29].

The latter method is, as insinuated, particularly appealing for its overall applicability and tunability of system parameters. Optical traps may be achieved using interfering laser light, by way of for instance retro-reflexive interference, or interfering opposing or parallel lasers; the latter offering more experimental degrees of freedom for instance by allowing for tuning lattice spacing through adjustments of the relative angles of the interfering lasers, as well as by allowing for an induced velocity of the lattice, by detuning the phases of the interfering lasers [27]. In essence, the principle behind an optical trap is the AC Stark shift: By placing a neutral atom in a light field, a dipole moment is induced in the former by the oscillating electric field of the latter, leading to a shift in the atomic energy level. A red-detuned light field, for which the frequency of the light field is lower than the atomic resonance frequency, leads to a gradient field that guides the atoms to regions of intensity maxima. The opposite, a blue-detuned light field, may also be employed, instead generating a gradient field guiding atoms to intensity minima [29]. As is explained in detail by O. Morsch *et al.* in Ref. [27], one may lower the rate of spontaneous photon scattering by atoms at the center of the traps by increasing the detuning, and further evaporative cooling may be achieved by gradually lowering the trap depth, by way of

decreasing the laser intensity. Further details may be found in Ref. [27], and in another review by I. Bloch *et al.* in Ref. [30]. In the context of a Bose–Hubbard model, several tunable parameters of an optical lattice trap may be directly translated to parameters of said model; for instance, the hopping parameter  $t$ —as well as the extent of the interaction potential  $U$ —of the Bose–Hubbard model may be tuned directly by way of tuning the lattice depth, which in physical terms alters the tunneling rate of the trapped particles across lattice sites; thus, the system becomes an invaluable tool to study this model experimentally [1, 28]. This does not only enable the study of the model for varying parameter inputs, but also for different *phases*, in particular the *superfluid* phase and the *Mott insulator* phase, occurring in the regimes of  $U/t \ll 1$  and  $U/t \gg 1$ —or, in terms of the properties of the lattice: shallow and deep traps—respectively [31]. Roughly, the former phase is characterized by a favoring of hopping across lattice sites, and the latter, by a strong binding to each site. For phase diagrams of a one- and three-dimensional optically trapped Bose–Einstein condensate described by the Bose–Hubbard model, the reader is referred to Ref. [32] by J. Mun *et al.*<sup>3</sup> This thesis will be concerned only with the weakly interacting superfluid phase due to limitations to the mean field approach to be employed in the analysis.

Experimental realizations of Bose–Einstein condensation in optical traps include the early work by D. M. Stamper-Kurn *et al.* [33]; a case of a harmonic one-dimensional trap by J. H. Denschlag *et al.* [34]; and a case of a two-dimensional harmonic trap by K. Jiménez-García *et al.* [35]. Another interesting example is the experimental realization by M. Greiner *et al.* [36], in which the transition from a superfluid phase to a Mott insulator phase in a BEC on a harmonic optical lattice was explored, as the lattice depth was increased. As suggested by D. Jaksch in Ref. [37], among the practical applications of Bose–Einstein condensates trapped in optical lattices, is quantum computing, due to the high level of control achievable for a system of trapped cold neutral atoms.

Of particular interest for this thesis is the analytic behavior of *two* weakly interacting Bose–Einstein condensates in a Bose gas trapped in an optical lattice. Such a system is adequately described by the Bose–Hubbard model, and, as mentioned, offers realizable methods for tuning model parameters.

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<sup>3</sup>This thesis will predominantly be concerned with the two-dimensional case, however; the diagrams referred to are but illustrative in this context.

For these particular systems, the energy spectra of quasi-particles<sup>4</sup> emerging from diagonalization procedures applied to non-diagonal Hamiltonians, have been calculated and explored in papers by J. Gu *et al.* [38], X. P. Liu [39], and more recently, by J. Linder *et al.* [1]. The two former papers did so under standard assumptions of nearest neighbor hopping and on-site interactions; the latter paper explored effects under longer-range conditions as well.

### 1.3 Engineering Synthetic Spin–Orbit Coupling

Spin–orbit coupling is a relativistic correction to the energy of a particle, coupling its spin to its orbital momentum. It plays an important—or even essential—role in several condensed matter phenomena, such as the spin Hall effect, and the electronic properties of GaAs, as well as playing a key role in systems such as topological insulators and spintronic devices [40]. However, the effects of an SOC is typically negligible under normal laboratory conditions. In 2002, J. Higbie *et al.* proposed an experimentally realizable method of inducing a *synthetic* SOC in a dilute atomic Bose gas [41]. By directing two lasers of appropriately tuned frequencies at the gas, one induces Raman transitions between two internal hyperfine states through absorption and stimulated re-emission, and by exploiting the Doppler effect, the atomic momentum couples to the transition rate by a momentum dependent detuning from the Raman resonance frequency. Thus, by treating the internal hyperfine states as pseudospin<sup>5</sup> states, one is effectively left with a spin–orbit coupled spin- $\frac{1}{2}$  system. The advantage of such systems is that the SOC is *tunable*, enabling a considerably more experimentally feasible study of the effects of an SOC; as such, they are suited to simulate the effects of an SOC on other systems as well, such as on electronic gases in crystal lattices, and on topological insulators [42]. A 2013 paper by V. Galitski *et al.* [43] expands on a

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<sup>4</sup>A quasi-particle is an effective particle emerging from the collective behavior of real particles. “Quasi-particle” and “particle” will be used interchangeably throughout this thesis; the context implies the nature of the particles.

<sup>5</sup>As the name suggests, “pseudospin” is not spin; rather, it is another feature or a set of states that may be engineered to emulate one or more desired effects of spin in a mathematically isomorphic manner. The terms “pseudospin” and “spin” will be used interchangeably throughout this thesis; the distinction is ultimately not of mathematical importance.

wider experimental implementation of synthetically spin–orbit coupled dilute Bose gases, enabling tunable two-dimensional Rashba and Dresselhaus SOC, as well as higher dimensional coupling such as Weyl SOC. Another very interesting feature of such a system, is that though emulating a spin- $\frac{1}{2}$  system, the particles involved are *bosons*, and as such, they are not subjected to fermionic constraints such as the Pauli exclusion principle, enabling the study of highly exotic phenomena; notably, and in the interest for this thesis, by cooling the gas to sufficiently low temperatures, one may produce two-component—or even multi-component—spin–orbit coupled Bose–Einstein condensates.

The first *experimental* realization of a synthetic SOC in a neutral atomic BEC was achieved in 2011 by Y.-J. Lin *et al.* [40], in which a one-dimensional Rashba and Dresselhaus SOC of equal strengths were engineered by the method of Raman transitions described above, directing two appropriately tuned lasers at a relative angle of  $90^\circ$  at a dilute gas of  $^{87}\text{Rb}$ , with the ground state and a complementary hyperfine internal state acting as pseudospin-up and pseudospin-down, respectively. SOC of tunable strength in an ultracold gas of  $^{87}\text{Rb}$  was achieved experimentally in 2015 by K. Jiménez-García *et al.* [44], by modulating the amplitude and the phase of the Raman lasers. Experimental realization of a *two-dimensional* SOC in a quantum degenerate gas remained challenging, but was achieved quite recently, in 2016, by Z. Wu *et al.*, again using the method of Raman lasers on an ultracold gas of  $^{87}\text{Rb}$ , inducing both a highly tunable SOC and an optical lattice trapping potential. Such a system may enable a broad experimental study of topological Hall effects, the Berry mechanism, and several exotic systems, such as Mott insulators of spin–orbit coupled interacting bosons, and topological superfluids [42].

## 1.4 Motivation and Outline of Thesis

In this Master’s thesis, the behavior of ultracold, synthetically spin–orbit coupled, weakly interacting, two-component Bose gases residing on Bravais lattices, is explored analytically. In particular, utilizing a mean field approach, general expressions for the chemical potentials are deduced for the superfluid phase, and non-diagonal expressions for the Hamiltonian are subsequently provided. An application of these expressions is presented for the case of a pure condensate residing on a square lattice, yielding an analytically derived phase diagram that coincides with numerical results found in the lit-

erature, in particular in Ref. [45]. This analysis is a generalization of the work by D. van Oosten *et al.* in Ref. [46], in which a similar analysis is performed for a non-spin–orbit coupled, weakly interacting, single-component Bose gas; in particular, the method by which D. van Oosten *et al.* deduces expressions for the chemical potentials in the superfluid phase, is applied in this thesis for the generalized case under consideration. Furthermore, the analysis draws many elements from the analysis of quasi-particle energy spectra conducted by J. Linder *et al.* in Ref. [1] for the non-spin–orbit coupled case, by S. Solli in Ref. [47] for the strongly<sup>6</sup> spin–orbit coupled case, and by the author in his 2017 project work [48], in which corrections were made to the thesis of S. Solli. The motivation for this analysis is to develop an analytic framework that describes the system under consideration; this is of practical interest for engineering experimentally feasible studies and simulations of the impact of spin–orbit couplings on fermionic systems such as electron gases in crystal lattices, as well as for exploring the exotic nature of synthetically spin–orbit coupled, weakly interacting Bose–Einstein condensates, both analytically and experimentally.

This thesis is structured as follows. Ch. 2 comprises preliminary material for Ch. 3 and 4, in particular reviewing relevant material for spin–orbit coupled, non-interacting Bose gases, and non-spin–orbit coupled, weakly interacting Bose gases. Additionally, a generalized diagonalization procedure is presented in Ch. 2, which may be of relevance for future work, as is elaborated in Ch. 6. In Ch. 3, a general analytic framework for an ultracold, spin–orbit coupled, weakly interacting two-component Bose gas on a Bravais lattice, is developed. In particular, expressions for the chemical potentials are deduced following the application of mean field theory to simplify the problem of diagonalizing the Hamiltonian. In Ch. 4, the framework developed in Ch. 3 is applied to a simple example of a pure condensate residing on a square lattice, which is shown to analytically reproduce numerical results found in the literature. Finally, miscellaneous discussion of the results in Ch. 3 and 4, and a summary and outlook, is presented in Ch. 5 and 6, respectively. The thesis is preceded by an appendix that may be helpful in understanding some of the results presented in Ch. 3, as well as presenting methods that may be used to generalize the materials of Ch. 3.

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<sup>6</sup>“Strong” in the sense that the coupling considered was assumed sufficiently strong to induce non-zero momenta among condensed bosons; the meaning of this will be made clear later in this thesis.

# CHAPTER 2

## *Preliminaries*

### 2.1 Notation and Conventions

The following notation and conventions are employed in this thesis:

- Vectorial quantities are written in bold font, e.g.  $\mathbf{v}$ .
- Lattice sites, condensate momenta and vectorial components are labeled by Latin lower indices such as  $i$  and  $j$ . Particle species, e.g. pseudospin states, are labeled by Greek upper indices such as  $\alpha$  and  $\beta$ .
- The Pauli spin matrices are labeled  $\sigma_i$ ,  $i = x, y, z$ , and the conventional definitions are used:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.1)$$

If  $\alpha, \beta = \uparrow, \downarrow$  are spin indices, the elements of these matrices are labeled  $\sigma_i^{\alpha\beta}$ , such that

$$\sigma_i = \begin{pmatrix} \sigma_i^{\uparrow\uparrow} & \sigma_i^{\uparrow\downarrow} \\ \sigma_i^{\downarrow\uparrow} & \sigma_i^{\downarrow\downarrow} \end{pmatrix}. \quad (2.2)$$

### 2.2 Quantum Mechanics on a Lattice

The analysis of this thesis revolves around the behavior of a Bose gas on a lattice, which effectively discretizes spatial translations. Realizable methods include radiation pressure traps, magnetic traps, and—for the interest of this thesis—optical dipole traps, for instance achievable by applying a sinusoidal standing wave potential using opposing lasers, inducing dipole forces that force atoms into intensity maxima or minima, depending on the specific detuning of the frequency of the light field with respect to the gaps between



the atomic ground state and the excited states [30, Sec. II.A.]. In-depth reviews of these methods are found in I. Bloch *et al.* [30], R. Grimm *et al.* [29] and C. J. Pethick *et al.* [15]. Optical traps offer easily realizable methods for tuning important system parameters: For instance, the energy cost of hopping—i.e., the tunneling rate across lattice sites—may be tuned simply by altering the intensity of the laser, leading to deeper or shallower traps; and both the strength *and* the sign of the interaction of particles may be tuned by way of *Feshback resonance*, wherein the energy of a bound state  $E_{\text{res}}$  is tuned—for instance by way of applying a uniform magnetic field to the optical trap, which is not possible in a magnetic trap—such that the energy of interacting particles  $E$  lies in the vicinity of  $E_{\text{res}}$ . The bound state acts as an intermediate state, leading to a resonant alteration of the scattering length

$$a_s \sim \frac{C}{E - E_{\text{res}}}, \quad (2.3)$$

where  $C$  is a constant [15, Ch. 4.2.2 & Ch. 5.4.2].

The exact eigenstates of a system subjected to a periodic lattice potential are Bloch functions. These are, however, extended across the entire lattice in real space [30, Sec. II.B.]. Wannier functions  $w(\mathbf{r} - \mathbf{R}_i)$ —related to Bloch functions by an inverse Fourier transform with respect to the lattice vectors—are localized around each lattice site  $i$  located at the fixed position  $\mathbf{R}_i$ , and constitute a more appropriate basis for describing discrete events on a lattice, such as hopping. In the *deep-lattice limit*, the amplitude of the Wannier functions decay exponentially around each lattice site, and their overlap across sites rapidly decays to zero [30, Sec. II.B.]. Thus, in this limit, choosing an appropriate normalization, the localized, lowest-band Wannier functions constitute an orthonormalized basis into which we may expand the field operators

$$\psi(\mathbf{r}) = \sum_i w(\mathbf{r} - \mathbf{r}_i) b_i, \quad (2.4)$$

where the  $b_i$  are annihilation operators for particles at the respective lattice sites [1]. This leads to a discretization of any Hamiltonian  $\mathcal{H}$  in terms of annihilation and creation operators.

## 2.3 The Bose–Hubbard Model

The system of interest for this thesis is a zero-temperature two-component Bose gas residing on a Bravais lattice, subject to a synthetic SOC and weak interactions, i.e. interactions for which only two-body scatterings significantly contribute to the system Hamiltonian  $\mathcal{H}$ ; three-body, four-body or higher order scattering events are of negligible impact. In physical terms, such a system could be a gas of neutral bosonic atoms residing on an optical lattice, cooled significantly *below the critical temperature* for Bose–Einstein condensation to occur—for which momenta are sufficiently small for us to only consider *s*-wave scattering—and which is *sufficiently dilute* for two-body scattering to be the only significant contribution to  $\mathcal{H}$ , given by the condition  $|a_s| \ll n^{-1/3}$ , where  $a_s$  is the *s*-wave scattering length; and  $n^{-1/3}$  is the average distance between particles, given by the inverse cube root of the particle density [14].

Consider a second-quantized system comprising an ensemble of two distinct bosonic particle species labeled  $\alpha, \beta = \uparrow, \downarrow$ <sup>1</sup> and of masses  $m^\alpha$ , residing on a Bravais lattice, subject to a two-body scattering potential  $v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|)$ , where  $\mathbf{r}$  and  $\mathbf{r}'$  denote the position of the two respective particles of species  $\alpha$  and  $\beta$ . Then, the general system Hamiltonian is

$$\begin{aligned} \mathcal{H} = & \sum_{\alpha} \int d\mathbf{r} \psi^{\alpha\dagger}(\mathbf{r}) h^{\alpha}(\mathbf{r}) \psi^{\alpha}(\mathbf{r}) \\ & + \frac{1}{2} \sum_{\alpha\beta} \int d\mathbf{r} \int d\mathbf{r}' \psi^{\alpha\dagger}(\mathbf{r}) \psi^{\beta\dagger}(\mathbf{r}') v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|) \psi^{\beta}(\mathbf{r}') \psi^{\alpha}(\mathbf{r}), \end{aligned} \quad (2.5)$$

where  $h^{\alpha}(\mathbf{r})$  is the single-particle Hamiltonian, given by

$$h^{\alpha}(\mathbf{r}) = -\frac{\nabla^2}{2m^{\alpha}} - \mu^{\alpha} + V(\mathbf{r}) \in \mathbb{R},^2 \quad (2.6)$$

where  $\mu^{\alpha}$  is a species-dependent chemical potential, and  $V(\mathbf{r})$  is a Bravais lattice potential [1]; therefore, if

$$\mathbf{v}_n, \quad n = 1, \dots, d, \quad (2.7)$$

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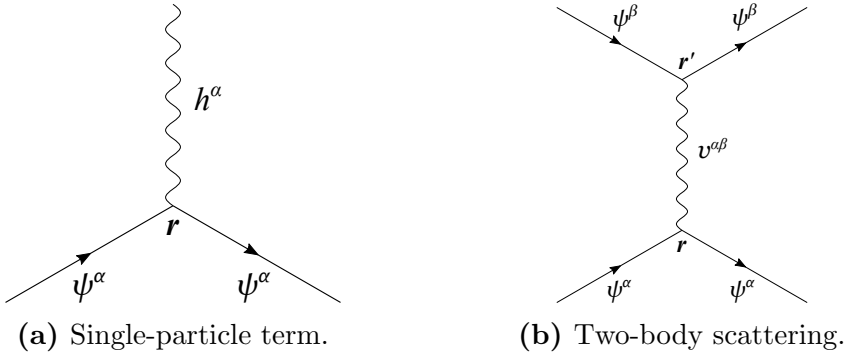
<sup>1</sup>These labels, of course, allude to the function of these species as pseudospin states.

are the  $d$  primitive vectors of the Bravais lattice,

$$V(\mathbf{r} + n_1\mathbf{v}_1 + n_2\mathbf{v}_2 + \cdots + n_d\mathbf{v}_d) = V(\mathbf{r}) \quad (2.8)$$

$$\Rightarrow h^\alpha(\mathbf{r} + n_1\mathbf{v}_1 + n_2\mathbf{v}_2 + \cdots + n_d\mathbf{v}_d) = h^\alpha(\mathbf{r}), \quad n_1, \dots, n_d \in \mathbb{Z}. \quad (2.9)$$

In addition, invariance of the potential  $v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|) = v^{\beta\alpha}(|\mathbf{r} - \mathbf{r}'|)$  with respect to a permutation of the species indices will be assumed, amounting physically to a quite natural assumption that the inter-species two-body scattering events depend only on relative species configurations. The terms in Eq. (2.5) may be visualized using Feynman diagrams, as presented in Fig. 2.1.



**Figure 2.1:** A visualization of the general Hamiltonian (2.5) for a system of bosonic particles of species  $\alpha, \beta$  subject to a two-body scattering potential  $v^{\alpha\beta}(\mathbf{r}, \mathbf{r}')$ .  $h^\alpha(\mathbf{r})$  is the single-particle Hamiltonian. Time progresses from left to right.

Writing the field operators  $\psi^\alpha(\mathbf{r})$  in terms of the Wannier basis (2.4) leads

<sup>2</sup>The reader may recognize “ $h^\alpha(\mathbf{r}) \in \mathbb{R}$ ” as abuse of notation. Formally, one would write “ $h^\alpha : \mathbb{R}^3 \rightarrow \mathbb{R}$ ” to indicate that  $h^\alpha$  maps real 3-vectors to a subset of the real numbers. However, for the remainder of this thesis, the former notation will be used to avoid clutter; whether it indicates a set membership or a mapping is implied by whether the left side of the expression is a number or a function, respectively. The domain of any mapping is understood by the context.

to

$$\begin{aligned}
 \mathcal{H} &= \sum_{\alpha} \int d\mathbf{r} \sum_{ij} w^{\alpha*}(\mathbf{r} - \mathbf{r}_i) b_i^{\alpha\dagger} h^{\alpha}(\mathbf{r}) w^{\alpha}(\mathbf{r} - \mathbf{r}_j) b_j^{\alpha} \\
 &\quad + \frac{1}{2} \sum_{\alpha\beta} \int d\mathbf{r} \int d\mathbf{r}' \sum_{ijkl} w^{\alpha*}(\mathbf{r} - \mathbf{r}_i) b_i^{\alpha\dagger} w^{\beta*}(\mathbf{r}' - \mathbf{r}_j) b_j^{\beta\dagger} \\
 &\quad \quad \quad \cdot v^{\alpha\beta}(\mathbf{r}, \mathbf{r}') w^{\beta}(\mathbf{r}' - \mathbf{r}_k) b_k^{\beta} w^{\alpha}(\mathbf{r} - \mathbf{r}_l) b_l^{\alpha} \quad (2.10) \\
 &= - \sum_{\alpha} \sum_{i \neq j} t_{ij}^{\alpha} b_i^{\alpha\dagger} b_j^{\alpha} - \sum_{\alpha} \sum_i \mu_i^{\alpha} b_i^{\alpha\dagger} b_i^{\alpha} \\
 &\quad + \frac{1}{2} \sum_{\alpha\beta} \sum_{ijkl} U_{ijkl}^{\alpha\beta} b_i^{\alpha\dagger} b_j^{\beta\dagger} b_k^{\beta} b_l^{\alpha},
 \end{aligned}$$

where

$$t_{ij}^{\alpha} \equiv - \int d\mathbf{r} w^{\alpha*}(\mathbf{r} - \mathbf{r}_i) h^{\alpha}(\mathbf{r}) w^{\alpha}(\mathbf{r} - \mathbf{r}_j), \quad (2.11)$$

$$\begin{aligned}
 \mu_i^{\alpha} &\equiv - \int d\mathbf{r} h^{\alpha}(\mathbf{r}) |w^{\alpha}(\mathbf{r} - \mathbf{r}_i)|^2 \\
 &\stackrel{(2.9)}{=} - \int d\mathbf{r} h^{\alpha}(\mathbf{r}) |w^{\alpha}(\mathbf{r})|^2 \equiv \mu^{\alpha} \in \mathbb{R},
 \end{aligned} \quad (2.12)$$

$$\begin{aligned}
 U_{ijkl}^{\alpha\beta} &\equiv \int d\mathbf{r} \int d\mathbf{r}' w^{\alpha*}(\mathbf{r} - \mathbf{r}_i) w^{\beta*}(\mathbf{r}' - \mathbf{r}_j) \\
 &\quad \cdot v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|) w^{\beta}(\mathbf{r}' - \mathbf{r}_k) w^{\alpha}(\mathbf{r} - \mathbf{r}_l),
 \end{aligned} \quad (2.13)$$

and where  $\mathbf{r}_i, \dots, \mathbf{r}_l$  denote the fixed positions of the lattice sites  $i, \dots, l$ , respectively, cf. Sec. 2.2. The first term of  $\mathcal{H}$  comprises contributions from hopping between two lattice sites; the second term is the self-energy of particles at every lattice site, with  $\mu^{\alpha}$  the chemical potential for particles of species  $\alpha$ ; and the final term is the interaction term, expressing interactions across as many as four lattice sites. It is evident that  $t_{ij}^{\alpha} = t_{ji}^{\alpha*}$ , and that  $U_{ijkl}^{\alpha\beta} = U_{lkji}^{\alpha\beta*} = U_{jilk}^{\beta\alpha}$ , the latter upon a relabeling of the integration variables.

For the remainder of this thesis, we will assume that there only be *nearest neighbor hopping* and *on-site interactions*. This may be achieved experimentally by increasing lattice depths to a point for which the overlap of non-neighboring Wannier functions is negligible, known as the *tight-binding limit*.

Thus,  $v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|)$  takes the form

$$v^{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|) = \gamma^{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}') \in \mathbb{R}, \quad (2.14)$$

where

$$\gamma^{\alpha\beta} = \gamma^{\beta\alpha} = \frac{2\pi(m^\alpha + m^\beta)a^{\alpha\beta}}{m^\alpha m^\beta}. \quad (2.15)$$

That is, the particles are subjected to mass-dependent point-interactions proportional to the intra- and inter-species  $s$ -wave scattering lengths  $a^{\alpha\beta}$  [1]. In addition, because the bosons reside on a periodic Bravais lattice, the dependency on lattice site positions is assumed only to be through the relative displacements

$$\boldsymbol{\delta}_{ji} \equiv \mathbf{r}_j - \mathbf{r}_i. \quad (2.16)$$

These assumptions amount to a considerably simpler  $\mathcal{H}$ ,

$$\begin{aligned} \mathcal{H} &= - \sum_{\alpha} \sum_{\langle i,j \rangle} t_{ij}^{\alpha} b_i^{\alpha\dagger} b_j^{\alpha} - \sum_{\alpha} \mu^{\alpha} \sum_i b_i^{\alpha\dagger} b_i^{\alpha} \\ &\quad + \frac{1}{2} \sum_{\alpha\beta} \sum_i U_{iiii}^{\alpha\beta} b_i^{\alpha\dagger} b_i^{\beta\dagger} b_i^{\beta} b_i^{\alpha} \\ &= - \sum_{\alpha} \sum_{\langle i,j \rangle} t_{ij}^{\alpha} b_i^{\alpha\dagger} b_j^{\alpha} - \sum_{\alpha} \mu^{\alpha} \sum_i b_i^{\alpha\dagger} b_i^{\alpha} \\ &\quad + \frac{1}{2} \sum_{\alpha\beta} U^{\alpha\beta} \sum_i b_i^{\alpha\dagger} b_i^{\beta\dagger} b_i^{\beta} b_i^{\alpha}, \end{aligned} \quad (2.17)$$

where  $\langle i, j \rangle$  denotes nearest neighbor lattice site indices, and

$$t_{ij}^{\alpha} = - \int d\mathbf{r} w^{\alpha*}(\mathbf{r}) h^{\alpha}(\mathbf{r}) w^{\alpha}(\mathbf{r} - \boldsymbol{\delta}_{ji}), \quad (2.18)$$

$$\begin{aligned} U_{iiii}^{\alpha\beta} &\stackrel{(2.14)}{=} \int d\mathbf{r} \int d\mathbf{r}' w^{\alpha*}(\mathbf{r} - \mathbf{r}_i) w^{\beta*}(\mathbf{r}' - \mathbf{r}_i) \\ &\quad \cdot \gamma^{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}') w^{\beta}(\mathbf{r}' - \mathbf{r}_i) w^{\alpha}(\mathbf{r} - \mathbf{r}_i) \\ &= \int d\mathbf{r} \gamma^{\alpha\beta} |w^{\alpha}(\mathbf{r})|^2 |w^{\beta}(\mathbf{r})|^2 \equiv U^{\alpha\beta} = U^{\beta\alpha} \in \mathbb{R}. \end{aligned} \quad (2.19)$$

The nearest neighbor displacement vectors  $\boldsymbol{\delta}_{\langle j,i \rangle}$  are

$$\boldsymbol{\delta}_{\langle j,i \rangle} \equiv \{\pm \mathbf{a}_1, \dots, \pm \mathbf{a}_{\ell}\}, \quad (2.20)$$

where  $\{\mathbf{a}_1, \dots, \mathbf{a}_n\}$  is the set of all  $n$  non-parallel nearest neighbor displacement vectors; the vectors in this set are by definition of equal magnitude. The hopping coupling  $t_{ij}^\alpha$  will be assumed to be real and equal for all nearest neighbor hoppings. Therefore, upon defining

$$t_{\langle i,j \rangle}^\alpha \equiv t^\alpha \in \mathbb{R}, \quad (2.21)$$

the expression for  $\mathcal{H}$  becomes

$$\begin{aligned} \mathcal{H} = & - \sum_{\alpha} t^\alpha \sum_{\langle i,j \rangle} b_i^{\alpha\dagger} b_j^\alpha - \sum_{\alpha} \mu^\alpha \sum_i b_i^{\alpha\dagger} b_i^\alpha \\ & + \frac{1}{2} \sum_{\alpha\beta} U^{\alpha\beta} \sum_i b_i^{\alpha\dagger} b_i^{\beta\dagger} b_i^\beta b_i^\alpha. \end{aligned} \quad (2.22)$$

Eq. (2.22) is the version of the *Bose–Hubbard model* that will be used in this thesis.  $t^\alpha$ ,  $\mu^\alpha$  and  $U^{\alpha\beta}$  will be assumed to be positive, meaning that hopping and increasing the number of particles in the system is energetically favorable, and that interactions are energetically unfavorable.

The behavior of an ultracold Bose gas is closely related to the momentum distribution of its constituent particles. Therefore, it is convenient to proceed further analyses in momentum space, by Fourier transforming the Hamiltonian (2.22). In terms of the basis  $\{A_{\mathbf{k}}^\alpha\}$  of operators annihilating particles of species  $\alpha$  and momentum  $k$ , the operators

$$b_i^\alpha = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} A_{\mathbf{k}}^\alpha e^{-i\mathbf{k}\cdot\mathbf{r}_i}. \quad (2.23)$$

The new operators  $A_{\mathbf{k}}^\alpha$  are readily shown to be bosonic: Using the inverse expression

$$A_{\mathbf{k}}^\alpha = \frac{1}{\sqrt{N_s}} \sum_i b_i^\alpha e^{i\mathbf{k}\cdot\mathbf{r}_i}, \quad (2.24)$$

one finds that

$$\begin{aligned} [A_{\mathbf{k}}^\alpha, A_{\mathbf{k}'}^{\beta\dagger}] &= \frac{1}{N_s} \sum_{ij} \left( b_i^{\alpha\dagger} b_j^{\beta\dagger} e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{i\mathbf{k}'\cdot\mathbf{r}_j} - b_j^{\beta\dagger} b_i^\alpha e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{i\mathbf{k}'\cdot\mathbf{r}_j} \right) \\ &= \frac{1}{N_s} \sum_{ij} [b_i^\alpha, b_j^{\beta\dagger}] e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{i\mathbf{k}'\cdot\mathbf{r}_j} \\ &= \delta^{\alpha\beta} \frac{1}{N_s} \sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} \\ &\stackrel{(2.27)}{=} \delta_{\mathbf{k}\mathbf{k}'} \delta^{\alpha\beta}. \end{aligned} \quad (2.25)$$

Now, inserting Eq. (2.23) into Eq. (2.22) leads to

$$\begin{aligned}
 \mathcal{H} = & -\frac{1}{N_s} \sum_{\alpha} t^{\alpha} \sum_{\langle i,j \rangle} \sum_{\mathbf{k}\mathbf{k}'} A_{\mathbf{k}}^{\alpha\dagger} e^{i\mathbf{k}\cdot\mathbf{r}_i} A_{\mathbf{k}'}^{\alpha} e^{-i\mathbf{k}'\cdot\mathbf{r}_j} \\
 & -\frac{1}{N_s} \sum_{\alpha} \mu^{\alpha} \sum_i \sum_{\mathbf{k}\mathbf{k}'} A_{\mathbf{k}}^{\alpha\dagger} e^{i\mathbf{k}\cdot\mathbf{r}_i} A_{\mathbf{k}'}^{\alpha} e^{-i\mathbf{k}'\cdot\mathbf{r}_i} \\
 & +\frac{1}{2N_s^2} \sum_{\alpha\beta} U^{\alpha\beta} \sum_i \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} A_{\mathbf{k}}^{\alpha\dagger} e^{i\mathbf{k}\cdot\mathbf{r}_i} A_{\mathbf{k}'}^{\beta\dagger} e^{i\mathbf{k}'\cdot\mathbf{r}_i} A_{\mathbf{p}}^{\beta} e^{-i\mathbf{p}\cdot\mathbf{r}_i} A_{\mathbf{p}'}^{\alpha} e^{-i\mathbf{p}'\cdot\mathbf{r}_i}.
 \end{aligned} \tag{2.26}$$

Applying the relation

$$\frac{1}{N_s} \sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} = \delta_{\mathbf{k},\mathbf{k}'}, \tag{2.27}$$

and using the fact that

$$e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{-i\mathbf{k}'\cdot\mathbf{r}_j} = e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{-i\mathbf{k}'\cdot(\mathbf{r}_j-\mathbf{r}_i+\mathbf{r}_i)} = e^{-i\mathbf{k}'\cdot\delta_{ji}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_i}, \tag{2.28}$$

Eq. (2.26) simplifies to

$$\begin{aligned}
 \mathcal{H} = & -\sum_{\alpha} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\langle i,j \rangle} t^{\alpha} e^{-i\mathbf{k}'\cdot\delta_{ji}} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\alpha} \left( \frac{1}{N_s} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_i} \right) \\
 & -\sum_{\alpha} \mu^{\alpha} \sum_{\mathbf{k}\mathbf{k}'} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\alpha} \left( \frac{1}{N_s} \sum_i e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_i} \right) \\
 & +\frac{1}{2N_s} \sum_{\alpha\beta} U^{\alpha\beta} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \left( \frac{1}{N_s} \sum_i e^{-i(\mathbf{p}+\mathbf{p}'-\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} \right) \\
 = & -\sum_{\alpha} \sum_{\mathbf{k}\mathbf{k}'} \underbrace{\left( \sum_{\delta \in \delta_{\langle i,j \rangle}} t^{\alpha} e^{-i\mathbf{k}'\cdot\delta} \right)}_{\equiv \epsilon_{\mathbf{k}}^{\alpha}} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\alpha} \underbrace{\left( \frac{1}{N_s} \sum_i e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_i} \right)}_{\delta_{\mathbf{k},\mathbf{k}'}} \\
 & -\sum_{\alpha} \mu^{\alpha} \sum_{\mathbf{k}\mathbf{k}'} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\alpha} \delta_{\mathbf{k},\mathbf{k}'} \\
 & +\frac{1}{2N_s} \sum_{\alpha\beta} U^{\alpha\beta} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'}
 \end{aligned} \tag{2.29}$$

$$\begin{aligned}
 \Rightarrow \mathcal{H} = & - \sum_{\mathbf{k}} \sum_{\alpha} (\epsilon_{\mathbf{k}}^{\alpha} + \mu^{\alpha}) A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^{\alpha} \\
 & + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}', \mathbf{p}+\mathbf{p}'},
 \end{aligned} \tag{2.30}$$

where

$$\begin{aligned}
 \epsilon_{\mathbf{k}}^{\alpha} & \equiv t^{\alpha} \sum_{\boldsymbol{\delta} \in \boldsymbol{\delta}_{\langle i,j \rangle}} e^{-i\mathbf{k} \cdot \boldsymbol{\delta}} \\
 & \stackrel{(2.20)}{=} t^{\alpha} \sum_n (e^{i\mathbf{k} \cdot \mathbf{a}_n} + e^{-i\mathbf{k} \cdot \mathbf{a}_n}) \\
 & = 2t^{\alpha} \sum_n \cos(\mathbf{k} \cdot \mathbf{a}_n).
 \end{aligned} \tag{2.31}$$

Eq. (2.30) is the expression for  $\mathcal{H}$  that will be used in the subsequent analysis. In the next section, the method by which the two bosonic particle species may be engineered to emulate the states of a spin- $\frac{1}{2}$  system in the presence of a synthetic spin-orbit coupling, is explored, and an analytic expression for the contribution to the Hamiltonian due to this coupling, is deduced.

## 2.4 Synthetic Spin–Orbit Coupling

### 2.4.1 Introduction and Experimental Realization

Spin–orbit coupling is a relativistic coupling between the spin and the orbital momentum of a particle. For an electron moving in an electrostatic potential, the SOC may be derived by taking the non-relativistic limit of the Dirac equation [49, 50]. Effectively, it may be viewed as an effect of changing the frame of reference: When an electron carrying a momentum  $\mathbf{p}$  moves through a static electric field  $\mathbf{E}$ , an effective magnetic field  $\mathbf{B}_{\text{eff}} \propto \mathbf{E} \times \mathbf{p}$  is induced in its rest frame, which in turn couples to its spin  $\mathbf{S} \propto \boldsymbol{\sigma}$  through the Zeeman interaction, producing a so-called *Rashba SOC*, an example of which is given in Eq. (2.32) [40, 50, 51]. For a gas of electrons constrained to a two-dimensional crystal lattice, Rashba SOC is attributed to broken *mirror* symmetry of the system, whereas another coupling, the Dresselhaus SOC, is



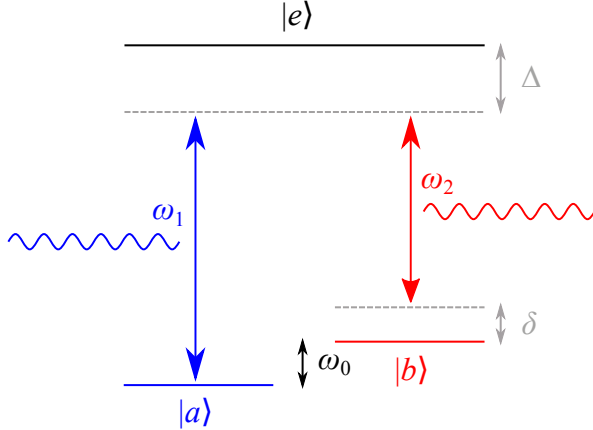
attributed to broken *inversion* symmetry [43]; however, this thesis will be concerned only with Rashba SOC.

Being a relativistic effect, unless the electrons are moving at sufficiently high velocities, or are subjected to sufficiently strong electric fields, natural SOC is typically of negligible impact. A more easily realizable, effectively spin-orbit coupled system, is that of a dilute Bose gas comprising two hyperfine states, coupled to each other and their momenta through Raman scattering and the Doppler shift. Such an experimentally realizable method was first proposed by J. Higbie *et al.* in Ref. [41]. In essence, one considers a dilute and uniform atomic Bose gas comprising two internal hyperfine states  $|a\rangle$  and  $|b\rangle$  with a relative difference in energy  $\hbar\omega_0$ , and an excited state  $|e\rangle$ , cf. Fig. 2.2. Two laser beams are directed at the gas: One laser beam carries a momentum  $\mathbf{k}_1$ , and a frequency  $\omega_1$  red-detuned<sup>3</sup> by an amount  $\Delta$  from the resonant frequency of the transition between the states  $|a\rangle$  and  $|e\rangle$ ; and the second laser beam carries a momentum  $\mathbf{k}_2$ , and a frequency  $\omega_2$  red-detuned by the same amount  $\Delta$  from the resonant frequency of the transition between the states  $|b\rangle$  and  $|e\rangle$ . The red-detuning  $\Delta$  ensures that the hyperfine states do not couple resonantly to the excited state; instead, photons inelastically scatter off the atoms in a two-photon Raman transition between internal states  $|a\rangle$  and  $|b\rangle$  via an intermediate energy level, by way of absorption and stimulated re-emission. In addition, another detuning  $\delta = (\omega_1 - \omega_2) - \omega_0$  of the transition frequencies leads to deviations from Raman resonance; this detuning depends on the atomic momenta through the Doppler shift, which leads to an altering of the laser frequencies in the rest frame of the respective atoms. As the absorption and re-emission of photons imparts a momentum transfer on the atoms, the combination of Raman scattering and the Doppler shift thus induces momentum dependent transitions between the two hyperfine states, the rate of which depends on the atomic momenta via the detuning  $\delta$ . This is effectively a synthetically spin-orbit coupled spin- $\frac{1}{2}$  system, offering flexible tuning of the coupling parameters. Since the atoms are bosonic—and therefore not subjected to fermionic constraints of a real spin- $\frac{1}{2}$  system, such as the Pauli exclusion principle—such a system gives rise to exotic and novel behavior: Notably, and in the interest of this thesis, such a synthetic coupling may induce non-zero momenta among condensed bosons. Variations of this method may be used to engineer both Rashba and Dresselhaus SOC, and enable a considerably more experimentally feasible study of

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<sup>3</sup>That is, adjusted to a lower frequency.

the effects of an SOC than by studying systems subjected to a natural SOC [43, 42].



**Figure 2.2:** Illustration of a mechanism by which a synthetic SOC may be induced. A Raman transition occurs between two hyperfine states  $|a\rangle$  and  $|b\rangle$  with a relative difference in energy  $\hbar\omega_0$ , via an intermediate energy level. Two photons of frequency  $\omega_1$  and  $\omega_2$  are absorbed and re-emitted; these are red-detuned from the resonant frequencies between the hyperfine states and the excited state  $|e\rangle$  by an amount  $\Delta$ , to suppress transitions to this state. Another detuning  $\delta$ , from Raman resonance, affects the transition rate between the hyperfine states, and depends on the atomic momenta through the Doppler effect. Thus, one achieves a coupling between the hyperfine states and their momenta.

## 2.4.2 Analytic Framework

In this section, an analytic expression for a synthetic SOC coupling the components of a two-component Bose gas on a Bravais lattice, is deduced. For a system of electrons moving through a static electric field  $\mathbf{E} \equiv E_0 \hat{\mathbf{z}}$ , the contribution to the Hamiltonian from a two-dimensional Rashba SOC takes the form [43, 47]

$$\mathcal{H}_{\text{SOC}} = \lambda_R(\sigma_x k_y - \sigma_y k_x), \quad (2.32)$$

where the  $\sigma_i$  are the Pauli spin matrices (2.1), and the precise form of the coupling strength  $\lambda_R$  is  $\lambda_R = e\hbar^2 E_0 / 4m_e^2 c^2$  [47], which will be assumed to

be non-negative. In Ref. [47, Sec. 3.2.1], S. Solli presents a heuristic two-dimensional generalization of spin-orbit coupling on a one-dimensional lattice presented by S. B. Sjømark in Ref. [52], which will be presented in this section, and applied to the subsequent analysis.

The component  $k_{\hat{\mathbf{a}}_n} \equiv \mathbf{k} \cdot \hat{\mathbf{a}}_n$  of  $\mathbf{k}$  along the direction  $\hat{\mathbf{a}}_n \equiv \mathbf{a}_n/|\mathbf{a}_n|$  of the non-parallel<sup>4</sup> nearest neighbor lattice vector  $\mathbf{a}_n$  is discretized such that

$$\begin{aligned} k_{\hat{\mathbf{a}}_n} &= -i \sum_i \left( b_i^\dagger b_{i+n} - b_i^\dagger b_{i-n} \right) \\ &= -i \sum_i \left( b_i^\dagger b_{i+n} - b_{i+n}^\dagger b_i \right), \end{aligned} \tag{2.33}$$

where the lower indices  $i \pm n$  refer to the lattice sites displaced by  $\pm \mathbf{a}_n$  relative to the site at  $\mathbf{r}_i$ , and

$$b_i \equiv \begin{pmatrix} b_i^\uparrow \\ b_i^\downarrow \end{pmatrix}. \tag{2.34}$$

A change in the summation variable  $i \rightarrow i+n$  was performed in the second equality in (2.33). Then

$$\begin{aligned} k_y &= \sum_n k_{\hat{\mathbf{a}}_n} \hat{\mathbf{a}}_n \cdot \hat{\mathbf{y}} \\ &= -i \sum_i \sum_n \left( b_i^\dagger b_{i+n} - b_{i+n}^\dagger b_i \right) (\hat{\mathbf{a}}_n \cdot \hat{\mathbf{y}}). \end{aligned} \tag{2.35}$$

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<sup>4</sup>That is,  $\mathbf{a}_n$  is one of the  $n$  mutually non-parallel nearest neighbor lattice vectors.

Inserting this into Eq. (2.32), the discretized  $\mathcal{H}_{\text{SOC}}$  becomes

$$\begin{aligned}
 \mathcal{H}_{\text{SOC}} &= i\lambda_R \sum_{\alpha\beta} \sum_i \sum_n \left( b_i^{\alpha\dagger} (-\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}})) b_{i+n}^\beta \right. \\
 &\quad \left. - b_{i+n}^{\alpha\dagger} (-\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}})) b_i^\beta \right) \\
 &= i\lambda_R \sum_{\alpha\beta} \sum_i \sum_n \left( b_i^{\alpha\dagger} (-\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}})) b_{i+n}^\beta \right. \\
 &\quad \left. - b_{i+n}^{\beta\dagger} (-\sigma_x^{\beta\alpha}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) + \sigma_y^{\beta\alpha}(\mathbf{a}_n \cdot \hat{\mathbf{x}})) b_i^\alpha \right) \\
 &= i\lambda_R \sum_{\alpha\beta} \sum_i \sum_n \left( b_i^{\alpha\dagger} (-\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}})) b_{i+n}^\beta \right. \\
 &\quad \left. - \text{H.c.} \right),^5
 \end{aligned} \tag{2.36}$$

where ‘‘H.c.’’ denotes the Hermitian conjugate of the preceding term, and the hermiticity  $\sigma_i^{\beta\alpha} = \sigma_i^{\alpha\beta*}$  of the Pauli matrices was used in the third equality.

As before, due to the close behavioral relationship between an ultracold Bose gas and the particle momentum distribution, it is of interest to perform further analyses in momentum space. Applying relation (2.23) to the expression (2.36) yields

$$\begin{aligned}
 \mathcal{H}_{\text{SOC}} &= i\lambda_R \sum_{\alpha\beta} \sum_i \sum_n \left( \left( \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} A_{\mathbf{k}}^{\alpha\dagger} e^{i\mathbf{k}\cdot\mathbf{r}_i} \right) \left( -\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) \right. \right. \\
 &\quad \left. \left. + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}}) \right) \left( \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}'} A_{\mathbf{k}'}^\beta e^{-i\mathbf{k}'\cdot(\mathbf{r}_i+\mathbf{a}_n)} \right) + \text{H.c.} \right) \\
 &\stackrel{(2.27)}{=} i\lambda_R \sum_{\mathbf{k}} \sum_{\alpha\beta} \sum_n \left( A_{\mathbf{k}}^{\alpha\dagger} \left( -\sigma_x^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{y}}) \right. \right. \\
 &\quad \left. \left. + \sigma_y^{\alpha\beta}(\mathbf{a}_n \cdot \hat{\mathbf{x}}) \right) A_{\mathbf{k}}^\beta e^{-i\mathbf{k}\cdot\mathbf{a}_n} + \text{H.c.} \right).
 \end{aligned} \tag{2.37}$$

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<sup>5</sup>This step in deducing a discretized expression for  $\mathcal{H}_{\text{SOC}}$  is heuristic, not rigorous. The Pauli matrices were implicitly moved inside products of vectors of operators in transitioning from the matricial expression (2.32) to the scalar expression (2.36). The final expression (2.36) is nevertheless a variation of the Kane–Mele model; the reader is referred to the 2005 paper by C. L. Kane *et al.* [53] for details.

Now, using the explicit expressions (2.1) for the Pauli matrices, and writing out the sum over spin indices, one finds that

$$\begin{aligned}
 \mathcal{H}_{\text{SOC}} &= \lambda_R \sum_{\mathbf{k}} \sum_n \left( A_{\mathbf{k}}^{\uparrow\uparrow} \left( -i\mathbf{a}_n \cdot \hat{\mathbf{y}} + \mathbf{a}_n \cdot \hat{\mathbf{x}} \right) \right. \\
 &\quad \left. \cdot A_{\mathbf{k}}^{\downarrow} \left( e^{-i\mathbf{k} \cdot \mathbf{a}_n} - e^{i\mathbf{k} \cdot \mathbf{a}_n} \right) + \text{H.c.} \right) \\
 &= \sum_{\mathbf{k}} \left( A_{\mathbf{k}}^{\uparrow\uparrow} \left( -2\lambda_R \sum_n \left( \mathbf{a}_n \cdot \hat{\mathbf{y}} + i\mathbf{a}_n \cdot \hat{\mathbf{x}} \right) \sin(\mathbf{k} \cdot \mathbf{a}_n) \right) \right. \\
 &\quad \left. \cdot A_{\mathbf{k}}^{\downarrow} + \text{H.c.} \right) \\
 &= \sum_{\mathbf{k}} \left( A_{\mathbf{k}}^{\uparrow\uparrow} s_{\mathbf{k}} A_{\mathbf{k}}^{\downarrow} + \text{H.c.} \right),
 \end{aligned} \tag{2.38}$$

where

$$s_{\mathbf{k}} \equiv -2\lambda_R \sum_n \left( \mathbf{a}_n \cdot \hat{\mathbf{y}} + i\mathbf{a}_n \cdot \hat{\mathbf{x}} \right) \sin(\mathbf{k} \cdot \mathbf{a}_n) \tag{2.39}$$

is the spin-orbit coupling.

The full momentum space expression for the Hamiltonian of a synthetically spin-orbit coupled, weakly interacting Bose gas on a Bravais lattice may now be obtained by adding the expression (2.38) to the Hamiltonian (2.30):

$$\begin{aligned}
 \mathcal{H} &= - \sum_{\mathbf{k}} \sum_{\alpha} (\epsilon_{\mathbf{k}}^{\alpha} + \mu^{\alpha}) A_{\mathbf{k}}^{\alpha\uparrow} A_{\mathbf{k}}^{\alpha} + \sum_{\mathbf{k}} \left( A_{\mathbf{k}}^{\uparrow\uparrow} s_{\mathbf{k}} A_{\mathbf{k}}^{\downarrow} + \text{H.c.} \right) \\
 &\quad + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}}^{\alpha\uparrow} A_{\mathbf{k}'}^{\beta\uparrow} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'} \\
 &= \sum_{\mathbf{k}} \left( A_{\mathbf{k}}^{\uparrow\uparrow} \right)^{\dagger} \begin{pmatrix} -\epsilon_{\mathbf{k}}^{\uparrow} - \mu^{\uparrow} & s_{\mathbf{k}} \\ s_{\mathbf{k}}^* & -\epsilon_{\mathbf{k}}^{\downarrow} - \mu^{\downarrow} \end{pmatrix} \begin{pmatrix} A_{\mathbf{k}}^{\uparrow\uparrow} \\ A_{\mathbf{k}}^{\downarrow} \end{pmatrix} \\
 &\quad + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}}^{\alpha\uparrow} A_{\mathbf{k}'}^{\beta\uparrow} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'} \\
 &= \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\uparrow} A_{\mathbf{k}}^{\beta} + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}}^{\alpha\uparrow} A_{\mathbf{k}'}^{\beta\uparrow} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'},
 \end{aligned} \tag{2.40}$$

where

$$\eta_{\mathbf{k}} = \begin{pmatrix} \eta_{\mathbf{k}}^{\uparrow\uparrow} & \eta_{\mathbf{k}}^{\uparrow\downarrow} \\ \eta_{\mathbf{k}}^{\downarrow\uparrow} & \eta_{\mathbf{k}}^{\downarrow\downarrow} \end{pmatrix} \equiv \begin{pmatrix} -\epsilon_{\mathbf{k}}^{\uparrow} - \mu^{\uparrow} & s_{\mathbf{k}} \\ s_{\mathbf{k}}^* & -\epsilon_{\mathbf{k}}^{\downarrow} - \mu^{\downarrow} \end{pmatrix} \quad (2.41)$$

is the spin basis single-particle coupling.

## 2.5 Synthetically Spin–Orbit Coupled, Non-Interacting Bose Gas

In this section, a brief exploration of the analytic behavior of a synthetically spin–orbit coupled, non-interacting, two-component Bose gas on a Bravais lattice is performed, using the expression for the synthetic SOC derived in the previous section. This is a precursor to the analysis of the weakly interacting case, which is the primary focus of this thesis. The Hamiltonian is

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta}. \quad (2.42)$$

In particular, we are interested in the behavior of the *quasi-particles* of the system, i.e. the collections of pseudospin particles that effectively behave as decoupled free particles. Mathematically, this amounts to finding a new basis of particle operators

$$\{B_{\mathbf{k}}^{\alpha}\}, \quad \alpha = \pm, \quad (2.43)$$

by a canonical transformation, such that

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{\alpha} \lambda_{\mathbf{k}}^{\alpha\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta}, \quad (2.44)$$

where

$$\lambda_{\mathbf{k}} = \begin{pmatrix} \lambda_{\mathbf{k}}^{++} & \lambda_{\mathbf{k}}^{+-} \\ \lambda_{\mathbf{k}}^{-+} & \lambda_{\mathbf{k}}^{--} \end{pmatrix} \equiv \begin{pmatrix} \lambda_{\mathbf{k}}^{+} & 0 \\ 0 & \lambda_{\mathbf{k}}^{-} \end{pmatrix}. \quad (2.45)$$

Additionally, the transformation should preserve the canonical commutation relation, such that

$$[B_{\mathbf{k}}^{\alpha}, B_{\mathbf{k}'}^{\beta\dagger}] = \delta_{\mathbf{k}\mathbf{k}'} \delta^{\alpha\beta}; \quad (2.46)$$

---

<sup>6</sup>These labels allude to the function of these species as pseudohelicity states, provided  $s_{\mathbf{k}} \neq 0$ , as will be justified later in this section.

that is, the resulting quasi-particles should be bosonic. An expression for  $\lambda_{\mathbf{k}}$  may be obtained by conventional diagonalization of the matrix (2.41):

$$\eta_{\mathbf{k}} = \mathcal{P}_{\mathbf{k}}^{-1} \mathcal{P}_{\mathbf{k}} \eta_{\mathbf{k}} \mathcal{P}_{\mathbf{k}}^{-1} \mathcal{P}_{\mathbf{k}} = \mathcal{P}_{\mathbf{k}}^{-1} \lambda_{\mathbf{k}} \mathcal{P}_{\mathbf{k}}, \quad (2.47)$$

where

$$\mathcal{P}_{\mathbf{k}} \equiv \begin{pmatrix} \chi_{\mathbf{k}}^+ & \chi_{\mathbf{k}}^- \end{pmatrix} \quad (2.48)$$

is the invertible diagonalizing matrix, the columns of which are orthonormalized eigenvectors  $\chi_{\mathbf{k}}^{\pm}$  of  $\eta_{\mathbf{k}}$ . Thus,

$$\begin{pmatrix} B_{\mathbf{k}}^+ \\ B_{\mathbf{k}}^- \end{pmatrix} = \mathcal{P}_{\mathbf{k}} \begin{pmatrix} A_{\mathbf{k}}^{\uparrow} \\ A_{\mathbf{k}}^{\downarrow} \end{pmatrix} = \chi_{\mathbf{k}}^+ A_{\mathbf{k}}^{\uparrow} + \chi_{\mathbf{k}}^- A_{\mathbf{k}}^{\downarrow}. \quad (2.49)$$

The eigenvalues  $\lambda_{\mathbf{k}}^{\pm}$  of  $\eta_{\mathbf{k}}$  are

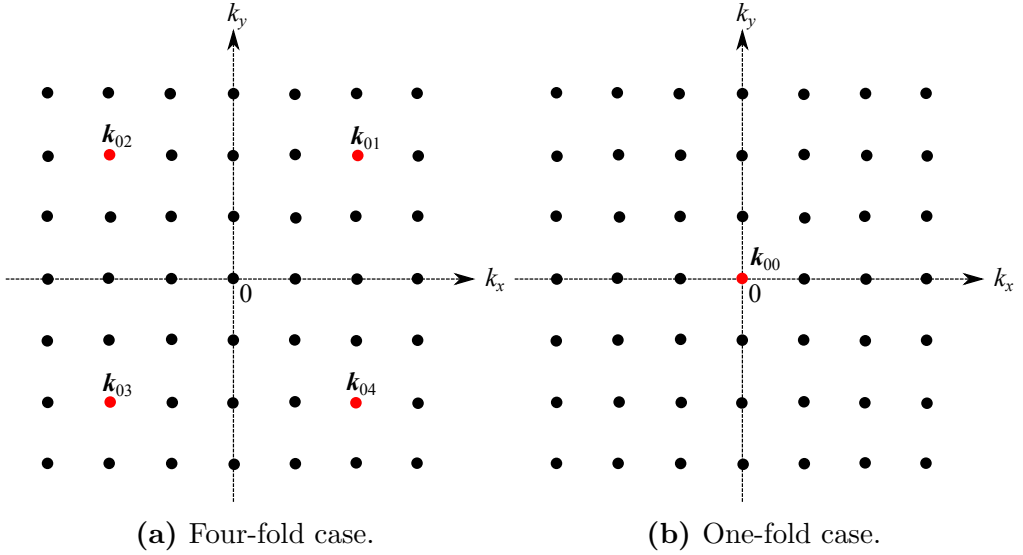
$$\eta_{\mathbf{k}} \chi_{\mathbf{k}}^{\pm} = \lambda_{\mathbf{k}}^{\pm} \chi_{\mathbf{k}}^{\pm} \Rightarrow (\eta_{\mathbf{k}} - \lambda_{\mathbf{k}}^{\pm}) \chi_{\mathbf{k}}^{\pm} = 0 \Rightarrow \det(\eta_{\mathbf{k}} - \lambda_{\mathbf{k}}^{\pm}) = 0 \quad (2.50)$$

$$\begin{aligned} \Rightarrow \lambda_{\mathbf{k}}^{\pm} &= \frac{1}{2} \left( -(\epsilon_{\mathbf{k}}^{\uparrow} + \epsilon_{\mathbf{k}}^{\downarrow}) - (\mu^{\uparrow} + \mu^{\downarrow}) \right) \\ &\pm \sqrt{4|s_{\mathbf{k}}|^2 + \left( (\epsilon_{\mathbf{k}}^{\uparrow} - \epsilon_{\mathbf{k}}^{\downarrow}) + (\mu^{\uparrow} - \mu^{\downarrow}) \right)^2}. \end{aligned} \quad (2.51)$$

These are the quasi-particle energy spectra. Observe that at  $\mathbf{k} = \mathbf{0}$ , there is a *Zeeman splitting*

$$\begin{aligned} \lambda_{\mathbf{0}}^+ - \lambda_{\mathbf{0}}^- &= \sqrt{4|s_{\mathbf{0}}|^2 + \left( (\epsilon_{\mathbf{0}}^{\uparrow} - \epsilon_{\mathbf{0}}^{\downarrow}) + (\mu^{\uparrow} - \mu^{\downarrow}) \right)^2} \\ &\stackrel{(2.39)}{=} \sqrt{\left( (\epsilon_{\mathbf{0}}^{\uparrow} - \epsilon_{\mathbf{0}}^{\downarrow}) + (\mu^{\uparrow} - \mu^{\downarrow}) \right)^2} \end{aligned} \quad (2.52)$$

of the energy bands, dependent on the differences in the no-SOC single-particle energies  $\epsilon_{\mathbf{0}}^{\uparrow} - \epsilon_{\mathbf{0}}^{\downarrow}$ , and in the chemical potentials  $\mu^{\uparrow} - \mu^{\downarrow}$ . Furthermore, within the first Brillouin zone, the  $\epsilon_{\mathbf{k}}^{\alpha}$  are minimal at  $\mathbf{k} = \mathbf{0}$ , while  $|s_{\mathbf{k}}|$  has its minima at  $\mathbf{k} \neq \mathbf{0}$ , cf. Eq. (2.31) and (2.39). Evidently, a sufficiently strong coupling strength  $\lambda_R$  may therefore displace the minima of the lowest energy band to non-zero values.



**Figure 2.3:** Momentum space illustration of a two-dimensional square lattice. The red points denote the possible ground state momenta  $\mathbf{k}_{0i}$ . Note that (a) is just one possible four-fold case, as the magnitude of the condensate momenta depends on the spin–orbit coupling strength.

Consider the case of the bosons residing on a *two-dimensional square lattice* of lattice constant  $a$ , such that  $\mathbf{a}_n = \{a\hat{\mathbf{x}}, a\hat{\mathbf{y}}\}$ . Furthermore, let pseudospin states be treated equally, i.e.

$$\mu^\uparrow = \mu^\downarrow \equiv \mu, \quad (2.53)$$

$$t^\uparrow = t^\downarrow \equiv t \quad (2.54)$$

$$\Rightarrow \epsilon_{\mathbf{k}}^\uparrow = \epsilon_{\mathbf{k}}^\downarrow \equiv \epsilon_{\mathbf{k}}, \quad (2.55)$$

such that there is no Zeeman splitting. Then

$$s_{\mathbf{k}} \stackrel{(2.39)}{=} -2\lambda_R(\sin(k_y a) + i \sin(k_x a)), \quad (2.56)$$

$$\epsilon_{\mathbf{k}} \stackrel{(2.31)}{=} 2t(\cos(k_x a) + \cos(k_y a)), \quad (2.57)$$

and the quasi-particle energy spectra reduce to

$$\lambda_{\mathbf{k}}^\pm = -\epsilon_{\mathbf{k}} - \mu \pm |s_{\mathbf{k}}|. \quad (2.58)$$



Treating  $k_x$  and  $k_y$  as continuous variables, the minima of  $\lambda_{\mathbf{k}}^-$  are readily found to occur at

$$k_x, k_y = \pm \frac{\arcsin\left(\frac{\lambda_R/t}{\sqrt{2+(\lambda_R/t)^2}}\right)}{a}, \quad (2.59)$$

from which it is clear that in this case, *any* non-zero  $\lambda_R$  induces one or more of four distinct non-zero momenta among ground state quasi-particles; see Fig. 2.3 and 2.4. The minimum value  $\lambda_0$  of  $\lambda_{\mathbf{k}}^-$  is given by  $\lambda_{\mathbf{k}}^-$  evaluated at either of these four points in  $k$ -space, and is equal to

$$\lambda_0 = -4t\sqrt{\frac{2\lambda_R^2}{t^2} + 1} - \mu. \quad (2.60)$$

The ground state energy cannot be negative, by the physical argument that the Hamiltonian (2.44) needs to be bounded from below. This may be solved as follows.  $\lambda_0$  may be subtracted from the energy spectra and treated as a contribution to the chemical potential as follows:

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \sum_{\alpha} \lambda_{\mathbf{k}}^{\alpha\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta} \\ &= \lambda_0 \sum_{\mathbf{k}} \sum_{\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta} + \sum_{\mathbf{k}} \sum_{\alpha} (\lambda_{\mathbf{k}}^{\alpha\alpha} - \lambda_0) B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta} \\ &= \lambda_0 N_a + \sum_{\mathbf{k}} \sum_{\alpha} \Delta\lambda_{\mathbf{k}}^{\alpha\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta}, \end{aligned} \quad (2.61)$$

where

$$N_a \equiv \sum_{\mathbf{k}} \sum_{\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta} \quad (2.62)$$

is the total number of quasi-particles in this particular system,<sup>7</sup> and

$$\Delta\lambda_{\mathbf{k}}^{\pm} \equiv \lambda_{\mathbf{k}}^{\pm} - \lambda_0; \quad (2.63)$$

the minimum value of the lower band  $\Delta\lambda_{\mathbf{k}}^-$  is now 0. If the ground state is dominant and comprises quasi-particles of non-zero momenta, one may neglect the contribution to the energy from the positive helicity quasi-particles

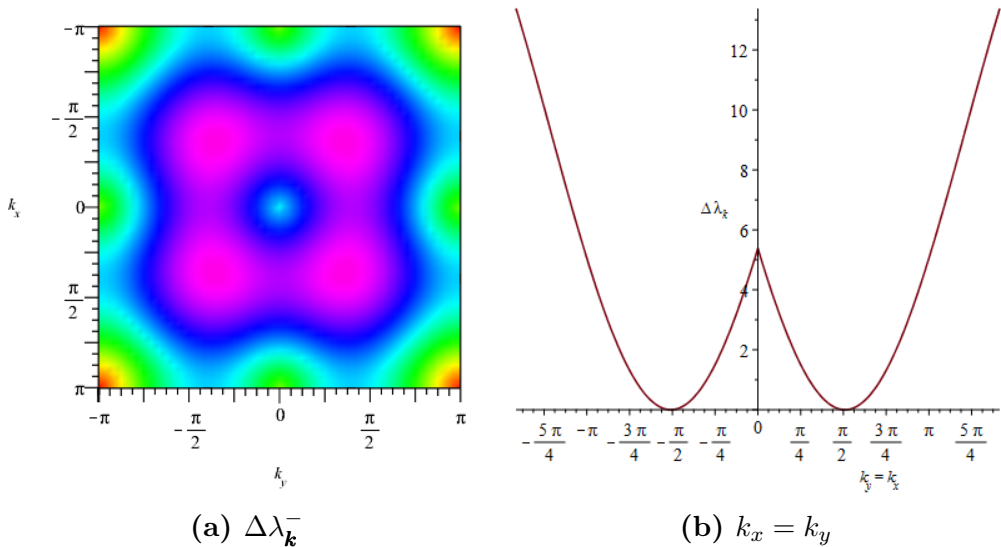
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<sup>7</sup>The total number of quasi-particles is in general *not* equal to the total number of real particles, cf. [14, Ch. 4.3].

carrying a ground state momentum, as these are four excited states associated with significantly higher energies than the ground state; cf. the expressions (2.58). In this case, since the lower energy band  $\Delta\lambda_{\mathbf{k}}^-$  by definition is zero at its minimum value, one may rewrite the final expression in (2.61) as

$$\mathcal{H} = \lambda_0 N_a + \sum_{\mathbf{k}}' \sum_{\alpha} \Delta\lambda_{\mathbf{k}}^{\alpha\alpha} B_{\mathbf{k}}^{\alpha\dagger} B_{\mathbf{k}}^{\beta}, \quad (2.64)$$

where the sum  $\sum_{\mathbf{k}}'$  excludes all ground state momenta.



**Figure 2.4:** Plots of the lowest energy band  $\Delta\lambda_{\mathbf{k}}^-$ —cf. Eq. (2.63)—associated with the quasi-particles in a spin-orbit coupled non-interacting Bose gas on a square lattice, with  $t = a = 1.0$  and  $\lambda_R = 3.0$ . In Fig. 2.4a, the regions of lowest energy are colored in pink, and the regions of highest energy, in red; cf. Fig. 2.4b, which shows the cross-section of Fig. 2.4a along the diagonal  $k_x = k_y$ . Note the four-fold symmetry in the band due to the symmetry of the lattice, and the displacement of the minima from the origin due to the SOC.

Furthermore, the eigenvectors  $\chi_{\mathbf{k}}^{\pm}$  of  $\eta_{\mathbf{k}}$  are found to be

$$\{\chi^{\pm}\} = \begin{cases} \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}, & s_{\mathbf{k}} = 0, \\ \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\gamma_{\mathbf{k}}} \\ 1 \end{pmatrix} \right\}, & s_{\mathbf{k}} \neq 0, \end{cases} \quad (2.65)$$

where

$$e^{-i\gamma_{\mathbf{k}}} \equiv \frac{s_{\mathbf{k}}}{|s_{\mathbf{k}}|}, \quad s_{\mathbf{k}} \neq 0 \wedge \gamma_{\mathbf{k}} \in [0, 2\pi). \quad (2.66)$$

Consequently, by Eq. (2.49), there is either no change in basis if  $s_{\mathbf{k}} = 0$ , or

$$\begin{pmatrix} B_{\mathbf{k}}^+ \\ B_{\mathbf{k}}^- \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\gamma_{\mathbf{k}}} (A_{\mathbf{k}}^{\uparrow} - A_{\mathbf{k}}^{\downarrow}) \\ A_{\mathbf{k}}^{\uparrow} + A_{\mathbf{k}}^{\downarrow} \end{pmatrix}, \quad (2.67)$$

if  $s_{\mathbf{k}} \neq 0$ . Alternatively, by an inversion,

$$\begin{pmatrix} A_{\mathbf{k}}^{\uparrow} \\ A_{\mathbf{k}}^{\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} B_{\mathbf{k}}^- + e^{i\gamma_{\mathbf{k}}} B_{\mathbf{k}}^+ \\ B_{\mathbf{k}}^- - e^{i\gamma_{\mathbf{k}}} B_{\mathbf{k}}^+ \end{pmatrix}, \quad (2.68)$$

if  $s_{\mathbf{k}} \neq 0$ . Inserting the expressions (2.67) into the requirement (2.46),  $B_{\mathbf{k}}^{\alpha}$  are readily confirmed to be bosonic operators:

$$\begin{aligned} [B_{\mathbf{k}}^{\alpha}, B_{\mathbf{k}'}^{\beta\dagger}] &\propto [(A_{\mathbf{k}}^{\uparrow} \pm A_{\mathbf{k}}^{\downarrow}), (A_{\mathbf{k}'}^{\uparrow} \mp A_{\mathbf{k}'}^{\downarrow})^{\dagger}] \\ &= [A_{\mathbf{k}}^{\uparrow}, A_{\mathbf{k}'}^{\uparrow\dagger}] - [A_{\mathbf{k}}^{\downarrow}, A_{\mathbf{k}'}^{\downarrow\dagger}] = 0, \quad \alpha \neq \beta, \end{aligned} \quad (2.69)$$

$$\begin{aligned} [B_{\mathbf{k}}^{\alpha}, B_{\mathbf{k}'}^{\alpha\dagger}] &= \frac{1}{2} \left( [(A_{\mathbf{k}}^{\uparrow} \pm A_{\mathbf{k}}^{\downarrow}), (A_{\mathbf{k}'}^{\uparrow} \pm A_{\mathbf{k}'}^{\downarrow})^{\dagger}] \right) \\ &= \frac{1}{2} \left( [A_{\mathbf{k}}^{\uparrow}, A_{\mathbf{k}'}^{\uparrow\dagger}] + [A_{\mathbf{k}}^{\downarrow}, A_{\mathbf{k}'}^{\downarrow\dagger}] \right) = \delta_{\mathbf{k}\mathbf{k}'}, \end{aligned} \quad (2.70)$$

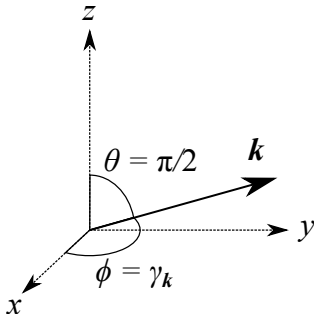
$$\Rightarrow [B_{\mathbf{k}}^{\alpha}, B_{\mathbf{k}'}^{\beta\dagger}] = \delta_{\mathbf{k}\mathbf{k}'} \delta^{\alpha\beta}. \quad (2.71)$$

Comparing the expressions (2.65) in the case of  $s_{\mathbf{k}} \neq 0$  to the general expressions for helicity eigenvectors,

$$\{\xi^+, \xi^-\} = \left\{ \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix}, \begin{pmatrix} -e^{-i\phi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} \right\}, \quad (2.72)$$

where  $\theta$  and  $\phi$  are the conventionally defined polar and azimuth angle with respect to the particle momentum vector, respectively, one realizes upon an

appropriate scaling of the eigenvectors  $\chi^\pm$ , that  $\gamma_{\mathbf{k}} = \phi$ , and  $\theta = \pi/2$ ; the latter in line with the choice of orientation of the imagined<sup>8</sup> static electric field  $\mathbf{E} \propto \hat{\mathbf{z}}$ ; see Fig. 2.5. The new basis (2.67) is thus identified as a *pseudohelicity* basis.



**Figure 2.5:** Illustration of the interpretation of  $\gamma_{\mathbf{k}}$  as the azimuth angle  $\phi$  with respect to the particle momentum  $\mathbf{k}$ . The polar angle  $\theta$  is fixed and equal to  $\pi/2$ .

## 2.6 Weakly Interacting Bose Gas: The Bogoliubov Transformation

In this section, we investigate the behavior of a *single-component* weakly interacting Bose gas tightly bound to a Bravais lattice, and, in the process, review the *Bogoliubov transformation*. This system is described by the Hamiltonian (2.30) upon neglecting pseudospin indices:

$$\begin{aligned} \mathcal{H} = & - \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + \mu) A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \\ & + \frac{U}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} A_{\mathbf{k}}^\dagger A_{\mathbf{k}'}^\dagger A_{\mathbf{p}} A_{\mathbf{p}'} \delta_{\mathbf{k}+\mathbf{k}', \mathbf{p}+\mathbf{p}'}, \end{aligned} \quad (2.73)$$

where  $\mu$ ,  $U$  and  $\epsilon_{\mathbf{k}}$  are given by Eq. (2.12), (2.19) and (2.31), respectively, neglecting pseudospin indices; and  $A_{\mathbf{k}}$  is an annihilation operator for a boson of momentum  $\mathbf{k}$ . Specifically, we will deduce expressions for the quasi-particle

<sup>8</sup>Recall that these calculations are concerned with a bosonic pseudospin- $\frac{1}{2}$  system subjected to a synthetic SOC, modeled to emulate a system of electrons subjected to an SOC induced by movement in a static electric field  $\mathbf{E} = E_0 \hat{\mathbf{z}}$ .

operators, as well as the quasi-particle energy spectra, which will be used to explore the phenomenon of *ground state depletion*. This is what was done by D. van Oosten *et al.* in Ref. [46], to which the reader is referred for details, and on which the calculations in this section are largely based.

When the Bose gas is cooled significantly below the critical temperature for which Bose–Einstein condensation occurs,<sup>9</sup> the ground state—i.e. the  $\mathbf{k} = \mathbf{0}$  mode—may be assumed to be dominant, provided the ground state depletion is not too severe.<sup>10</sup> Thus, we may neglect terms in  $\mathcal{H}$  that are trilinear and quadrilinear in excitation operators:

$$\mathcal{H} \approx \mathcal{H}'_0 + \mathcal{H}'_2, \quad (2.74)$$

where

$$\mathcal{H}'_0 \equiv -(\epsilon_0 + \mu) A_0^\dagger A_0 + \frac{U}{2N_s} A_0^\dagger A_0^\dagger A_0 A_0, \quad (2.75)$$

$$\begin{aligned} \mathcal{H}'_2 \equiv & - \sum'_{\mathbf{k}} (\epsilon_{\mathbf{k}} + \mu) A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \\ & + \frac{U}{2N_s} \sum'_{\mathbf{k}} \left( A_0^\dagger A_0^\dagger A_{\mathbf{k}} A_{-\mathbf{k}} + 4A_0^\dagger A_{\mathbf{k}}^\dagger A_{\mathbf{k}} A_0 + A_{\mathbf{k}}^\dagger A_{-\mathbf{k}}^\dagger A_0 A_0 \right), \end{aligned} \quad (2.76)$$

where the sum  $\sum'_{\mathbf{k}}$  excludes  $\mathbf{k} = \mathbf{0}$ . This is the first step of the *Bogoliubov approach*. Note that due to conservation of momentum, i.e. the factor  $\delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'}$  in Eq. (2.73), there are no terms in  $\mathcal{H}$  that are linear in excitation operators, since e.g.  $\mathbf{k} = \mathbf{k}' = \mathbf{p} = \mathbf{0}$  would imply that also  $\mathbf{p}' = \mathbf{0}$ .

Now, the *Bogoliubov prescription* amounts to substituting the condensate operators  $A_0$  with an expectation value  $a_0$  plus a *small* fluctuation  $\delta A_0$ :

$$A_0 \longrightarrow a_0 + \delta A_0. \quad (2.77)$$

Here,  $a_0$  is a *c*-number and a mean field parameter, and  $\delta A_0$  is an operator. In the literature, including in Ref. [46],  $a_0$  is usually taken to be real and equal to the square root of the condensate particle number, i.e.  $\sqrt{N_0}$ ; however, for this thesis, we will let

$$a_0 \equiv \sqrt{N_0} e^{-i\theta_0} \in \mathbb{C}; \quad (2.78)$$

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<sup>9</sup>Here, it is implicitly assumed that Bose–Einstein condensation *does* occur.

<sup>10</sup>The meaning of this will be specified later in this section, after the concept of ground state depletion has been covered.

that is, though the modulus is still  $\sqrt{N_{\mathbf{0}}} \in \mathbb{R}$ ,  $a_{\mathbf{0}}$  may also carry a complex phase factor parameterized by the angle  $\theta_{\mathbf{0}} \in [0, 2\pi)$ . In accordance with Ch. 4 of H. Bruus *et al.* [54], the mean field parameters  $N_{\mathbf{0}}$  and  $\theta_{\mathbf{0}}$  may be determined by solving a set of self-consistent equations, *or*, equivalently, by minimizing the free energy  $F$  with respect to these parameters; the latter approach will be employed in this thesis. Observe that in fixing  $a_{\mathbf{0}}$ , and by extension the phase  $\theta_{\mathbf{0}}$ , the global  $U(1)$  symmetry of the Hamiltonian (2.5) with respect to the phase of the field operators, is formally broken, which in turn renders the ground state particle number non-conserved; in physical terms, one is effectively treating the condensate as a particle reservoir [14, Ch. 2.2].  $a_{\mathbf{0}}$  is a local *order parameter*<sup>11</sup> that characterizes the Bose–Einstein condensate phase.

Inserting Eq. (2.77) and (2.78) into Eq. (2.74), one finds that

$$\mathcal{H} \approx \mathcal{H}_0 + \mathcal{H}_{(1)} + \mathcal{H}_2, \quad (2.79)$$

where

$$\mathcal{H}_0 \equiv -(\epsilon_{\mathbf{0}} + \mu) N_{\mathbf{0}} + \frac{U}{2N_s} N_{\mathbf{0}}^2, \quad (2.80)$$

$$\mathcal{H}_{(1)} \equiv \left( -\epsilon_{\mathbf{0}} - \mu + \frac{U}{N_s} N_{\mathbf{0}} \right) \sqrt{N_{\mathbf{0}}} \left( e^{i\theta_{\mathbf{0}}} \delta A_{\mathbf{0}} + e^{-i\theta_{\mathbf{0}}} \delta A_{\mathbf{0}}^\dagger \right), \quad (2.81)$$

$$\begin{aligned} \mathcal{H}_2 \equiv & - \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + \mu) A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \\ & + \frac{U}{2N_s} N_{\mathbf{0}} \sum_{\mathbf{k}} \left( e^{2i\theta_{\mathbf{0}}} A_{\mathbf{k}} A_{-\mathbf{k}} + 4A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + e^{-2i\theta_{\mathbf{0}}} A_{\mathbf{k}}^\dagger A_{-\mathbf{k}}^\dagger \right). \end{aligned} \quad (2.82)$$

Observe that the sums over  $\mathbf{k}$  in the expression for  $\mathcal{H}_2$  are *unconstrained*, i.e. *including*  $\mathbf{k} = \mathbf{0}$ ; implicitly, we redefined

$$\delta A_{\mathbf{0}} \equiv A_{\mathbf{0}}, \quad (2.83)$$

such that  $A_{\mathbf{0}}$  hereafter refers to the zero-mode fluctuation about the expectation value  $a_{\mathbf{0}}$ . Now, because the free energy  $F$  is assumed to be minimal with

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<sup>11</sup>An order parameter characterizes a feature of order in a phase, and is interlinked with breaking of symmetries. What parameters constitute a measure of order may be highly non-trivial [55]. Note that the idea of relating Bose–Einstein condensation to spontaneous symmetry breaking is not entirely uncontroversial; A. J. Leggett expands on his objections in Ref. [21], in particular in Ch. III.D.

respect to the number of condensed particles  $N_{\mathbf{0}}$ ,  $\mathcal{H}_{(1)}$  must be zero, as it comprises all terms linear in zero-mode fluctuations. From this one deduces the expression for the chemical potential:

$$\mu = -\epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}}. \quad (2.84)$$

Treating  $\mu$  as an input parameter, one may immediately deduce that the expression for the number of condensed particles per lattice site is

$$\frac{N_{\mathbf{0}}}{N_s} = \frac{\epsilon_{\mathbf{0}} + \mu}{U}. \quad (2.85)$$

Now, inserting Eq. (2.84) into Eq. (2.79), and using

$$A_{\mathbf{k}}^\dagger A_{\mathbf{k}} = \frac{1}{2} \left( A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + A_{\mathbf{k}} A_{\mathbf{k}}^\dagger - 1 \right) \quad (2.86)$$

as well as  $\epsilon_{-\mathbf{k}} \stackrel{(2.31)}{=} \epsilon_{\mathbf{k}}$ , one may write the Hamiltonian (2.79) as

$$\begin{aligned} \mathcal{H} &= -\frac{U}{2N_s} N_{\mathbf{0}}^2 - \frac{1}{2} \sum_{\mathbf{k}} \left( -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} \right) \\ &+ \frac{1}{2} \sum_{\mathbf{k}} \begin{pmatrix} A_{\mathbf{k}} \\ A_{-\mathbf{k}}^\dagger \end{pmatrix}^\dagger \begin{pmatrix} -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} & \frac{U}{N_s} N_{\mathbf{0}} e^{2i\theta_{\mathbf{0}}} \\ \frac{U}{N_s} N_{\mathbf{0}} e^{-2i\theta_{\mathbf{0}}} & -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} \end{pmatrix} \begin{pmatrix} A_{\mathbf{k}} \\ A_{-\mathbf{k}}^\dagger \end{pmatrix} \\ &\equiv \tilde{\mathcal{H}}_0 + \frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}}^\dagger \mathcal{M} A_{\mathbf{k}}, \end{aligned} \quad (2.87)$$

where

$$\tilde{\mathcal{H}}_0 \equiv -\frac{U}{2N_s} N_{\mathbf{0}}^2 - \frac{1}{2} \sum_{\mathbf{k}} \left( -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} \right), \quad (2.88)$$

$$\mathbf{A}_{\mathbf{k}} \equiv \begin{pmatrix} A_{\mathbf{k}} \\ A_{-\mathbf{k}}^\dagger \end{pmatrix}, \quad (2.89)$$

$$\mathcal{M} \equiv \begin{pmatrix} -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} & \frac{U}{N_s} N_{\mathbf{0}} e^{2i\theta_{\mathbf{0}}} \\ \frac{U}{N_s} N_{\mathbf{0}} e^{-2i\theta_{\mathbf{0}}} & -\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{0}} + \frac{U}{N_s} N_{\mathbf{0}} \end{pmatrix}. \quad (2.90)$$

In order to find the quasi-particle operators and excitation spectra, one must diagonalize the Hamiltonian (2.87) such that

$$\mathcal{H} = \tilde{\mathcal{H}}_0 + \frac{1}{2} \sum_{\mathbf{k}} \hbar\omega(\mathbf{k}) \left( D_{\mathbf{k}}^\dagger D_{\mathbf{k}} + \frac{1}{2} \right), \quad (2.91)$$

where  $D_{\mathbf{k}}$  is an annihilation operator for a quasi-particle of momentum  $\mathbf{k}$ , and  $\hbar\omega(\mathbf{k})$  is the corresponding quasi-particle energy spectrum.  $D_{\mathbf{k}}$  may be deduced by using the *Bogoliubov transformation*, named after N. N. Bogoliubov, who first applied this procedure in a paper published in 1947 to describe superfluidity in a non-ideal Bose gas [56], and later, in 1958, generalized the procedure in order to find solutions to the then recently developed BCS theory of superconductivity [57]; the generalized method is what is presented in the following. In the Bogoliubov approach, one postulates that one may perform a canonical transformation such that

$$\begin{pmatrix} A_{\mathbf{k}} \\ A_{-\mathbf{k}}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^* & v_{\mathbf{k}} \\ v_{\mathbf{k}}^* & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} D_{\mathbf{k}} \\ D_{-\mathbf{k}}^\dagger \end{pmatrix}. \quad (2.92)$$

Inserting this into Eq. (2.5) and demanding that the resulting Hamiltonian be on the form (2.91), one finds that the coefficients of the off-diagonal terms in the new basis must be zero, i.e.

$$(u_{\mathbf{k}}^2 e^{2i\theta_0} + v_{\mathbf{k}}^2 e^{-2i\theta_0}) \frac{U}{N_s} N_0 + 2u_{\mathbf{k}} v_{\mathbf{k}} \left( -\epsilon_{\mathbf{k}} + \epsilon_0 + \frac{U}{N_s} N_0 \right) = 0, \quad (2.93)$$

and that the diagonal terms must be equal to  $\hbar\omega(\mathbf{k})$ , i.e.

$$\begin{aligned} & (|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2) \left( -\epsilon_{\mathbf{k}} + \epsilon_0 + \frac{U}{N_s} N_0 \right) \\ & + (u_{\mathbf{k}} v_{\mathbf{k}}^* e^{2i\theta_0} + u_{\mathbf{k}}^* v_{\mathbf{k}} e^{-2i\theta_0}) \frac{U}{N_s} N_0 = \hbar\omega(\mathbf{k}). \end{aligned} \quad (2.94)$$

The canonical transformation should preserve the canonical commutation relation, implying

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1; \quad (2.95)$$

that is, the resulting quasi-particles of the system should be bosonic. Solving these equations for  $\hbar\omega(\mathbf{k})$ ,  $|u_{\mathbf{k}}|^2$  and  $|v_{\mathbf{k}}|^2$  yields

$$\hbar\omega(\mathbf{k}) = \sqrt{\left( -\epsilon_{\mathbf{k}} + \epsilon_0 \right) \left( -\epsilon_{\mathbf{k}} + \epsilon_0 + 2\frac{U}{N_s} N_0 \right)}, \quad (2.96)$$

$$|v_{\mathbf{k}}|^2 = |u_{\mathbf{k}}|^2 - 1 = \frac{1}{2} \left( \frac{-\epsilon_{\mathbf{k}} + \epsilon_0 + \frac{U}{N_s} N_0}{\hbar\omega(\mathbf{k})} - 1 \right). \quad (2.97)$$



The quasi-particle energy spectrum possesses two significant asymptotic features: a) Since  $\epsilon_{\mathbf{k}}$ , as given by Eq. (2.31) upon neglecting the pseudospin index, is asymptotically quadratic in  $|\mathbf{k}|$  as  $|\mathbf{k}| \rightarrow \mathbf{0}$ , the energy spectrum is asymptotically *linear* in  $|\mathbf{k}|$ —i.e. phonon-like—as  $|\mathbf{k}| \rightarrow \mathbf{0}$ ; and b) the energy spectrum approaches that of bosons in a non-interacting system, i.e.  $\hbar\omega(\mathbf{k}) \rightarrow -\epsilon_{\mathbf{k}} + \epsilon_0$ , as  $|\mathbf{k}|$  approaches the boundary of the first Brillouin zone.

Now, we turn our attention to the phenomenon of *ground state depletion*. The total number of particles  $N$  is given by

$$\begin{aligned}
 N &= N_0 + \sum'_{\mathbf{k}} \langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle \\
 &\stackrel{(2.92)}{=} N_0 + \sum'_{\mathbf{k}} \left\langle \left( u_{\mathbf{k}}^* D_{\mathbf{k}} - v_{\mathbf{k}} D_{-\mathbf{k}}^\dagger \right)^\dagger \left( u_{\mathbf{k}}^* D_{\mathbf{k}} - v_{\mathbf{k}} D_{-\mathbf{k}}^\dagger \right) \right\rangle \\
 &= N_0 + \sum'_{\mathbf{k}} \left( |u_{\mathbf{k}}|^2 \langle D_{\mathbf{k}}^\dagger D_{\mathbf{k}} \rangle - u_{\mathbf{k}} v_{\mathbf{k}} \langle D_{\mathbf{k}}^\dagger D_{-\mathbf{k}}^\dagger \rangle \right. \\
 &\quad \left. - u_{\mathbf{k}}^* v_{\mathbf{k}}^* \langle D_{\mathbf{k}} D_{-\mathbf{k}} \rangle + |v_{\mathbf{k}}|^2 \langle D_{-\mathbf{k}} D_{-\mathbf{k}}^\dagger \rangle \right) \\
 &= N_0 + \sum'_{\mathbf{k}} \left( \left( |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 \right) \langle D_{\mathbf{k}}^\dagger D_{\mathbf{k}} \rangle + |v_{\mathbf{k}}|^2 \right),
 \end{aligned} \tag{2.98}$$

where the marked sum excludes  $\mathbf{k} = \mathbf{0}$ , and the property that  $\mathcal{H}$  is diagonal with respect to the new bosonic basis defined by  $D_{\mathbf{k}}$  and  $D_{-\mathbf{k}}^\dagger$ , was used to cancel off-diagonal terms in the third to last equality. Furthermore, due to the property of diagonality, the quantity  $\langle D_{\mathbf{k}}^\dagger D_{\mathbf{k}} \rangle$  is the Bose–Einstein distribution;

$$N = N_0 + \sum'_{\mathbf{k}} \left( \frac{|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2}{e^{\beta\hbar\omega(\mathbf{k})} - 1} + |v_{\mathbf{k}}|^2 \right), \tag{2.99}$$

where

$$\beta \equiv \frac{1}{k_B T}, \tag{2.100}$$

and  $T$  is the temperature of the system. At zero  $T$ , the number of condensed particles is therefore

$$N_0 = N - \sum'_{\mathbf{k}} |v_{\mathbf{k}}|^2. \tag{2.101}$$

Observe the generally non-zero quantity subtracted from the total number of particles. Evidently, introducing weak, two-body scattering interactions to the single-component Bose gas has led to a depletion of the ground state, even at zero temperature. For a plot of the condensate fraction  $N_0/N$  as a function of the interaction strength  $U$  relative to the hopping coupling  $t$ , see Fig. 1 in Ref. [46]. Note by inspection of Eq. (2.97) and (2.101) that  $U/t \gg 1$  leads to a severe depletion of the ground state, in which case the assumption preceding Eq. (2.79) that the ground state is dominant, does no longer hold true. As noted by D. van Oosten *et al.* in Ref. [46], the system is expected to be in the Mott insulator phase when  $U/t \gg 1$ , and the present mean field approach fails to describe this phase due to the neglect of trilinear and quadrilinear terms in excitation operators that lead to Eq. (2.79); for this reason, this analysis is restricted to the superfluid phase, which is expected to occur for  $U/t \ll 1$ .

### 2.6.1 The Free Energy

The final quantity that remains to be addressed is the variational parameter  $\theta_0$ . As was elaborated below Eq. (2.78), the free energy  $F$  needs to be minimized with respect to this in order to determine its value [54]. In this section, a general expression for  $F$  is derived and applied. The derivation below is based on the one presented by S. Solli in Ref. [47], with some adjustments.

The diagonalized Hamiltonian  $\mathcal{H}$  is assumed to be on the form

$$\mathcal{H} = \tilde{\mathcal{H}}_0 + \frac{1}{2} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) \left( C_{\mathbf{k}\sigma}^{\dagger} C_{\mathbf{k}\sigma} + \frac{1}{2} \right), \quad (2.102)$$

where  $C_{\mathbf{k}\sigma}$  constitutes a basis of bosonic quasi-particle operators for which  $\mathcal{H}$  is diagonal,  $\sigma$  labels the branch, and the quantity  $\tilde{\mathcal{H}}_0$  comprises additional operator-independent terms. Let  $|\tilde{N}_m\rangle \equiv \prod_{i=1}^m |N_i\rangle$ ,  $N_i \equiv N_{\mathbf{k}\sigma} \equiv C_{\mathbf{k}\sigma}^{\dagger} C_{\mathbf{k}\sigma}$ , be

a many-particle Fock basis. The partition function  $Z$  is then

$$\begin{aligned}
 Z &= \text{tr} (e^{-\beta\mathcal{H}}) \\
 &= \sum_m \langle \tilde{N}_m | e^{-\beta\mathcal{H}} | \tilde{N}_m \rangle \\
 &\stackrel{(2.102)}{=} e^{-\beta\tilde{\mathcal{H}}_0} \exp \left( -\frac{\beta}{4} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) \right) \\
 &\quad \cdot \sum_m \langle \tilde{N}_m | \exp \left( -\frac{\beta}{2} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) N_{\mathbf{k}\sigma} \right) | \tilde{N}_m \rangle \\
 &= e^{-\beta\tilde{\mathcal{H}}_0} \exp \left( -\frac{\beta}{4} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) \right) \prod_{\mathbf{k}\sigma} \sum_{N_{\mathbf{k}\sigma}} \exp \left( -\frac{\beta}{2} \hbar\omega_{\sigma}(\mathbf{k}) N_{\mathbf{k}\sigma} \right) \\
 &= e^{-\beta\tilde{\mathcal{H}}_0} \exp \left( -\frac{\beta}{4} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) \right) \prod_{\mathbf{k}\sigma} \frac{1}{1 - \exp \left( -\frac{\beta}{2} \hbar\omega_{\sigma}(\mathbf{k}) \right)}.
 \end{aligned} \tag{2.103}$$

$F$  is thus

$$\begin{aligned}
 F &= -\frac{1}{\beta} \ln Z \\
 &= \tilde{\mathcal{H}}_0 + \frac{1}{4} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}) + \frac{1}{\beta} \sum_{\mathbf{k}}' \sum_{\sigma} \ln \left( 1 - \exp \left( -\frac{\beta}{2} \hbar\omega_{\sigma}(\mathbf{k}) \right) \right) \\
 &\xrightarrow{\beta \rightarrow \infty} \tilde{\mathcal{H}}_0 + \frac{1}{4} \sum_{\mathbf{k}}' \sum_{\sigma} \hbar\omega_{\sigma}(\mathbf{k}),
 \end{aligned} \tag{2.104}$$

where the final line expresses the limit of  $T \rightarrow 0$ . Furthermore, for a pure condensate, for which  $\mathcal{H} = \mathcal{H}_0$ , where the quantity  $\mathcal{H}_0$  is operator-independent,  $F$  is simply

$$F = \mathcal{H}_0. \tag{2.105}$$

Upon substituting the quantities in Eq. (2.104) for the appropriate expressions given by Eq. (2.88) and (2.96), one finds that  $F$  is independent of  $\theta_0$ . It may therefore be fixed to any value in its range; the conventional choice in the literature is  $\theta_0 = 0$ . Note that this trivial relationship between the phase and the free energy needs not be the case in general, in particular regarding the system under consideration in Ch. 3.

## 2.7 Generalized Diagonalization Procedure<sup>12</sup>

We proceed to review and develop a diagonalization method that generalizes the Bogoliubov procedure presented in Sec. 2.6. The contents of this section are largely based on the theory developed by C. Tsallis in Ref. [58] and by D. van Hemmen in Ref. [59], and will only be of importance for the summary and outlook presented in Ch. 6 at the end of this thesis.

Let

$$\mathcal{J} \equiv \text{diag}(\underbrace{1, 1, \dots, 1}_n, \underbrace{-1, \dots, -1, -1}_n), \quad (2.106)$$

and let  $\mathbf{A} \equiv (A_1 \ A_2 \ \dots \ A_n \ A_1^\dagger \ A_2^\dagger \ \dots \ A_n^\dagger)^T$ , where the  $A_i$  are  $n$  bosonic field operators, i.e.

$$[\mathbf{A}, \mathbf{A}^\dagger] = \mathcal{J}. \quad (2.107)$$

Now, in diagonalizing a general Hamiltonian  $\mathcal{H}$  that may be written in terms of bilinear products of these  $n$  bosonic operators, one finds that

$$\begin{aligned} \mathcal{H} &\equiv \mathbf{A}^\dagger \mathcal{M} \mathbf{A} = \mathbf{A}^\dagger (\mathcal{J} (\mathcal{T}^{-1} (\mathcal{J} \mathcal{J}) \mathcal{T}) \mathcal{J}) \mathcal{M} (\mathcal{T}^{-1} \mathcal{T}) \mathbf{A} \\ &= (\mathbf{A}^\dagger (\mathcal{J} \mathcal{T}^{-1} \mathcal{J})) (\mathcal{J} \mathcal{T} \mathcal{J} \mathcal{M} \mathcal{T}^{-1}) (\mathcal{T} \mathbf{A}) \\ &\equiv \mathbf{C}^\dagger \mathcal{J} \Omega \mathbf{C} \end{aligned} \quad (2.108)$$

where  $\mathcal{M}$  is a  $2n$ -by- $2n$  matrix comprising the coefficients in  $\mathcal{H}$  for every bilinear product; and  $\Omega$  is the diagonalized  $2n$ -by- $2n$  matrix, provided the  $2n$ -by- $2n$  transformation matrix  $\mathcal{T}$  diagonalizes  $\mathcal{J} \mathcal{M}$ , i.e.

$$\mathcal{T} \mathcal{J} \mathcal{M} \mathcal{T}^{-1} = \Omega, \quad (2.109)$$

and  $\mathbf{C}^\dagger$  is the adjoint of  $\mathbf{C}$ , i.e.

$$\mathcal{T}^\dagger = \mathcal{J} \mathcal{T}^{-1} \mathcal{J} \quad \Leftrightarrow \quad \mathcal{T}^\dagger \mathcal{J} \mathcal{T} = \mathcal{J}. \quad (2.110)$$

This last equation is equivalent to requiring that the resulting quasi-particles described by  $\mathbf{C}$  be bosons: If  $\mathbf{C} = \mathbf{A}^\dagger \mathcal{T}$  and  $\mathbf{C}^\dagger = \mathcal{T}^\dagger \mathbf{A}$ , then demanding that the boson commutation relation holds for  $\mathbf{C}$  implies

$$\mathcal{J} = [\mathbf{C}, \mathbf{C}^\dagger] = \mathcal{T}^\dagger [\mathbf{A}, \mathbf{A}^\dagger] \mathcal{T} \stackrel{(2.107)}{=} \mathcal{T}^\dagger \mathcal{J} \mathcal{T}. \quad (2.111)$$

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<sup>12</sup>This section is only relevant for Ch. 6, on summary and outlook.

Eq. (2.107) implies that  $\mathcal{M}$  can be symmetrized such that

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}_1 & \mathcal{M}_2 \\ \mathcal{M}_2^* & \mathcal{M}_1^* \end{pmatrix}, \quad (2.112)$$

where  $\mathcal{M}_1$  and  $\mathcal{M}_2$  are  $n$ -by- $n$  sub-matrices; the former being Hermitian, and the latter symmetric, as implied by the hermiticity of  $\mathcal{M}$ . The symmetries of this expression can be used to investigate the properties of  $\Omega$  and  $\mathcal{T}$ . Following the methods presented in Ref. [59, Sec. 4], we define an operator  $\mathcal{K} : \mathbb{C}^{2n} \rightarrow \mathbb{C}^{2n}$  acting on  $(\mathbf{u}^T \ \mathbf{v}^T)^T$ ,  $\mathbf{u}, \mathbf{v} \in \mathbb{C}^n$ , such that

$$\mathcal{K} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} \mathbf{v}^* \\ \mathbf{u}^* \end{pmatrix}. \quad (2.113)$$

Then  $\{\mathcal{J}, \mathcal{K}\} = 0$  and  $[\mathcal{M}, \mathcal{K}] = 0$ . Consequently, if  $\mathbf{x}_i = (\mathbf{u}^T \ \mathbf{v}^T)^T$  is an eigenvector of  $\mathcal{J}\mathcal{M}$  with a corresponding eigenvalue  $\omega_i$ , then  $\mathcal{K}\mathbf{x}_i = (\mathbf{v}^{*T} \ \mathbf{u}^{*T})^T$  is also an eigenvector of  $\mathcal{J}\mathcal{M}$ , with a corresponding eigenvalue  $-\omega_i$ :

$$\mathcal{J}\mathcal{M}\mathcal{K}\mathbf{x}_i = -\mathcal{K}\mathcal{J}\mathcal{M}\mathbf{x}_i = -\mathcal{K}\omega_i\mathbf{x}_i = -\omega_i\mathcal{K}\mathbf{x}_i. \quad (2.114)$$

Accordingly, one may construct an  $\Omega$  on the form

$$\Omega = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n), \quad (2.115)$$

leading to a  $\mathcal{T}$  on the form

$$\mathcal{T} = \left( \begin{pmatrix} \mathcal{T}_1 \\ \mathcal{T}_2^* \end{pmatrix} \ \mathcal{K} \begin{pmatrix} \mathcal{T}_1 \\ \mathcal{T}_2^* \end{pmatrix} \right) = \begin{pmatrix} \mathcal{T}_1 & \mathcal{T}_2 \\ \mathcal{T}_2^* & \mathcal{T}_1^* \end{pmatrix}, \quad (2.116)$$

where the columns are the eigenvectors of  $\mathcal{J}\mathcal{M}$ . Then, by Eq. (2.108), the diagonal matrix associated with  $\mathcal{M}$  is  $\mathcal{J}\Omega = \text{diag}(\omega_1, \dots, \omega_n, \omega_1, \dots, \omega_n)$ , and so the  $\omega_i$  are real by virtue of  $\mathcal{M}$  being Hermitian.

$\mathcal{T}$  as given by Eq. (2.116) may now be shown to satisfy Eq. (2.110). Re-expressing  $\mathcal{T}$  in terms of the eigenvectors  $\mathbf{x}_i$ ,  $i = 1 \dots n$ ,

$$\mathcal{T} = (\mathbf{x}_1 \ \dots \ \mathbf{x}_n \ \mathcal{K}(\mathbf{x}_1 \ \dots \ \mathbf{x}_n)), \quad (2.117)$$

Eq. (2.110) is found to be equivalent to

$$(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu) = \mathcal{J}_{\mu\nu}, \quad (2.118)$$

where  $(\cdot, \cdot)$  denotes the conventional inner product. We note that

$$(\mathcal{K}\mathbf{x}_\mu, \mathcal{J}\mathcal{K}\mathbf{x}_\nu) = (\mathcal{K}\mathbf{x}_\mu, -\mathcal{K}\mathcal{J}\mathbf{x}_\nu) = -(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu)^*. \quad (2.119)$$

Furthermore, using the fact that  $\mathcal{M}$  and  $\mathcal{J}$  are Hermitian,

$$\begin{aligned} \omega_\mu(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu) &= (\omega_\mu\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu) = (\mathcal{J}\mathcal{M}\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu) = (\mathbf{x}_\mu, \mathcal{M}\mathcal{J}\mathcal{J}\mathbf{x}_\nu) \\ &= (\mathbf{x}_\mu, \mathcal{M}\mathbf{x}_\nu) = (\mathbf{x}_\mu, \mathcal{J}\mathcal{J}\mathcal{M}\mathbf{x}_\nu) = (\mathbf{x}_\mu, \mathcal{J}\omega_\nu\mathbf{x}_\nu) = \omega_\nu(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu). \end{aligned} \quad (2.120)$$

If  $\omega_\mu \neq \omega_\nu$ , then Eq. (2.120) implies that  $(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\nu) = 0$ . If  $\omega_\mu = \omega_\nu$ ,  $\mu \neq \nu$ , then the Gram–Schmidt method can be applied in order to orthonormalize the basis of the corresponding eigenspace. Finally, noting that  $\mathbf{C}^\dagger \mathcal{J} \Omega \mathbf{C}$  corresponds to  $2n$  harmonic oscillators, and discarding the possibility of  $\omega_i = 0$ , one must have  $\omega_i > 0$ , since there would otherwise be no lower limit for the energy of the system. Hence,  $\mathcal{M}$  is positive-definite, and so, by the first and fourth equality of Eq. (2.120),

$$\omega_\mu(\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\mu) = (\mathbf{x}_\mu, \mathcal{M}\mathbf{x}_\mu) > 0 \quad \Rightarrow \quad (\mathbf{x}_\mu, \mathcal{J}\mathbf{x}_\mu) > 0, \quad \mu = 1 \dots n, \quad (2.121)$$

since  $\omega_\mu > 0$ . Now, because eigenvectors may be scaled by arbitrary non-zero scalars, the first  $n$  column vectors of  $\mathcal{T}$  may be scaled such that the first  $n$  diagonal entries of the left-hand side of Eq. (2.118) are 1. Then Eq. (2.119) implies that the remaining  $n$  diagonal entries are  $-1$ . Hence  $\mathcal{T}$  as defined by (2.116) either satisfies, or can be made to satisfy, the boson relation (2.110). Therefore, if the Hamiltonian has the form (2.112), and the associated diagonal matrix has the form (2.115), then these conditions suffice to ensure that the resulting quasi-particles are bosons.

# CHAPTER 3

## *Spin–Orbit Coupled, Weakly Interacting Bose Gas*

Our starting point is the Hamiltonian (2.40),

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta} + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{p}}^{\beta} A_{\mathbf{p}'}^{\alpha} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{p}+\mathbf{p}'}, \quad (3.1)$$

where  $A_{\mathbf{k}}^{\alpha}$  is an annihilation operator for a boson of pseudospin  $\alpha$  and momentum  $\mathbf{k}$ , as given by Eq. (2.24) and (2.25);  $N_s$  is the number of lattice points; and the delta function expresses conservation of momentum. Furthermore,  $U^{\alpha\beta} = U^{\beta\alpha}$  defined by Eq. (2.14) is the on-site interaction coupling, and  $\eta_{\mathbf{k}}$  is the single-particle coupling (2.41),

$$\eta_{\mathbf{k}} = \begin{pmatrix} \eta_{\mathbf{k}}^{\uparrow\uparrow} & \eta_{\mathbf{k}}^{\uparrow\downarrow} \\ \eta_{\mathbf{k}}^{\downarrow\uparrow} & \eta_{\mathbf{k}}^{\downarrow\downarrow} \end{pmatrix} \equiv \begin{pmatrix} -\epsilon_{\mathbf{k}}^{\uparrow} - \mu^{\uparrow} & s_{\mathbf{k}} \\ s_{\mathbf{k}}^* & -\epsilon_{\mathbf{k}}^{\downarrow} - \mu^{\downarrow} \end{pmatrix}, \quad (3.2)$$

where  $\mu^{\alpha}$  is the chemical potential associated with particles of pseudospin  $\alpha$ ,  $\epsilon_{\mathbf{k}}^{\alpha}$  is the no-SOC single-particle energies defined in Eq. (2.31), and  $s_{\mathbf{k}}$  is the SOC. For a square lattice of lattice constant  $a$ , oriented as in Fig. 2.3,

$$\epsilon_{\mathbf{k}}^{\alpha} = 2t^{\alpha}(\cos(k_x a) + \cos(k_y a)), \quad (3.3)$$

$$s_{\mathbf{k}} = -2\lambda_R(\sin(k_y a) + i \sin(k_x a)). \quad (3.4)$$

Here,  $t^{\alpha}$  is the hopping coupling, and  $\lambda_R$  is the SOC strength.

Because the temperature of the ultracold Bose gas is assumed to be significantly lower than the critical temperature for Bose–Einstein condensation to occur,<sup>1</sup> the condensate operators  $A_{\mathbf{k}_0i}^{\alpha}$  may be assumed dominant, provided the phenomenon of ground state depletion described in Sec. 2.6 is not too severe; for this reason, the subsequent analysis is expected only to hold for the

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<sup>1</sup>As was also remarked in Sec. 2.6, here, it is implicitly assumed that Bose–Einstein condensation *does* occur.

superfluid phase, for which the hopping couplings are considerably stronger than the interaction couplings. Here, the  $\mathbf{k}_{0i}$  are the condensate momenta, with the *momentum index*  $i = 0$  or  $i = 1, \dots, n$  depending on whether there is 1 or up to  $n > 1$  distinct possible condensate momenta, respectively, cf. Fig. 2.3; these cases are hereafter referred to as *one-fold*, and *many-fold* or *n-fold*, respectively. Any trilinear or quadrilinear contributions in excitation operators to  $\mathcal{H}$  are assumed negligible. All separate instances of *interaction* terms that are constant, linear and bilinear in excitation operators are presented in Tab. 3.1.<sup>2</sup>

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<sup>2</sup>S. Solli [47], S. T. H. Hartman [60] and the author [48] identified only a subset of the configurations presented in Tab. 3.1 in their respective thesis and project work. This subset of configurations does not appear to consistently describe any physical special case besides the case of zero-momentum condensed particles, rendering many—if not all—results regarding cases of non-zero momentum condensed particles, erroneous.



**Table 3.1:** Interaction term momentum configurations

Case	$\mathbf{k}$	$\mathbf{k}'$	$\mathbf{p}$	$\mathbf{p}'$	$\#_6$	$\#_4$	$\#_2$	$\#_1$	$\#_n$ ( $n \geq 2$ )
1:	$\mathbf{k}_{0i}$	$\mathbf{k}_{0j}$	$\mathbf{k}_{0i'}$	$\mathbf{k}_{0j'}$	90	36	6	1	$3n(n-1)$
2:	$\mathbf{k}_{0i}$	$\mathbf{k}_{0j}$	$\mathbf{k}_{0i'}$	$\mathbf{p}'$	126	28	2	0	$n(n^2 - 3(n-1))$
3:	$\mathbf{k}_{0i}$	$\mathbf{k}_{0j}$	$\mathbf{p}$	$\mathbf{k}_{0j'}$	126	28	2	0	$n(n^2 - 3(n-1))$
4:	$\mathbf{k}_{0i}$	$\mathbf{k}'$	$\mathbf{k}_{0i'}$	$\mathbf{k}_{0j'}$	126	28	2	0	$n(n^2 - 3(n-1))$
5:	$\mathbf{k}$	$\mathbf{k}_{0j}$	$\mathbf{k}_{0i'}$	$\mathbf{k}_{0j'}$	126	28	2	0	$n(n^2 - 3(n-1))$
6:	$\mathbf{k}_{0i}$	$\mathbf{k}_{0j}$	$\mathbf{p}$	$\mathbf{p}'$	36	16	4	1	$n^2$
7:	$\mathbf{k}_{0i}$	$\mathbf{k}'$	$\mathbf{k}_{0i'}$	$\mathbf{p}'$	36	16	4	1	$n^2$
8:	$\mathbf{k}_{0i}$	$\mathbf{k}'$	$\mathbf{p}$	$\mathbf{k}_{0j'}$	36	16	4	1	$n^2$
9:	$\mathbf{k}$	$\mathbf{k}'$	$\mathbf{k}_{0i'}$	$\mathbf{k}_{0j'}$	36	16	4	1	$n^2$
10:	$\mathbf{k}$	$\mathbf{k}_{0j}$	$\mathbf{p}$	$\mathbf{k}_{0j'}$	36	16	4	1	$n^2$
11:	$\mathbf{k}$	$\mathbf{k}_{0j}$	$\mathbf{k}_{0i'}$	$\mathbf{p}'$	36	16	4	1	$n^2$

Table of all momentum configurations in the two-body scattering terms.  $\#_n$  is the number of permissible configurations in the respective cases when the condensate comprises particles of one or more of  $n$  distinct momenta symmetrically distributed about the origin in  $k$ -space. Entries that are not denoted by a condensate momentum such as  $\mathbf{k}_{0i}$ , are implicitly assumed *not* to be condensate momenta. For a derivation of the expressions for  $\#_n$  when  $n \geq 2$ , see the text preceding the table; for a visual method of counting, see appendix A. Observe that in the many-fold cases, there are instances of permissible configurations that are *linear* in non-condensate momenta; neither the author nor his supervisor have found this explored in the literature.

In case 6–11 in Tab. 3.1, the number of configurations is  $n^2$  as the momentum indices may take on any of the  $n$  values. In case 1–5, however, the number of configurations is non-trivial because all momenta are constrained, either by being assumed to be a condensate momentum, or by conservation of momentum. For details on a visual, iterative method to count these con-

figurations, see appendix A.

The general expressions for  $\#_n$  presented in Tab. 3.1—i.e. the number of configurations of condensate momenta for the two-body scattering terms in the  $n$ -fold case, assuming the terms are either bilinear, trilinear or quadrilinear in condensate particle operators—may be derived as follows. The incoming and outgoing particle momenta are constrained only by conservation of momentum. Systematically examining the cases presented in Tab. 3.1, one finds the following:

- a) In case 6–11, conservation of momentum is on the form

$$\mathbf{k}_{0i} + \mathbf{k}' = \mathbf{k}_{0i'} + \mathbf{p}'. \quad (3.5)$$

where  $\mathbf{k}'$  and  $\mathbf{p}'$  are assumed to be non-condensate momenta. In these cases, conservation of momentum does not constrain the number of permissible configurations of condensate momenta. In other words, the momentum indices  $i, i'$  may take on any of the  $n$  possible values, and so

$$\#_n = n^2. \quad (3.6)$$

- b) In case 1, conservation of momentum is on the form

$$\mathbf{k}_{0i} + \mathbf{k}_{0j} = \mathbf{k}_{0i'} + \mathbf{k}_{0j'}. \quad (3.7)$$

By inspection of this equation, one finds that the permissible configurations are exhausted by permutations on the following forms:

$$1 : \mathbf{k}_{0i} = \mathbf{k}_{0j} = \mathbf{k}_{0i'} = \mathbf{k}_{0j'}, \quad (3.8)$$

$$2 : \mathbf{k}_{0i} = \mathbf{k}_{0j'} \neq \mathbf{k}_{0j} = \mathbf{k}_{0i'}, \quad n \geq 2, \quad (3.9)$$

$$3 : \mathbf{k}_{0i} = \mathbf{k}_{0i'} \neq \mathbf{k}_{0j} = \mathbf{k}_{0j'}, \quad n \geq 2, \quad (3.10)$$

$$4 : \mathbf{k}_{0i} = -\mathbf{k}_{0j}, \quad \mathbf{k}_{0i'} = -\mathbf{k}_{0j'} \neq \pm\mathbf{k}_{0i}, \quad n \geq 4. \quad (3.11)$$

The last line follows from the inversion symmetry of the Bravais lattice. Thus, the total number of permissible configurations is

$$\#_n = \begin{cases} 1, & n = 1, \\ n + n(n-1) + n(n-1) + n(n-2) = 3n(n-1), & n \geq 2. \end{cases} \quad (3.12)$$

- c) In case 2–5, conservation of momentum is on the form

$$\mathbf{k}_{0i} + \mathbf{k}_{0j} = \mathbf{k}_{0i'} + \mathbf{p}'. \quad (3.13)$$

If one is interested only in the number of permissible configurations, one may proceed by treating  $\mathbf{p}'$  as an unconstrained momentum, from which it follows that the number of permissible configurations in these cases is equal to the total number of configurations of  $\mathbf{k}_{0i}, \mathbf{k}_{0j}, \mathbf{k}_{0i'}$ , save the configurations that leave  $\mathbf{p}'$  equal to a condensate momentum, i.e.

$$\#_n \stackrel{(3.12)}{=} \begin{cases} 1^3 - 1 = 0, & n = 1, \\ n^3 - 3n(n-1) = n(n^2 - 3(n-1)), & n \geq 2. \end{cases} \quad (3.14)$$

However, it may also be of interest to identify all permutations that exhaust the constraint of conservation of momentum in these cases. By inspection of Eq. (3.13), one finds that these permutations are on the following forms:

$$1 : \mathbf{k}_{0i} = \mathbf{k}_{0j} \neq \mathbf{k}_{0i'}, \quad n \geq 2, \quad (3.15)$$

$$2 : \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0i}, \quad \mathbf{k}_{0i'} \neq \mathbf{k}_{0j} \neq \mathbf{k}_{0i}, \quad n \geq 2. \quad (3.16)$$

Thus, the number of permissible configurations is

$$\#_n = \begin{cases} 0, & n = 1, \\ n(n-1) + n(n-2)^2 = n(n^2 - 3(n-1)), & n \geq 2. \end{cases} \quad (3.17)$$

which coincides with the expression (3.14), derived by a different line of reasoning. Note that in the one-fold case, there are no terms in  $\mathcal{H}$  that are linear in non-condensate momenta, since, for instance,

$$\mathbf{k}_{00} + \mathbf{k}_{00} = \mathbf{k}_{00} + \mathbf{p}' \quad \Rightarrow \quad \mathbf{p}' = \mathbf{k}_{00}, \quad (3.18)$$

contrary to the assumption that  $\mathbf{p}'$  is not a condensate momentum. This holds more generally for any condensate presumed to comprise quasi-particles of only one momentum:

$$\mathbf{k}_{0i} + \mathbf{k}_{0i} = \mathbf{k}_{0i} + \mathbf{p}' \quad \Rightarrow \quad \mathbf{p}' = \mathbf{k}_{0i}, \quad (3.19)$$

for a specified value of  $i$ . However, in the many-fold cases, there *are* permissible configurations that are linear in non-condensate momenta; as such, it is a qualitatively new aspect from the one-fold case, and neither the author nor his supervisor have found this explored in the literature.

$\mathcal{H}$  may now be written as

$$\mathcal{H} \approx \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2, \quad (3.20)$$

where

$$\begin{aligned} \mathcal{H}_0 \equiv & \sum_i \sum_{\alpha\beta} \eta_{\mathbf{k}_{0i}}^{\alpha\beta} A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0i}}^\beta \\ & + \frac{1}{2N_s} \sum_{ijj'} \sum_{\alpha\beta} U^{\alpha\beta} A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}_{0i'}}^\beta A_{\mathbf{k}_{0j'}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}}, \end{aligned} \quad (3.21)$$

$$\begin{aligned} \mathcal{H}_1 \equiv & \frac{1}{2N_s} \sum_{\mathbf{k}}' \sum_{ijj'} \sum_{\alpha\beta} U^{\alpha\beta} \left( A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}_{0i'}}^\beta A_{\mathbf{k}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}} \right. \\ & + A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}}^\beta A_{\mathbf{k}_{0i'}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}+\mathbf{k}_{0i'}} \\ & + A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}_{0i'}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}_{0j}+\mathbf{k}_{0i'}} \\ & \left. + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}_{0i}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}_{0i'}}^\alpha \delta_{\mathbf{k}+\mathbf{k}_{0i}, \mathbf{k}_{0j}+\mathbf{k}_{0i'}} \right), \end{aligned} \quad (3.22)$$

and

$$\begin{aligned} \mathcal{H}_2 \equiv & \sum_{\mathbf{k}}' \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^\beta \\ & + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'}'' \sum_{ij} \sum_{\alpha\beta} U^{\alpha\beta} \left( A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}}^\beta A_{\mathbf{k}'}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}+\mathbf{k}'} \right. \\ & + A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}'}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}_{0j}+\mathbf{k}'} \\ & + A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\beta A_{\mathbf{k}_{0j}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}} \\ & + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{k}_{0i}}^\beta A_{\mathbf{k}_{0j}}^\alpha \delta_{\mathbf{k}+\mathbf{k}', \mathbf{k}_{0i}+\mathbf{k}_{0j}} \\ & + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}_{0i}}^{\beta\dagger} A_{\mathbf{k}'}^\beta A_{\mathbf{k}_{0j}}^\alpha \delta_{\mathbf{k}+\mathbf{k}_{0i}, \mathbf{k}'+\mathbf{k}_{0j}} \\ & \left. + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}_{0i}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}'}^\alpha \delta_{\mathbf{k}+\mathbf{k}_{0i}, \mathbf{k}_{0j}+\mathbf{k}'} \right), \end{aligned} \quad (3.23)$$

where the sum  $\sum_{\mathbf{k}}'$  excludes all  $\mathbf{k} = \mathbf{k}_{0i} \forall i$ , and the sum  $\sum_{\mathbf{k}\mathbf{k}'}''$  excludes all configurations of  $\mathbf{k}$  and  $\mathbf{k}'$  for which either one or both are equal to a condensate momentum; note that in relation to the sum  $\sum_{\mathbf{k}\mathbf{k}'}''$ , if e.g.  $\mathbf{k}$  is set equal to an *arbitrary* non-condensate momentum,  $\mathbf{k}'$  *might* be a condensate

momentum due to conservation of momentum, which is a configuration that is excluded from the sum.<sup>3</sup>  $\mathcal{H}_1$  and  $\mathcal{H}_2$  may be simplified by applying the commutator relation (2.25) and permuting momentum indices, in conjunction with the fact that  $U^{\alpha\beta} = U^{\beta\alpha}$ , cf. Eq. (2.19):

$$\begin{aligned} \mathcal{H}_1 \equiv & \frac{1}{N_s} \sum'_{\mathbf{k}} \sum_{ijj'} \sum_{\alpha\beta} U^{\alpha\beta} \left( A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}_{0i'}}^{\beta} A_{\mathbf{k}}^{\alpha} \right. \\ & \left. + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}_{0i'}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^{\beta} A_{\mathbf{k}_{0i}}^{\alpha} \right) \delta_{\mathbf{k}+\mathbf{k}_{0i'}, \mathbf{k}_{0j}+\mathbf{k}_{0i}}, \end{aligned} \quad (3.24)$$

$$\begin{aligned} \mathcal{H}_2 \equiv & \sum'_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta} \\ & + \frac{1}{2N_s} \sum''_{\mathbf{k}\mathbf{k}'} \sum_{ij} \sum_{\alpha\beta} U^{\alpha\beta} \left( (A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}_{0j}}^{\beta\dagger} A_{\mathbf{k}}^{\beta} A_{\mathbf{k}'}^{\alpha} \right. \\ & \left. + A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{k}_{0i}}^{\beta} A_{\mathbf{k}_{0j}}^{\alpha}) \delta_{\mathbf{k}+\mathbf{k}', \mathbf{k}_{0i}+\mathbf{k}_{0j}} \right. \\ & \left. + 2(A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}_{0j}}^{\beta} A_{\mathbf{k}'}^{\alpha} \right. \\ & \left. + A_{\mathbf{k}_{0i}}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^{\beta} A_{\mathbf{k}_{0j}}^{\alpha}) \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}} \right). \end{aligned} \quad (3.25)$$

### 3.1 Mean Field Theory

To simplify further analyses, a mean field approach is applied to the general expression (3.20) for  $\mathcal{H}$ , which in conjunction with an assumption that the condensate be dominant, renders  $\mathcal{H}$  at most bilinear in excitation operators, effectively reducing the many-particle problem to a single-particle problem. This is analogous to what was done in the non-SOC case presented in Sec. 2.6. The mean field approach leads to the introduction of a number of variational parameters. In accordance with Ch. 4 of H. Bruus *et al.* [54], these may be determined by solving a set of self-consistent equations, *or*, equivalently, by minimizing the free energy  $F$  with respect to these parameters; the latter approach will be employed in this thesis.

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<sup>3</sup>This latter point does not appear to be addressed consistently in the literature; see e.g. D. Toniolo *et al.* [61, Eq. (5)], where  $\mathbf{k} = 3\mathbf{K}_0$  produces terms involving operators for particles carrying a possible condensate momentum  $2\mathbf{K}_0 - \mathbf{k} = -\mathbf{K}_0$ , which is not addressed beyond an implicit assumption that the *mean field parameters* associated with these operators, are zero.

The mean field approach amounts to substituting the condensate operators  $A_{\mathbf{k}_{0i}}^\alpha$  with an expectation value  $a_{\mathbf{k}_{0i}}^\alpha$  plus a *small* fluctuation  $\delta A_{\mathbf{k}_{0i}}^\alpha$ :

$$A_{\mathbf{k}_{0i}}^\alpha \longrightarrow a_{\mathbf{k}_{0i}}^\alpha + \delta A_{\mathbf{k}_{0i}}^\alpha. \quad (3.26)$$

Here,  $a_{\mathbf{k}_{0i}}^\alpha$  is a *c*-number, and  $\delta A_{\mathbf{k}_{0i}}^\alpha$  is an operator. In the literature,  $a_{\mathbf{k}_{0i}}^\alpha$  is usually taken to be real and equal to the square root of the appropriate condensate particle number, i.e.  $\sqrt{N_{\mathbf{k}_{0i}}^\alpha}$ ; however, for this thesis, we will let

$$a_{\mathbf{k}_{0i}}^\alpha \equiv \sqrt{N_{\mathbf{k}_{0i}}^\alpha} e^{-i\theta_{\mathbf{k}_{0i}}^\alpha} \in \mathbb{C}; \quad (3.27)$$

that is, though the modulus is still  $\sqrt{N_{\mathbf{k}_{0i}}^\alpha} \in \mathbb{R}$ ,  $a_{\mathbf{k}_{0i}}^\alpha$  may also carry a complex phase factor parameterized by the angle  $\theta_{\mathbf{k}_{0i}}^\alpha \in [0, 2\pi)$ .

Following the same procedure as van Oosten *et al.* [46], Eq. (3.26) is applied to Eq. (3.21), (3.24) and (3.25). To lowest order in the condensate fluctuations, only terms that are constant or linear in fluctuations, save terms that contain the product of a fluctuation and an excitation operator, are kept, while the remainder is neglected. The contribution to  $\mathcal{H}$  that comprises all

terms that are linear in condensate fluctuations, is

$$\begin{aligned}
 \mathcal{H}_{(1)} &\equiv \sum_i \sum_{\alpha\beta} \eta_{\mathbf{k}_{0i}}^{\alpha\beta} \left( (a_{\mathbf{k}_{0i}}^\alpha)^* \delta A_{\mathbf{k}_{0i}}^\beta + a_{\mathbf{k}_{0i}}^\beta \delta A_{\mathbf{k}_{0i}}^{\alpha\dagger} \right) \\
 &\quad + \frac{1}{2N_s} \sum_{ij'j'} \sum_{\alpha\beta} U^{\alpha\beta} \left( (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta a_{\mathbf{k}_{0j'}}^\alpha \delta A_{\mathbf{k}_{0i}}^{\alpha\dagger} \right. \\
 &\quad \quad \quad + (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0i'}}^\beta a_{\mathbf{k}_{0j'}}^\alpha \delta A_{\mathbf{k}_{0j}}^{\beta\dagger} \\
 &\quad \quad \quad + (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0j'}}^\alpha \delta A_{\mathbf{k}_{0i'}}^\beta \\
 &\quad \quad \quad \left. + (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta \delta A_{\mathbf{k}_{0j'}}^\alpha \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \\
 &= \sum_i \sum_{\alpha\beta} \eta_{\mathbf{k}_{0i}}^{\alpha\beta} \left( (a_{\mathbf{k}_{0i}}^\alpha)^* \delta A_{\mathbf{k}_{0i}}^\beta + a_{\mathbf{k}_{0i}}^\beta \delta A_{\mathbf{k}_{0i}}^{\alpha\dagger} \right) \\
 &\quad + \frac{1}{N_s} \sum_{ij'j'} \sum_{\alpha\beta} U^{\alpha\beta} \left( (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta a_{\mathbf{k}_{0j'}}^\alpha \delta A_{\mathbf{k}_{0i}}^{\alpha\dagger} \right. \\
 &\quad \quad \quad \left. + a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* (a_{\mathbf{k}_{0j'}}^\beta)^* \delta A_{\mathbf{k}_{0i}}^\beta \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \\
 &= \sum_i \sum_{\alpha\beta} \left( \delta A_{\mathbf{k}_{0i}}^\beta \left( \eta_{\mathbf{k}_{0i}}^{\alpha\beta} (a_{\mathbf{k}_{0i}}^\alpha)^* \right. \right. \\
 &\quad \quad \quad \left. \left. + \frac{1}{N_s} U^{\alpha\beta} \sum_{j'j'} a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* (a_{\mathbf{k}_{0j'}}^\beta)^* \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \right) \right. \\
 &\quad \quad \quad \left. + \delta A_{\mathbf{k}_{0i}}^{\alpha\dagger} \left( \eta_{\mathbf{k}_{0i}}^{\alpha\beta} a_{\mathbf{k}_{0i}}^\beta \right. \right. \\
 &\quad \quad \quad \left. \left. + \frac{1}{N_s} U^{\alpha\beta} \sum_{j'j'} (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta a_{\mathbf{k}_{0j'}}^\alpha \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \right) \right) \\
 &= \sum_i \sum_{\alpha\beta} \left( \delta A_{\mathbf{k}_{0i}}^\beta \left( \eta_{\mathbf{k}_{0i}}^{\alpha\beta} (a_{\mathbf{k}_{0i}}^\alpha)^* \right. \right. \\
 &\quad \quad \quad \left. \left. + \frac{1}{N_s} U^{\alpha\beta} \sum_{j'j'} a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* (a_{\mathbf{k}_{0j'}}^\beta)^* \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \right) \right. \\
 &\quad \quad \quad \left. + \text{H.c.} \right),
 \end{aligned} \tag{3.28}$$

where ‘‘H.c.’’ denotes the Hermitian conjugate of the preceding term. Because  $F$  is to be minimized with respect to the variational parameters  $a_{\mathbf{k}_{0i}}^\alpha$ ,  $\mathcal{H}_{(1)}$  must be zero. Thus, we conclude that to lowest order in condensate

fluctuations, the chemical potentials  $\mu^\alpha$  in Eq. (2.41) exactly cancel the remainder of  $\mathcal{H}_{(1)}$ .

For the moment, we neglect the contributions from interactions.  $\mathcal{H}_{(1)}$  written out in terms of pseudospin indices is

$$\begin{aligned} \mathcal{H}_{(1)} = \sum_i & \left( \delta A_{\mathbf{k}_{0i}}^\uparrow \left( - \left( \epsilon_{\mathbf{k}_{0i}}^\uparrow + \mu^\uparrow \right) (a_{\mathbf{k}_{0i}}^\uparrow)^* + s_{\mathbf{k}_{0i}}^* (a_{\mathbf{k}_{0i}}^\downarrow)^* \right) \right. \\ & \delta A_{\mathbf{k}_{0i}}^{\uparrow\uparrow} \left( - \left( \epsilon_{\mathbf{k}_{0i}}^\uparrow + \mu^\uparrow \right) a_{\mathbf{k}_{0i}}^\uparrow + s_{\mathbf{k}_{0i}} a_{\mathbf{k}_{0i}}^\downarrow \right) \\ & \delta A_{\mathbf{k}_{0i}}^\downarrow \left( - \left( \epsilon_{\mathbf{k}_{0i}}^\downarrow + \mu^\downarrow \right) (a_{\mathbf{k}_{0i}}^\downarrow)^* + s_{\mathbf{k}_{0i}} (a_{\mathbf{k}_{0i}}^\uparrow)^* \right) \\ & \left. \delta A_{\mathbf{k}_{0i}}^{\downarrow\downarrow} \left( - \left( \epsilon_{\mathbf{k}_{0i}}^\downarrow + \mu^\downarrow \right) a_{\mathbf{k}_{0i}}^\downarrow + s_{\mathbf{k}_{0i}}^* a_{\mathbf{k}_{0i}}^\uparrow \right) \right). \end{aligned} \quad (3.29)$$

There are two scenarios of particular interest:

- a)  $s_{\mathbf{k}_{0i}} = 0$ : This is the case when either the SOC strength  $\lambda_R$  is sufficiently weak, or  $\mathbf{k}_{0i} = \mathbf{0}$ . In this case,

$$\mu^\uparrow = -\epsilon_{\mathbf{k}_{0i}}^\uparrow, \quad (3.30)$$

$$\mu^\downarrow = -\epsilon_{\mathbf{k}_{0i}}^\downarrow. \quad (3.31)$$

The momentum index  $i$  is not problematic, as the Bravais lattice symmetry dictates that  $\epsilon_{\mathbf{k}_{0i}}^\alpha \stackrel{(2.31)}{=} \epsilon_{\mathbf{k}_{0j}}^\alpha \forall i, j$ ; hence, there is no dependency of  $\mu^\alpha$  on this index.

- b)  $s_{\mathbf{k}_{0i}} \neq 0$ : In this case, one cannot have  $a_{\mathbf{k}_{0i}}^\uparrow \neq a_{\mathbf{k}_{0i}}^\downarrow = 0$  or vice versa; otherwise, there would be no way to render  $\mathcal{H}_{(1)} = 0$ , contrary to the assumption that the free energy be minimal with respect to the variational parameters. Therefore, for any value of  $i$ ,  $a_{\mathbf{k}_{0i}}^\uparrow$  and  $a_{\mathbf{k}_{0i}}^\downarrow$  must both either be zero or non-zero. The instances of  $i$  for which both are zero give no information about the chemical potentials, as the respective contributions to the sum in Eq. (3.29) are zero. Therefore, assuming there *is* a condensate, i.e. that there exists at least one pair

$$a_{\mathbf{k}_{0i}}^\uparrow, a_{\mathbf{k}_{0i}}^\downarrow \neq 0, \quad (3.32)$$



$\mathcal{H}_{(1)} = 0$  implies

$$\mu^\uparrow = -\epsilon_{\mathbf{k}_{0i}}^\uparrow + s_{\mathbf{k}_{0i}}^* \left( \frac{a_{\mathbf{k}_{0i}}^\downarrow}{a_{\mathbf{k}_{0i}}^\uparrow} \right)^* = -\epsilon_{\mathbf{k}_{0i}}^\uparrow + s_{\mathbf{k}_{0i}} \frac{a_{\mathbf{k}_{0i}}^\downarrow}{a_{\mathbf{k}_{0i}}^\uparrow}, \quad (3.33)$$

$$\mu^\downarrow = -\epsilon_{\mathbf{k}_{0i}}^\downarrow + s_{\mathbf{k}_{0i}} \left( \frac{a_{\mathbf{k}_{0i}}^\uparrow}{a_{\mathbf{k}_{0i}}^\downarrow} \right)^* = -\epsilon_{\mathbf{k}_{0i}}^\downarrow + s_{\mathbf{k}_{0i}}^* \frac{a_{\mathbf{k}_{0i}}^\uparrow}{a_{\mathbf{k}_{0i}}^\downarrow}. \quad (3.34)$$

Eq. (3.33) and (3.34) are equivalent to requiring  $\mu^\alpha \in \mathbb{R}$ . Inserting the expressions (3.27) for  $a_{\mathbf{k}_{0i}}^\alpha$ , one finds that Eq. (3.33) and (3.34) both imply that

$$e^{i(\gamma_{\mathbf{k}_{0i}} + \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\uparrow)} = e^{-i(\gamma_{\mathbf{k}_{0i}} + \theta_{\mathbf{k}_{0i}}^\uparrow - \theta_{\mathbf{k}_{0i}}^\downarrow)}, \quad (3.35)$$

where  $e^{-i\gamma_{\mathbf{k}_{0i}}} = s_{\mathbf{k}_{0i}}/|s_{\mathbf{k}_{0i}}|$ , cf. Eq. (2.66). Therefore,

$$\sin(\gamma_{\mathbf{k}_{0i}} + \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\uparrow) = 0 \quad (3.36)$$

$$\Rightarrow \gamma_{\mathbf{k}_{0i}} + \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\uparrow = \ell\pi, \quad \ell \in \{0, 1\}. \quad (3.37)$$

Note that the value  $\ell\pi$  of  $\gamma_{\mathbf{k}_{0i}} + \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\uparrow$  is *fixed*, as  $\mu^\alpha$  must be invariant with respect to  $i$ . An appropriate value of  $\ell$  must therefore be chosen. Now,

$$\mu^\uparrow = -\epsilon_{\mathbf{k}_{0i}}^\uparrow \pm |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\downarrow}{N_{\mathbf{k}_{0i}}^\uparrow}}, \quad (3.38)$$

$$\mu^\downarrow = -\epsilon_{\mathbf{k}_{0i}}^\downarrow \pm |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\uparrow}{N_{\mathbf{k}_{0i}}^\downarrow}}, \quad (3.39)$$

where the sign of the SOC term in the chemical potentials depends on the value of  $\ell$ . As will be at the end of Ch. 4, choosing a negative sign is necessary in order to reproduce results from the literature, which will therefore be assumed for the remainder of this thesis, i.e.

$$\mu^\uparrow = -\epsilon_{\mathbf{k}_{0i}}^\uparrow - |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\downarrow}{N_{\mathbf{k}_{0i}}^\uparrow}}, \quad (3.40)$$

$$\mu^\downarrow = -\epsilon_{\mathbf{k}_{0i}}^\downarrow - |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\uparrow}{N_{\mathbf{k}_{0i}}^\downarrow}}. \quad (3.41)$$

Again,  $\epsilon_{\mathbf{k}_{0i}}^\alpha \stackrel{(2.31)}{=} \epsilon_{\mathbf{k}_{0j}}^\alpha \forall i, j$  introduces no dependency on the momentum index  $i$ . The Bravais lattice symmetry also implies that the quantity

$$|s_{\mathbf{k}}| \stackrel{(2.39)}{=} \lambda_R \left( \left( \sum_n \mathbf{a}_n \cdot \hat{\mathbf{y}} \sin(\mathbf{k} \cdot \mathbf{a}_n) \right)^2 + \left( \sum_n \mathbf{a}_n \cdot \hat{\mathbf{x}} \sin(\mathbf{k} \cdot \mathbf{a}_n) \right)^2 \right)^{\frac{1}{2}} \quad (3.42)$$

satisfies  $|s_{\mathbf{k}_{0i}}| = |s_{\mathbf{k}_{0j}}| \forall i, j$ . However, one must require that the ratios

$$\sqrt{\frac{N_{\mathbf{k}_{0i}}^\downarrow}{N_{\mathbf{k}_{0i}}^\uparrow}} = \sqrt{\frac{N_{\mathbf{k}_{0j}}^\downarrow}{N_{\mathbf{k}_{0j}}^\uparrow}}, \quad i \neq j, \quad (3.43)$$

are invariant with respect to values of the momentum indices for which the pairs  $N_{\mathbf{k}_{0i}}^\uparrow, N_{\mathbf{k}_{0i}}^\downarrow$  are non-zero. Note that these conclusions only apply to cases for which  $s_{\mathbf{k}_{0i}} \neq 0$ .

Now, we include interactions; i.e., the full expression (3.28) for  $\mathcal{H}_{(1)}$  is taken into consideration. Suppose that  $a_{\mathbf{k}_{0i}}^\uparrow$  is non-zero for some value of  $i$ . Then the condition  $\mathcal{H}_{(1)} = 0$  leads to

$$\begin{aligned} \mu^\uparrow = \mu^{\uparrow*} = & -\epsilon_{\mathbf{k}_{0i}}^\uparrow - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\downarrow}{N_{\mathbf{k}_{0i}}^\uparrow}} \right]_{s_{\mathbf{k}_{0\ell}} \neq 0} \\ & + \frac{1}{N_s} \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^\uparrow}{a_{\mathbf{k}_{0i}}^\uparrow} \right)^* a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}, \end{aligned} \quad (3.44)$$

where the square brackets  $[\dots]_{s_{\mathbf{k}_{0\ell}} \neq 0}$  is a reminder that the term enclosed by them contributes to the chemical potential only if  $s_{\mathbf{k}_{0\ell}} \neq 0$ .  $\mu^\uparrow = \mu^{\uparrow*}$  implies

$$\begin{aligned} & \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^\uparrow}{a_{\mathbf{k}_{0i}}^\uparrow} \right)^* a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\ & = \left( \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^\uparrow}{a_{\mathbf{k}_{0i}}^\uparrow} \right)^* a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right)^*, \end{aligned} \quad (3.45)$$

i.e.

$$\Im \left( \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^{\uparrow}}{a_{\mathbf{k}_{0i}}^{\uparrow}} \right)^* a_{\mathbf{k}_{0j}}^{\alpha} (a_{\mathbf{k}_{0i'}}^{\alpha})^* \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} \right) = 0, \quad (3.46)$$

$$\stackrel{(3.27)}{\Rightarrow} \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\alpha} N_{\mathbf{k}_{0i'}}^{\alpha}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \cdot \sin(\theta_{\mathbf{k}_{0j'}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\alpha} + \theta_{\mathbf{k}_{0i'}}^{\alpha}) \delta_{\mathbf{k}_{0i}+\mathbf{k}_{0j}, \mathbf{k}_{0i'}+\mathbf{k}_{0j'}} = 0 \quad (3.47)$$

The delta function may be eliminated by rewriting the sum over momentum indices in terms of the configurations (3.8)–(3.11), resulting in

$$\begin{aligned} & \sum_{\substack{j \\ j \neq i \\ n \geq 2}} U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0j}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\downarrow} N_{\mathbf{k}_{0i}}^{\downarrow}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \sin(\theta_{\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\downarrow} + \theta_{\mathbf{k}_{0i}}^{\downarrow}) \\ & + \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0i} \\ n \geq 4}} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0i}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \sin(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{-\mathbf{k}_{0i}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) = 0, \end{aligned} \quad (3.48)$$

where  $n$  is the number of distinct possible momenta among condensed particles. Since the above condition only applies to many-fold cases, the SOC is necessarily non-zero when the condition applies. Therefore, using the relation (3.37),

$$\theta_{\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\downarrow} + \theta_{\mathbf{k}_{0i}}^{\downarrow} = \gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0i}}. \quad (3.49)$$

Furthermore, recalling the interpretation of  $\gamma_{\mathbf{k}}$  as the angle between  $\mathbf{k}$  and the  $x$ -axis, as was illustrated in Fig. 2.5,

$$\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0i}} = \gamma_{-\mathbf{k}_{0i}} - \gamma_{\mathbf{k}_{0i}} = \pi, \quad j \neq i \wedge n = 2, \quad (3.50)$$

where the inversion symmetry of the Bravais lattice was used. Thus, the condition (3.48) automatically holds true for  $n = 2$ ; more generally, the term in the first sum in Eq. (3.48) for which  $\mathbf{k}_{0j} = -\mathbf{k}_{0i}$ , is always zero. Upon

applying Eq. (3.43), Eq. (3.48) may therefore finally be reduced to

$$\begin{aligned}
 & \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0i} \\ n \geq 4}} \left( U^{\uparrow\downarrow} N_{\mathbf{k}_{0j}}^{\downarrow} \sin(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0i}}) \right. \\
 & \left. + \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0i}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \sin(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{-\mathbf{k}_{0i}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \right) = 0.
 \end{aligned} \tag{3.51}$$

It is interesting to note that this condition leads to constraints on the variational parameters only if  $n \geq 4$  in order to ensure  $\mu^{\uparrow} \in \mathbb{R}$ ; this is a qualitatively new aspect relative to the simplest of many-fold cases, i.e.  $n = 2$ , for which this is automatically true.

Now that the imaginary part of the interaction terms in the expression (3.44) has been set to zero, one may write

$$\begin{aligned}
 \mu^{\uparrow} &= -\epsilon_{\mathbf{k}_{0i}}^{\uparrow} - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^{\downarrow}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \right]_{s_{\mathbf{k}_{0\ell}} \neq 0} \\
 &+ \frac{1}{N_s} \Re \left( \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^{\uparrow}}{a_{\mathbf{k}_{0i}}^{\uparrow}} \right)^* a_{\mathbf{k}_{0j}}^{\alpha} (a_{\mathbf{k}_{0i'}}^{\alpha})^* \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right) \\
 &\stackrel{(3.27)}{=} -\epsilon_{\mathbf{k}_{0i}}^{\uparrow} - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^{\downarrow}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \right]_{s_{\mathbf{k}_{0\ell}} \neq 0} \\
 &+ \frac{1}{N_s} \sum_{j'i'j'} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\alpha} N_{\mathbf{k}_{0i'}}^{\alpha}}{N_{\mathbf{k}_{0i}}^{\uparrow}}} \\
 &\quad \cdot \cos(\theta_{\mathbf{k}_{0j'}}^{\uparrow} - \theta_{\mathbf{k}_{0i}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\alpha} + \theta_{\mathbf{k}_{0i'}}^{\alpha}) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}.
 \end{aligned} \tag{3.52}$$

In order to ensure that  $\mu^{\uparrow}$  is invariant with respect to the momentum index

$i$ , one must also require

$$\begin{aligned}
 & \sum_{j'j'} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\alpha} N_{\mathbf{k}_{0i'}}^{\alpha}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\theta_{\mathbf{k}_{0j'}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\alpha} + \theta_{\mathbf{k}_{0i'}}^{\alpha}) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 & = \sum_{ji'j'} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\alpha} N_{\mathbf{k}_{0i'}}^{\alpha}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\theta_{\mathbf{k}_{0j'}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{\mathbf{k}_{0j}}^{\alpha} + \theta_{\mathbf{k}_{0i'}}^{\alpha}) \delta_{\mathbf{k}_{0\ell'} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}
 \end{aligned} \tag{3.53}$$

for all values of  $\ell$  and  $\ell' \neq \ell$  for which  $N_{\mathbf{k}_{0\ell}}^{\uparrow}, N_{\mathbf{k}_{0\ell'}}^{\uparrow} \neq 0$ ; because  $\ell' \neq \ell$ , this condition only applies to many-fold cases, i.e.  $n \geq 2$ . Again eliminating the delta functions by rewriting the sum over momentum indices in terms of the configurations (3.8)–(3.11), results in

$$\begin{aligned}
 & \sum_{\alpha} U^{\uparrow\alpha} \left( N_{\mathbf{k}_{0\ell}}^{\alpha} + \sum_{\substack{j \\ j \neq \ell \\ n \geq 2}} N_{\mathbf{k}_{0j}}^{\alpha} \right. \\
 & + \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0\ell} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \Bigg) \\
 & + \sum_{\substack{j \\ j \neq \ell \\ n \geq 2}} \left( U^{\uparrow\uparrow} N_{\mathbf{k}_{0j}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0j}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\downarrow} N_{\mathbf{k}_{0\ell}}^{\downarrow}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0\ell}}) \right) \\
 & = \sum_{\alpha} U^{\uparrow\alpha} \left( N_{\mathbf{k}_{0\ell'}}^{\alpha} + \sum_{\substack{j \\ j \neq \ell' \\ n \geq 2}} N_{\mathbf{k}_{0j}}^{\alpha} \right. \\
 & + \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0\ell'} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell'}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell'}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \Bigg) \\
 & + \sum_{\substack{j \\ j \neq \ell' \\ n \geq 2}} \left( U^{\uparrow\uparrow} N_{\mathbf{k}_{0j}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0j}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\downarrow} N_{\mathbf{k}_{0\ell'}}^{\downarrow}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0\ell'}}) \right).
 \end{aligned} \tag{3.54}$$

Because  $n \geq 2$ , the above expressions may be compacted slightly, to

$$\begin{aligned}
 & \sum_{\alpha} U^{\uparrow\alpha} \left( \sum_{\substack{j \\ n \geq 2}} N_{\mathbf{k}_{0j}}^{\alpha} \right. \\
 & + \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0\ell} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \Bigg) \\
 & + \sum_{\substack{j \\ j \neq \ell \\ n \geq 2}} \left( U^{\uparrow\uparrow} N_{\mathbf{k}_{0j}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0j}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\downarrow} N_{\mathbf{k}_{0\ell}}^{\downarrow}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0\ell}}) \right) \\
 & = \sum_{\alpha} U^{\uparrow\alpha} \left( \sum_{\substack{j \\ n \geq 2}} N_{\mathbf{k}_{0j}}^{\alpha} \right. \\
 & + \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0\ell'} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell'}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell'}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \Bigg) \\
 & + \sum_{\substack{j \\ j \neq \ell' \\ n \geq 2}} \left( U^{\uparrow\uparrow} N_{\mathbf{k}_{0j}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0j}}^{\uparrow} N_{\mathbf{k}_{0j}}^{\downarrow} N_{\mathbf{k}_{0\ell'}}^{\downarrow}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0\ell'}}) \right).
 \end{aligned} \tag{3.55}$$

Cancelling all terms that appear on both sides of the equation, one finds that

$$\begin{aligned}
 & \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell'} \\ \mathbf{k}_{0\ell'}\neq\pm\mathbf{k}_{0\ell} \\ n\geq 4}} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \\
 & + U^{\uparrow\uparrow} N_{\mathbf{k}_{0\ell'}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0\ell'}}^{\uparrow} N_{\mathbf{k}_{0\ell'}}^{\downarrow} N_{\mathbf{k}_{0\ell}}^{\downarrow}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \\
 = & \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell} \\ \mathbf{k}_{0\ell}\neq\pm\mathbf{k}_{0\ell'} \\ n\geq 4}} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell'}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell'}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \\
 & + U^{\uparrow\uparrow} N_{\mathbf{k}_{0\ell}}^{\uparrow} + U^{\uparrow\downarrow} \sqrt{\frac{N_{\mathbf{k}_{0\ell}}^{\uparrow} N_{\mathbf{k}_{0\ell}}^{\downarrow} N_{\mathbf{k}_{0\ell'}}^{\downarrow}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\gamma_{\mathbf{k}_{0\ell}} - \gamma_{\mathbf{k}_{0\ell'}}).
 \end{aligned} \tag{3.56}$$

Finally, applying the relation (3.43) and rearranging terms, one is left with

$$\begin{aligned}
 & \sum_{\alpha} U^{\uparrow\alpha} \left( \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell'} \\ \mathbf{k}_{0\ell'}\neq\pm\mathbf{k}_{0\ell} \\ n\geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \right. \\
 & \left. - \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell} \\ \mathbf{k}_{0\ell}\neq\pm\mathbf{k}_{0\ell'} \\ n\geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^{\uparrow} N_{-\mathbf{k}_{0\ell'}}^{\alpha} N_{\mathbf{k}_{0j}}^{\alpha}}{N_{\mathbf{k}_{0\ell'}}^{\uparrow}}} \cos(\theta_{-\mathbf{k}_{0j}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell'}}^{\alpha} + \theta_{\mathbf{k}_{0j}}^{\alpha}) \right) \\
 & + U^{\uparrow\uparrow} \left( N_{\mathbf{k}_{0\ell'}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) = 0.
 \end{aligned} \tag{3.57}$$

To recapitulate, these conditions, applicable only in many-fold cases, ensure that the chemical potential  $\mu^{\uparrow}$  does not depend on any momentum index. There is one such relation for every combination  $\ell \neq \ell'$  for which  $N_{\mathbf{k}_{0\ell}}^{\uparrow}, N_{\mathbf{k}_{0\ell'}}^{\uparrow} \neq 0$ . As will be shown in a moment after performing the same calculations for  $\mu^{\downarrow}$ , these condition may be further simplified.

Now, suppose that  $a_{\mathbf{k}_{0i}}^{\downarrow}$  is non-zero for some value of  $i$ . Then the condition

$\mathcal{H}_{(1)} = 0$  leads to

$$\begin{aligned} \mu^\downarrow = \mu^{\downarrow*} = & -\epsilon_{\mathbf{k}_{0i}}^\downarrow - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\uparrow}{N_{\mathbf{k}_{0i}}^\downarrow}} \right]_{s_{\mathbf{k}_{0\ell}} \neq 0} \\ & + \frac{1}{N_s} \sum_{jj'j'} \sum_{\alpha} U^{\downarrow\alpha} \left( \frac{a_{\mathbf{k}_{0j'}}^\downarrow}{a_{\mathbf{k}_{0i}}^\downarrow} \right)^* a_{\mathbf{k}_{0j}}^\alpha (a_{\mathbf{k}_{0i'}}^\alpha)^* \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}. \end{aligned} \quad (3.58)$$

Analogously to the conclusions that were drawn for  $\mu^\uparrow$ , for  $\mu^\downarrow$  to be real, one finds that

$$\begin{aligned} & \sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0i} \\ n \geq 4}} \left( U^{\uparrow\downarrow} N_{\mathbf{k}_{0j}}^\uparrow \sin(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0i}}) \right. \\ & \left. + \sum_{\alpha} U^{\downarrow\alpha} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^\downarrow N_{-\mathbf{k}_{0i}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0i}}^\downarrow}} \sin(\theta_{-\mathbf{k}_{0j}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{-\mathbf{k}_{0i}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha) \right) = 0, \end{aligned} \quad (3.59)$$

and for the value of  $\mu^\downarrow$  to not depend on the momentum index  $i$ , one finds that

$$\begin{aligned} & \sum_{\alpha} U^{\downarrow\alpha} \left( \sum_{\substack{\mathbf{k}_{0j} = \pm \mathbf{k}_{0\ell'} \\ \mathbf{k}_{0\ell'} \neq \pm \mathbf{k}_{0\ell} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^\downarrow N_{-\mathbf{k}_{0\ell}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0\ell}}^\downarrow}} \cos(\theta_{-\mathbf{k}_{0j}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{-\mathbf{k}_{0\ell}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha) \right. \\ & \left. - \sum_{\substack{\mathbf{k}_{0j} = \pm \mathbf{k}_{0\ell} \\ \mathbf{k}_{0\ell} \neq \pm \mathbf{k}_{0\ell'} \\ n \geq 4}} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^\downarrow N_{-\mathbf{k}_{0\ell'}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0\ell'}}^\downarrow}} \cos(\theta_{-\mathbf{k}_{0j}}^\downarrow - \theta_{\mathbf{k}_{0\ell'}}^\downarrow - \theta_{-\mathbf{k}_{0\ell'}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha) \right) \\ & + U^{\downarrow\downarrow} \left( N_{\mathbf{k}_{0\ell'}}^\downarrow - N_{\mathbf{k}_{0\ell}}^\downarrow \right) + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^\uparrow - N_{\mathbf{k}_{0\ell}}^\uparrow \right) = 0, \end{aligned} \quad (3.60)$$

for every combination  $\ell \neq \ell'$  for which  $N_{\mathbf{k}_{0\ell}}^\downarrow, N_{\mathbf{k}_{0\ell'}}^\downarrow \neq 0$ ; cf. Eq. (3.51) and (3.57).

Note that if two opposite points in  $k$ -space are occupied by the condensate, i.e.  $N_{\mathbf{k}_{0\ell'}}^\alpha = N_{-\mathbf{k}_{0\ell}}^\alpha \wedge N_{\mathbf{k}_{0\ell}}^\alpha, N_{-\mathbf{k}_{0\ell}}^\alpha \neq 0$ , then for these, the coupled equations



(3.57) and (3.60) reduce to

$$\begin{aligned} U^{\uparrow\uparrow} \left( N_{-\mathbf{k}_{0\ell}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) + U^{\uparrow\downarrow} \cos(\gamma_{-\mathbf{k}_{0\ell}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{-\mathbf{k}_{0\ell}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) \\ = U^{\uparrow\uparrow} \left( N_{-\mathbf{k}_{0\ell}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) - U^{\uparrow\downarrow} \left( N_{-\mathbf{k}_{0\ell}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) = 0, \end{aligned} \quad (3.61)$$

$$\begin{aligned} U^{\downarrow\downarrow} \left( N_{-\mathbf{k}_{0\ell}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) + U^{\uparrow\downarrow} \cos(\gamma_{-\mathbf{k}_{0\ell}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{-\mathbf{k}_{0\ell}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) \\ = U^{\downarrow\downarrow} \left( N_{-\mathbf{k}_{0\ell}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) - U^{\uparrow\downarrow} \left( N_{-\mathbf{k}_{0\ell}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) = 0, \end{aligned} \quad (3.62)$$

which are uniquely solved by

$$N_{\mathbf{k}_{0\ell}}^{\uparrow} = N_{-\mathbf{k}_{0\ell}}^{\uparrow}, \quad N_{\mathbf{k}_{0\ell}}^{\downarrow} = N_{-\mathbf{k}_{0\ell}}^{\downarrow}, \quad (3.63)$$

with the single exception of when

$$\frac{(U^{\uparrow\downarrow})^2}{U^{\uparrow\uparrow}U^{\downarrow\downarrow}} = 1. \quad (3.64)$$

In other words, in the presence of interactions, if the condensate contains particles of opposite momenta, then there must be equally many such particles in the condensate.

The above conclusion also holds in the event that  $\mathbf{k}_{0\ell'}$  and  $\mathbf{k}_{0\ell}$  are non-parallel, and either  $N_{-\mathbf{k}_{0\ell}}^{\alpha} = 0$  or  $N_{\mathbf{k}_{0\ell'}}^{\alpha} = 0$ , provided  $N_{\mathbf{k}_{0\ell}}^{\alpha}, N_{\mathbf{k}_{0\ell'}}^{\alpha} \neq 0$ . That is, the coupled equations (3.57) and (3.60) reduce to

$$U^{\uparrow\uparrow} \left( N_{\mathbf{k}_{0\ell'}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) = 0, \quad (3.65)$$

$$U^{\downarrow\downarrow} \left( N_{\mathbf{k}_{0\ell'}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) = 0, \quad (3.66)$$

which are uniquely solved by

$$N_{\mathbf{k}_{0\ell}}^{\uparrow} = N_{\mathbf{k}_{0\ell'}}^{\uparrow}, \quad N_{\mathbf{k}_{0\ell}}^{\downarrow} = N_{\mathbf{k}_{0\ell'}}^{\downarrow}, \quad (3.67)$$

with the single exception of when

$$\frac{(U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}))^2}{U^{\uparrow\uparrow}U^{\downarrow\downarrow}} = 1. \quad (3.68)$$

If, on the other hand,  $N_{-\mathbf{k}_{0\ell}}^\alpha, N_{-\mathbf{k}_{0\ell'}}^\alpha \neq 0$ , then Eq. (3.63) may be applied to simplify Eq. (3.57) and (3.60). Note that in this case, factors on the form

$$\begin{aligned} \sqrt{\frac{N_{-\mathbf{k}_{0j}}^\beta N_{-\mathbf{k}_{0\ell}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0\ell}}^\beta}} &= \sqrt{\frac{N_{\mathbf{k}_{0j}}^\beta N_{\mathbf{k}_{0\ell}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0\ell}}^\beta}} \\ &= \left\{ \begin{array}{ll} N_{\mathbf{k}_{0j}}^\alpha, & \alpha = \beta \\ \sqrt{\frac{N_{\mathbf{k}_{0j}}^\beta N_{\mathbf{k}_{0j}}^\alpha N_{\mathbf{k}_{0j}}^\alpha}{N_{\mathbf{k}_{0j}}^\beta}} = N_{\mathbf{k}_{0j}}^\alpha, & \alpha \neq \beta \end{array} \right\} = N_{\mathbf{k}_{0j}}^\alpha, \end{aligned} \quad (3.69)$$

where the relation (3.43) was used in the case of  $\alpha \neq \beta$ , and  $N_{\pm\mathbf{k}_{0j}}^\alpha \neq 0$  was assumed. Eq. (3.57) may now be written as

$$\begin{aligned} &\sum_{\alpha} U^{\uparrow\alpha} \left( N_{\mathbf{k}_{0\ell'}}^\alpha \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell'} \\ \mathbf{k}_{0\ell'} \neq \pm\mathbf{k}_{0\ell} \\ n \geq 4}} \cos(\theta_{-\mathbf{k}_{0j}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{-\mathbf{k}_{0\ell}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha) \right. \\ &\quad \left. - N_{\mathbf{k}_{0\ell}}^\alpha \sum_{\substack{\mathbf{k}_{0j}=\pm\mathbf{k}_{0\ell} \\ \mathbf{k}_{0\ell} \neq \pm\mathbf{k}_{0\ell'} \\ n \geq 4}} \cos(\theta_{-\mathbf{k}_{0j}}^\uparrow - \theta_{\mathbf{k}_{0\ell'}}^\uparrow - \theta_{-\mathbf{k}_{0\ell'}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha) \right) \\ &\quad + U^{\uparrow\uparrow} \left( N_{\mathbf{k}_{0\ell'}}^\uparrow - N_{\mathbf{k}_{0\ell}}^\uparrow \right) + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^\downarrow - N_{\mathbf{k}_{0\ell}}^\downarrow \right) = 0. \end{aligned} \quad (3.70)$$

Now, due to relation (3.37),

$$\gamma_{\mathbf{k}_{0\ell}} + \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow = \gamma_{-\mathbf{k}_{0\ell}} + \theta_{-\mathbf{k}_{0\ell}}^\downarrow - \theta_{-\mathbf{k}_{0\ell}}^\uparrow \quad (3.71)$$

$$\Rightarrow \theta_{\mathbf{k}_{0\ell}}^\uparrow + \theta_{-\mathbf{k}_{0\ell}}^\downarrow = \theta_{-\mathbf{k}_{0\ell}}^\uparrow + \theta_{\mathbf{k}_{0\ell}}^\downarrow + \gamma_{-\mathbf{k}_{0\ell}} - \gamma_{\mathbf{k}_{0\ell}} = \theta_{-\mathbf{k}_{0\ell}}^\uparrow + \theta_{\mathbf{k}_{0\ell}}^\downarrow \pm \pi. \quad (3.72)$$

Therefore, expressions on the form

$$\cos(\theta_{-\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0\ell'}}^\uparrow - \theta_{-\mathbf{k}_{0\ell'}}^\downarrow + \theta_{\mathbf{k}_{0\ell}}^\downarrow) + \cos(\theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0\ell'}}^\uparrow - \theta_{-\mathbf{k}_{0\ell'}}^\downarrow + \theta_{-\mathbf{k}_{0\ell}}^\downarrow) = 0, \quad (3.73)$$

and (3.70) reduces to

$$\begin{aligned} &U^{\uparrow\uparrow} \left( N_{\mathbf{k}_{0\ell'}}^\uparrow - N_{\mathbf{k}_{0\ell}}^\uparrow \right) \left( 1 - 2 \cos(\theta_{-\mathbf{k}_{0\ell'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{-\mathbf{k}_{0\ell}}^\uparrow + \theta_{\mathbf{k}_{0\ell'}}^\uparrow) \right) \\ &\quad + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^\downarrow - N_{\mathbf{k}_{0\ell}}^\downarrow \right) = 0. \end{aligned} \quad (3.74)$$

Conversely, Eq. (3.60) reduces to

$$U^{\downarrow\downarrow} \left( N_{\mathbf{k}_{0\ell'}}^{\downarrow} - N_{\mathbf{k}_{0\ell}}^{\downarrow} \right) \left( 1 - 2 \cos(\theta_{-\mathbf{k}_{0\ell'}}^{\downarrow} - \theta_{\mathbf{k}_{0\ell}}^{\downarrow} - \theta_{-\mathbf{k}_{0\ell}}^{\downarrow} + \theta_{\mathbf{k}_{0\ell'}}^{\downarrow}) \right) \\ + U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}) \left( N_{\mathbf{k}_{0\ell'}}^{\uparrow} - N_{\mathbf{k}_{0\ell}}^{\uparrow} \right) = 0. \quad (3.75)$$

Again, these are uniquely solved by

$$N_{\mathbf{k}_{0\ell}}^{\uparrow} = N_{\mathbf{k}_{0\ell'}}^{\uparrow}, \quad N_{\mathbf{k}_{0\ell}}^{\downarrow} = N_{\mathbf{k}_{0\ell'}}^{\downarrow}, \quad (3.76)$$

with the exception of when

$$\frac{(U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}))^2}{U^{\uparrow\uparrow} U^{\downarrow\downarrow} (1-A)(1-B)} = 1, \quad A, B \neq 1, \quad (3.77)$$

where

$$A \equiv 2 \cos(\theta_{-\mathbf{k}_{0\ell'}}^{\uparrow} - \theta_{\mathbf{k}_{0\ell}}^{\uparrow} - \theta_{-\mathbf{k}_{0\ell}}^{\uparrow} + \theta_{\mathbf{k}_{0\ell'}}^{\uparrow}), \quad (3.78)$$

$$B \equiv 2 \cos(\theta_{-\mathbf{k}_{0\ell'}}^{\downarrow} - \theta_{\mathbf{k}_{0\ell}}^{\downarrow} - \theta_{-\mathbf{k}_{0\ell}}^{\downarrow} + \theta_{\mathbf{k}_{0\ell'}}^{\downarrow}). \quad (3.79)$$

Additionally, because Eq. (3.63) was used, one must also have

$$\frac{(U^{\uparrow\downarrow})^2}{U^{\uparrow\uparrow} U^{\downarrow\downarrow}} \neq 1, \quad (3.80)$$

in order to ensure uniqueness of the solution. To recapitulate, due to the requirement that  $\mu^{\uparrow}$  and  $\mu^{\downarrow}$  be real and invariant with respect to momentum indices, the conclusions drawn so far imply that if the condensate comprises particles of different momenta, then the fractions of particles of a specific pseudospin state carrying the respective momenta, must be equal; that is,

$$N_{\mathbf{k}_{0\ell}}^{\uparrow} = N_{\mathbf{k}_{0\ell'}}^{\uparrow}, \quad N_{\mathbf{k}_{0\ell}}^{\downarrow} = N_{\mathbf{k}_{0\ell'}}^{\downarrow}, \quad (3.81)$$

for all combinations of  $\ell$  and  $\ell' \neq \ell$  for which there are particles present in the condensate carrying the momenta  $\mathbf{k}_{0\ell}$  and  $\mathbf{k}_{0\ell'}$ . For non-zero condensate particle numbers, one may therefore neglect the momentum index altogether. Assuming the condensate comprises particles of  $f$  distinct momenta, one may write

$$N_0^{\uparrow}/f \equiv N_{\mathbf{k}_{0\ell}}^{\uparrow}, \quad (3.82)$$

$$N_0^{\downarrow}/f \equiv N_{\mathbf{k}_{0\ell}}^{\downarrow}, \quad (3.83)$$

where  $N_0^\alpha$  is the total number of condensate particles of pseudospin  $\alpha$ , and  $\ell$  is any of the  $f$  values for which  $N_{\mathbf{k}_{0\ell}}^\alpha \neq 0$ . The above conclusions do not *necessarily* hold, however, in the event that either

$$\frac{(U^{\uparrow\downarrow})^2}{U^{\uparrow\uparrow}U^{\downarrow\downarrow}} = 1 \quad (3.84)$$

in general; or

$$\frac{(U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}))^2}{U^{\uparrow\uparrow}U^{\downarrow\downarrow}} = 1 \quad (3.85)$$

if  $\mathbf{k}_{0\ell'}$  and  $\mathbf{k}_{0\ell}$  are non-parallel, and either  $N_{-\mathbf{k}_{0\ell}}^\alpha = 0$  or  $N_{-\mathbf{k}_{0\ell'}}^\alpha = 0$ ; or

$$\frac{(U^{\uparrow\downarrow} \cos(\gamma_{\mathbf{k}_{0\ell'}} - \gamma_{\mathbf{k}_{0\ell}}))^2}{U^{\uparrow\uparrow}U^{\downarrow\downarrow} (1-A)(1-B)} = 1, \quad A, B \neq 1, \quad (3.86)$$

if  $N_{-\mathbf{k}_{0\ell}}^\alpha, N_{-\mathbf{k}_{0\ell'}}^\alpha \neq 0$ , where  $A$  and  $B$  are defined in Eq. (3.78) and (3.79), respectively.

In summary, the expression for  $\mu^\uparrow$  is

$$\begin{aligned} \mu^\uparrow = & -\epsilon_{\mathbf{k}_{0i}}^\uparrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\downarrow}{N_{\mathbf{k}_{0i}}^\uparrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\ & + \frac{1}{N_s} \sum_{j'j'} \sum_{\alpha} U^{\uparrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^\uparrow N_{\mathbf{k}_{0j}}^\alpha N_{\mathbf{k}_{0i'}}^\alpha}{N_{\mathbf{k}_{0i}}^\uparrow}} \\ & \left. \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0i}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right]_{\exists N_{\mathbf{k}_{0i}}^\uparrow : N_{\mathbf{k}_{0i}}^\uparrow \neq 0}, \end{aligned} \quad (3.87)$$

where the square brackets  $[\dots]_{\exists N_{\mathbf{k}_{0i}}^\uparrow : N_{\mathbf{k}_{0i}}^\uparrow \neq 0}$  indicate that the terms enclosed by them are present only if there exists a non-zero  $N_{\mathbf{k}_{0i}}^\uparrow$  for some value of  $i$ .

Conversely, the expression for  $\mu^\downarrow$  is

$$\begin{aligned} \mu^\downarrow = & -\epsilon_{\mathbf{k}_{0i}}^\downarrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_{\mathbf{k}_{0i}}^\uparrow}{N_{\mathbf{k}_{0i}}^\downarrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\ & + \frac{1}{N_s} \sum_{j'i'j'} \sum_{\alpha} U^{\downarrow\alpha} \sqrt{\frac{N_{\mathbf{k}_{0j'}}^\downarrow N_{\mathbf{k}_{0j}}^\alpha N_{\mathbf{k}_{0i'}}^\alpha}{N_{\mathbf{k}_{0i}}^\downarrow}} \\ & \left. \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right]_{\exists N_{\mathbf{k}_{0i}}^\downarrow : N_{\mathbf{k}_{0i}}^\downarrow \neq 0}, \end{aligned} \quad (3.88)$$

where the square brackets  $[\dots]_{\exists N_{\mathbf{k}_{0i}}^\downarrow : N_{\mathbf{k}_{0i}}^\downarrow \neq 0}$  indicate that the terms enclosed by them are present only if there exists a non-zero  $N_{\mathbf{k}_{0i}}^\downarrow$  for some value of  $i$ . These expressions were derived by demanding that  $\mathcal{H}_{(1)}$ —which comprises all terms linear in condensate fluctuations, and is given by Eq. (3.28)—is zero, a requirement that follows from the assumption that the free energy is minimal with respect to the variational parameters introduced by applying mean field theory to condensate particle operators. Furthermore, to ensure that the  $\mu^\alpha$  are real, the conditions (3.51) and (3.59) must be satisfied. Finally, to ensure that the expressions (3.87) and (3.88) for  $\mu^\alpha$  do not depend on the momentum index  $i$ , the conditions (3.37) and (3.43) must be satisfied if there is a non-zero SOC present, and the conditions (3.57) and (3.60) must be satisfied if there are interactions present. The conditions regarding interactions uniquely reduce to (3.81), save the cases for which either Eq. (3.84), (3.85) or (3.86) hold; that is, the fractions of condensed particles of a particular pseudospin state carrying any of the  $f$  momenta presumed carried by particles in the condensate, are all equal. All of these constraints lead to a significant reduction in the number of degrees of freedom with respect to the variational parameters involved. If Eq. (3.81) holds, the expressions for

the chemical potentials reduce to

$$\begin{aligned}
 \mu^\uparrow = & -\epsilon_{\mathbf{k}_{0i}}^\uparrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_0^\downarrow}{N_0^\uparrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\
 & + \frac{1}{N_s f} \left( \sum_{j i' j'} \sum_{\alpha} \right)''' U^{\uparrow\alpha} N_0^\alpha \\
 & \left. \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0i}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right]_{\exists N_{\mathbf{k}_{0i}}^\uparrow : N_{\mathbf{k}_{0i}}^\uparrow \neq 0},
 \end{aligned} \tag{3.89}$$

$$\begin{aligned}
 \mu^\downarrow = & -\epsilon_{\mathbf{k}_{0i}}^\downarrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_0^\uparrow}{N_0^\downarrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\
 & + \frac{1}{N_s f} \left( \sum_{j i' j'} \sum_{\alpha} \right)''' U^{\downarrow\alpha} N_0^\alpha \\
 & \left. \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right]_{\exists N_{\mathbf{k}_{0i}}^\downarrow : N_{\mathbf{k}_{0i}}^\downarrow \neq 0}.
 \end{aligned} \tag{3.90}$$

Above, in the respective expressions for  $\mu^\beta$ , the sum  $\left( \sum_{j i' j'} \sum_{\alpha} \right)'''$  goes over the subset of values of  $j, i', j', \alpha$  for which  $N_{\mathbf{k}_{0j}}^\alpha \neq 0$ ,  $N_{\mathbf{k}_{0i'}}^\alpha \neq 0$  and  $N_{\mathbf{k}_{0j'}}^\beta \neq 0$ . The primed parentheses  $(\dots)'''$  will be re-used in related sums in later expressions, generally signaling that the sums which they enclose, only cover values of the summand that are non-zero before the application of relation (3.83); precisely what this entails will be specified under the respective expressions.

The complete expression for  $\mathcal{H}$  after applying mean field theory is

$$\mathcal{H} \approx \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2, \tag{3.91}$$

where

$$\begin{aligned}
 \mathcal{H}_0 \approx & \sum_i \sum_{\alpha\beta} \eta_{\mathbf{k}_{0i}}^{\alpha\beta} (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0i}}^\beta \\
 & + \frac{1}{2N_s} \sum_{ij i' j'} \sum_{\alpha\beta} U^{\alpha\beta} (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta a_{\mathbf{k}_{0j'}}^\alpha \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}},
 \end{aligned} \tag{3.92}$$

$$\begin{aligned}
 \mathcal{H}_1 \approx \frac{1}{N_s} \sum_{\mathbf{k}}' \sum_{ijj'} \sum_{\alpha\beta} U^{\alpha\beta} & \left( (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* a_{\mathbf{k}_{0i'}}^\beta A_{\mathbf{k}}^\alpha \right. \\
 & \left. + (a_{\mathbf{k}_{0i'}}^\beta)^* a_{\mathbf{k}_{0j}}^\beta a_{\mathbf{k}_{0i}}^\alpha A_{\mathbf{k}}^{\alpha\dagger} \right) \delta_{\mathbf{k}+\mathbf{k}_{0i'}, \mathbf{k}_{0j}+\mathbf{k}_{0i}},
 \end{aligned} \tag{3.93}$$

$$\begin{aligned}
 \mathcal{H}_2 \approx \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^\beta & + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij} \sum_{\alpha\beta} U^{\alpha\beta} \left( \left( (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* A_{\mathbf{k}}^\beta A_{\mathbf{k}'}^\alpha \right. \right. \\
 & + a_{\mathbf{k}_{0i}}^\alpha a_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}'}^{\alpha\dagger} A_{\mathbf{k}}^{\beta\dagger} \left. \right) \delta_{\mathbf{k}+\mathbf{k}', \mathbf{k}_{0i}+\mathbf{k}_{0j}} \\
 & + \left( (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\alpha \right. \\
 & + (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0j}}^\alpha A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\beta \\
 & + a_{\mathbf{k}_{0i}}^\alpha (a_{\mathbf{k}_{0j}}^\beta)^* A_{\mathbf{k}'}^{\alpha\dagger} A_{\mathbf{k}}^\beta \\
 & \left. \left. + a_{\mathbf{k}_{0i}}^\alpha (a_{\mathbf{k}_{0j}}^\alpha)^* A_{\mathbf{k}'}^{\beta\dagger} A_{\mathbf{k}}^\beta \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}} \right) \\
 = \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^\beta & + \frac{1}{2N_s} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij} \sum_{\alpha\beta} U^{\alpha\beta} \left( \left( (a_{\mathbf{k}_{0i}}^\alpha)^* (a_{\mathbf{k}_{0j}}^\beta)^* A_{\mathbf{k}}^\beta A_{\mathbf{k}'}^\alpha \right. \right. \\
 & + \text{H.c.} \left. \right) \delta_{\mathbf{k}+\mathbf{k}', \mathbf{k}_{0i}+\mathbf{k}_{0j}} \\
 & + \left( \left( (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0j}}^\beta A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\alpha \right. \right. \\
 & + (a_{\mathbf{k}_{0i}}^\alpha)^* a_{\mathbf{k}_{0j}}^\alpha A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\beta \\
 & \left. \left. + \text{H.c.} \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}} \right),
 \end{aligned} \tag{3.94}$$

where the reader should note that the sums over momenta in the above expression for  $\mathcal{H}_2$  are no longer constrained; analogously to what was done in the process of obtaining the expression (2.82), the condensate fluctuations were implicitly relabeled:

$$\delta A_{\mathbf{k}_{0i}}^\alpha \equiv A_{\mathbf{k}_{0i}}^\alpha, \tag{3.95}$$

such that  $A_{\mathbf{k}_{0i}}^\alpha$  hereafter refers to the condensate fluctuation about the expectation value  $a_{\mathbf{k}_{0i}}^\alpha$ . Assuming Eq. (3.81) holds,  $\mathcal{H}_0$  reduces to

$$\begin{aligned}
 \mathcal{H}_0 &\approx \frac{1}{f} \left( \sum_i \sum_{\alpha\beta} \right)''' \sqrt{N_0^\alpha N_0^\beta} \eta_{\mathbf{k}_{0i}}^{\alpha\beta} e^{-i(\theta_{\mathbf{k}_{0i}}^\beta - \theta_{\mathbf{k}_{0i}}^\alpha)} \\
 &\quad + \frac{1}{2N_s f^2} \left( \sum_{ij'j'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\alpha N_0^\beta \\
 &\quad \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= -\frac{1}{N_s f^2} \left( \sum_i \sum_\alpha \right)''' N_0^\alpha \left( \sum_{j'j'} \sum_\beta \right)''' U^{\alpha\beta} N_0^\beta \\
 &\quad \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &\quad + \frac{1}{2N_s f^2} \left( \sum_{ij'j'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\alpha N_0^\beta \\
 &\quad \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= -\frac{1}{2N_s f^2} \left( \sum_{ij'j'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\alpha N_0^\beta \\
 &\quad \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} ,
 \end{aligned} \tag{3.96}$$

where the second equality follows from inserting the expressions (3.89) and (3.90) for the chemical potentials, as well as applying (3.37) to the off-diagonal single-particle terms; the sum  $\left( \sum_i \sum_{\alpha\beta} \right)'''$  goes over the subset of values of  $i, \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$  and  $N_{\mathbf{k}_{0i}}^\beta \neq 0$ ; and, conversely, the sum  $\left( \sum_{ij'j'} \sum_{\alpha\beta} \right)'''$  goes over the subset of values of  $i, j, i', j', \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$ ,  $N_{\mathbf{k}_{0j}}^\beta \neq 0$ ,  $N_{\mathbf{k}_{0i'}}^\beta \neq 0$  and  $N_{\mathbf{k}_{0j'}}^\alpha \neq 0$ . Note that further simplifications may be made to Eq. (3.96) once a specific configuration of non-zero condensate particle numbers is assumed; for instance, if the configuration includes non-zero condensate particle numbers associated with opposite momenta, then Eq. (3.73) may be used to cancel certain terms. Note also that in the final expression in Eq. (3.96), the condensate numbers  $N_0^\alpha$  and  $N_0^\beta$  are *no longer* variational parameters; the free energy  $F$  has implicitly already



been minimized with respect to these in the derivation of the expressions (3.89) and (3.90) for the chemical potentials, which may be inverted to acquire explicit expressions for the condensate numbers, akin to what was done in order to arrive at the expression (2.85). Furthermore,

$$\mathcal{H}_1 \approx \frac{1}{N_s f^{\frac{3}{2}}} \sum_{\mathbf{k}}' \left( \sum_{ijj'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\beta \sqrt{N_0^\alpha} \cdot \left( e^{-i(\theta_{\mathbf{k}_{0i'}}^\beta - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta)} A_{\mathbf{k}}^\alpha + \text{H.c.} \right) \delta_{\mathbf{k}+\mathbf{k}_{0i'}, \mathbf{k}_{0j}+\mathbf{k}_{0i}}, \quad (3.97)$$

where, analogously to before, the sum  $\left( \sum_{ijj'} \sum_{\alpha\beta} \right)'''$  goes over the subset of values of  $i, j, i', \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$ ,  $N_{\mathbf{k}_{0j}}^\beta \neq 0$  and  $N_{\mathbf{k}_{0i'}}^\beta \neq 0$ ; and

$$\begin{aligned} \mathcal{H}_2 \approx & \sum_{\mathbf{k}} \sum_{\alpha\beta} \eta_{\mathbf{k}}^{\alpha\beta} A_{\mathbf{k}}^{\alpha\dagger} A_{\mathbf{k}}^\beta \\ & + \frac{1}{2N_s f} \sum_{\mathbf{k}\mathbf{k}'} \left( \sum_{ij} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} \sqrt{N_0^\alpha N_0^\beta} \\ & \cdot \left( \left( e^{-i(-\theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta)} A_{\mathbf{k}}^\beta A_{\mathbf{k}'}^\alpha + \text{H.c.} \right) \delta_{\mathbf{k}+\mathbf{k}', \mathbf{k}_{0i}+\mathbf{k}_{0j}} \right. \\ & \left. + \left( e^{-i(-\theta_{\mathbf{k}_{0i}}^\alpha + \theta_{\mathbf{k}_{0j}}^\beta)} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\alpha + \text{H.c.} \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}} \right) \\ & + \frac{1}{2N_s f} \sum_{\mathbf{k}\mathbf{k}'} \left( \sum_{ij} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\alpha \\ & \cdot \left( e^{-i(-\theta_{\mathbf{k}_{0i}}^\alpha + \theta_{\mathbf{k}_{0j}}^\alpha)} A_{\mathbf{k}}^{\beta\dagger} A_{\mathbf{k}'}^\beta + \text{H.c.} \right) \delta_{\mathbf{k}_{0i}+\mathbf{k}, \mathbf{k}'+\mathbf{k}_{0j}}, \end{aligned} \quad (3.98)$$

where the first instance of the sum  $\left( \sum_{ij} \sum_{\alpha\beta} \right)'''$  goes over the subset of values of  $i, j, \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$  and  $N_{\mathbf{k}_{0j}}^\beta \neq 0$ , and the second instance goes over the subset of values of  $i, j, \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$  and  $N_{\mathbf{k}_{0j}}^\alpha \neq 0$ . Note that these expressions reduce to those presented by van Oosten *et al.* in Ref. [46] upon equating and neglecting all pseudospin and momentum indices, as well as neglecting all phases.

# CHAPTER 4

## *Pure Condensate on a Square Lattice*

In this section, we explore the analytic behavior of a pure condensate on a square lattice. The lattice is oriented as illustrated in Fig. 2.3. The analytic results, in particular the phase diagram derived by minimization of the free energy  $F$ , will be compared to the numerical results by P. N. Galteland *et al.* [45] for the same system.

For a pure condensate, any contribution to the Hamiltonian  $\mathcal{H}$  proportional to an excitation operator, is neglected. Assuming the relation (3.63) holds, the expression for  $\mathcal{H}$  is

$$\mathcal{H} = \mathcal{H}_0 \stackrel{(3.96)}{\approx} - \frac{1}{2N_s f^2} \left( \sum_{ijj'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} N_0^\alpha N_0^\beta \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}, \quad (4.1)$$

where  $N_s$  is the number of lattice points;  $f$  is the number of distinct momenta carried by the bosons comprising the condensate;  $U^{\alpha\beta}$  are pseudospin-dependent interaction couplings;  $N_0^\alpha$  is the number of condensed particles in pseudospin state  $\alpha$ ;  $\theta_{\mathbf{k}_{0i}}^\alpha$  are the mean field phases defined in Eq. (3.27);  $\mathbf{k}_{0i}$  are the condensate momenta; the delta function expresses conservation of momentum; and the sum  $\left( \sum_{ijj'} \sum_{\alpha\beta} \right)'''$  goes over the subset of values of  $i, j, i', j', \alpha, \beta$  for which  $N_{\mathbf{k}_{0i}}^\alpha \neq 0$ ,  $N_{\mathbf{k}_{0j}}^\beta \neq 0$ ,  $N_{\mathbf{k}_{0i'}}^\beta \neq 0$  and  $N_{\mathbf{k}_{0j'}}^\alpha \neq 0$ , where the  $N_{\mathbf{k}_{0i}}^\alpha$  are the mean field condensate numbers defined in Eq. (3.27). Note that the  $N_0^\alpha$  are *not* variational parameters;  $F$  has implicitly already been minimized with respect to these in the derivation of the expressions (3.89) and (3.90) for the chemical potentials, which may be inverted to acquire explicit expressions for the condensate numbers. The variational parameters that must be determined by minimization of  $F$ , are the phases  $\theta_{\mathbf{k}_{0i}}^\alpha$ , and the

magnitude of the condensate momenta

$$\sqrt{2}k_0 \equiv |\mathbf{k}_{0i}| \quad (4.2)$$

in the event that they are non-zero. Because momentum is quantized,  $k_0$  is a discrete variable, but will be approximated as a continuous variable for the remainder of this chapter, so that one may differentiate  $F$  with respect to  $k_0$ . Furthermore, the free energy  $F$  is

$$F \stackrel{(2.105)}{=} \mathcal{H}_0; \quad (4.3)$$

and the chemical potentials are given by Eq. (3.89) and (3.90):

$$\begin{aligned} \mu^\uparrow = & -\epsilon_{\mathbf{k}_{0i}}^\uparrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_0^\downarrow}{N_0^\uparrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\ & + \frac{1}{N_{sf}} \left( \sum_{j'i'j'} \sum_{\alpha} \right)''' U^{\uparrow\alpha} N_0^\alpha \\ & \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0i}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \left. \right]_{\exists N_{\mathbf{k}_{0i}}^\uparrow : N_{\mathbf{k}_{0i}}^\uparrow \neq 0}, \end{aligned} \quad (4.4)$$

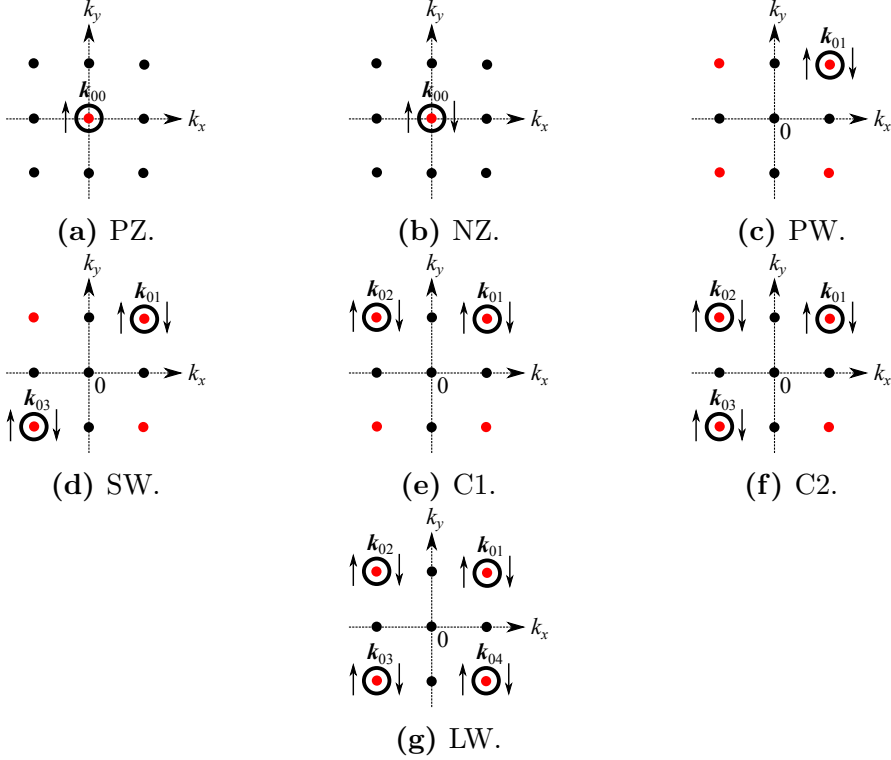
$$\begin{aligned} \mu^\downarrow = & -\epsilon_{\mathbf{k}_{0i}}^\downarrow + \left[ - \left[ |s_{\mathbf{k}_{0i}}| \sqrt{\frac{N_0^\uparrow}{N_0^\downarrow}} \right]_{s_{\mathbf{k}_{0i}} \neq 0} \right. \\ & + \frac{1}{N_{sf}} \left( \sum_{j'i'j'} \sum_{\alpha} \right)''' U^{\downarrow\alpha} N_0^\alpha \\ & \cdot \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0i}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \left. \right]_{\exists N_{\mathbf{k}_{0i}}^\downarrow : N_{\mathbf{k}_{0i}}^\downarrow \neq 0}, \end{aligned} \quad (4.5)$$

where, in the respective expressions for  $\mu^\beta$ , the sum  $\left( \sum_{j'i'j'} \sum_{\alpha} \right)'''$  goes over the subset of values of  $j, i', j', \alpha$  for which  $N_{\mathbf{k}_{0j}}^\alpha \neq 0$ ,  $N_{\mathbf{k}_{0i'}}^\alpha \neq 0$  and  $N_{\mathbf{k}_{0j'}}^\beta \neq 0$ ; and the quantities  $\epsilon_{\mathbf{k}_{0i}}^\alpha$  and  $|s_{\mathbf{k}_{0i}}|$  are given by

$$|s_{\mathbf{k}_{0i}}| \stackrel{(2.56),(4.2)}{=} 2\sqrt{2}\lambda_R |\sin(k_0 a)|, \quad (4.6)$$

$$\epsilon_{\mathbf{k}_{0i}} \stackrel{(2.57),(4.2)}{=} 4t \cos(k_0 a). \quad (4.7)$$

In order to write out the sums  $\left(\sum_{ij'j'} \sum_{\alpha\beta}\right)'''$  and  $\left(\sum_{ji'j'} \sum_{\alpha}\right)'''$  in the expressions for the Hamiltonian (4.1) and the chemical potentials (4.4) and (4.5), a configuration of condensate numbers  $N_{\mathbf{k}_{0i}}^{\alpha}$  must be assumed. In assuming the form (4.1) of  $\mathcal{H}$ , equal fractions of condensed bosons of a specific pseudospin carrying any of the available condensate momenta, was implicitly assumed. The condition (3.32) further limits the possible configurations in cases for which the SOC is non-zero. All remaining configurations that are not equivalent upon a rotation or an interchange of pseudospin states, are illustrated in Fig. 4.1.



**Figure 4.1:** All condensate configurations remaining after taking into consideration the constraints (3.32) and (3.63). All possible condensate momenta for a set of input parameters are colored in red. Condensate momenta assumed carried by the particles in the condensate are encircled and labeled  $\mathbf{k}_{0i}$ . The arrows indicate the pseudospin states present in the condensate. The configurations (a) and (b) are the polarized (PZ) and non-polarized (NZ) zero-momentum phase, respectively; the names are given due to their respective pseudospin imbalances, as well as the associated condensate momentum. The configurations (c), (d) and (g) are the plane (PW), stripe (SW) and lattice (LW) wave phase, respectively; the names are given due to the wave patterns they produce in real space. The configurations (e) and (f) have been given the arbitrary names C1 and C2, and will be shown to be impossible in the calculations proceeding this figure. The configurations (a)–(d) were analyzed numerically by P. N. Galteland *et al.* in Ref. [45]; the LW phase was not taken into account.

The configurations C1 and C2 in Fig. 4.1 may be dismissed as they do not satisfy the condition (3.51) that renders  $\mu^\uparrow$  real. These are four-fold cases, as there are four available condensate momenta. In both cases, the second term in the sum over  $j$  in Eq. (3.51) is zero, and the condition reduces to

$$\sum_{\substack{j \\ \mathbf{k}_{0j} \neq \pm \mathbf{k}_{0i} \\ n \geq 4}} N_{\mathbf{k}_{0j}}^\downarrow \sin(\gamma_{\mathbf{k}_{0j}} - \gamma_{\mathbf{k}_{0i}}) = 0. \quad (4.8)$$

In both cases, choose  $\mathbf{k}_{0i} = \mathbf{k}_{01}$ . Then Eq. (4.8) reduces to

$$N_{\mathbf{k}_{02}}^\downarrow = 0, \quad (4.9)$$

which contradicts the initial assumption  $N_{\mathbf{k}_{02}}^\downarrow \neq 0$ . Thus, neither of these configurations produces a real-valued chemical potential  $\mu^\uparrow$ , and may be dismissed.

For the PZ, NZ, PW and SW phase, the condition (3.51) is trivially satisfied, as the left-hand side is zero. For the LW phase, using Eq. (3.63) and choosing  $\mathbf{k}_{0i} = \mathbf{k}_{01}$ , condition (3.51) yields

$$\begin{aligned} & U^{\uparrow\downarrow} N_0^\downarrow (\sin(\gamma_{\mathbf{k}_{02}} - \gamma_{\mathbf{k}_{01}}) + \sin(\gamma_{\mathbf{k}_{04}} - \gamma_{\mathbf{k}_{01}})) \\ & + U^{\uparrow\downarrow} N_0^\downarrow \left( \sin(\theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{02}}^\downarrow) \right. \\ & \quad \left. + \sin(\theta_{\mathbf{k}_{02}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{04}}^\downarrow) \right) \\ & + U^{\uparrow\uparrow} N_0^\uparrow \left( \sin(\theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{02}}^\uparrow) \right. \\ & \quad \left. + \sin(\theta_{\mathbf{k}_{02}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{04}}^\uparrow) \right) \end{aligned} \quad (4.10)$$

$$\begin{aligned} & \stackrel{(3.50),(3.72)}{=} 2U^{\uparrow\uparrow} N_0^\uparrow \sin(\theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{02}}^\uparrow) = 0. \\ & \Rightarrow \theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{02}}^\uparrow = m^\uparrow \pi, \quad m^\uparrow \in \{0, 1\}. \end{aligned} \quad (4.11)$$

Conversely, for the LW phase, condition (3.59) leads to

$$\theta_{\mathbf{k}_{04}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{02}}^\downarrow = m^\downarrow \pi, \quad m^\downarrow \in \{0, 1\}. \quad (4.12)$$

In fact, using

$$\gamma_{\mathbf{k}_{0\ell}} + \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow = \gamma_{\mathbf{k}_{0\ell'}} + \theta_{\mathbf{k}_{0\ell'}}^\downarrow - \theta_{\mathbf{k}_{0\ell'}}^\uparrow \quad (4.13)$$

$$\Rightarrow \theta_{\mathbf{k}_{0\ell'}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\downarrow = \gamma_{\mathbf{k}_{0\ell}} - \gamma_{\mathbf{k}_{0\ell'}} + \theta_{\mathbf{k}_{0\ell'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow \quad (4.14)$$

one finds that

$$\theta_{\mathbf{k}_{04}}^{\uparrow} - \theta_{\mathbf{k}_{01}}^{\uparrow} - \theta_{\mathbf{k}_{03}}^{\uparrow} + \theta_{\mathbf{k}_{02}}^{\uparrow} = \theta_{\mathbf{k}_{04}}^{\downarrow} - \theta_{\mathbf{k}_{01}}^{\downarrow} - \theta_{\mathbf{k}_{03}}^{\downarrow} + \theta_{\mathbf{k}_{02}}^{\downarrow} + \pi \quad (4.15)$$

$$\Rightarrow m^{\uparrow} = m^{\downarrow} + 1 \equiv m \pmod{2}. \quad (4.16)$$

Note that the results (4.11) and (4.12) render  $A, B \neq 1$ , where  $A$  and  $B$  are defined in Eq. (3.78) and (3.79), respectively, in turn rendering the quantity (3.77) well-defined provided  $U^{\uparrow\uparrow}, U^{\downarrow\downarrow} \neq 0$ .

The sums  $\left(\sum_{iji'j'} \sum_{\alpha\beta}\right)'''$  and  $\left(\sum_{jj'j'} \sum_{\alpha}\right)'''$  in the expressions for the Hamiltonian (4.1) and the chemical potentials (4.4) and (4.5) may now be written out for each of the remaining phases. The sets of values that the momentum and pseudospin indices may take for the respective phases that are not equivalent upon a rotation or an interchange of pseudospin states, are summarized in Tab. 4.1.

**Table 4.1:** Sets of values for momentum and pseudospin indices

Phase	Momentum indices	Pseudospin indices
PZ	{0}	{↑}
NZ	{0}	{↑, ↓}
PW	{1}	{↑, ↓}
SW	{1, 3}	{↑, ↓}
LW	{1, 2, 3, 4}	{↑, ↓}

Table of the sets of values for momentum and pseudospin indices in the sums  $\left(\sum_{iji'j'} \sum_{\alpha\beta}\right)'''$  and  $\left(\sum_{jj'j'} \sum_{\alpha}\right)'''$  for the respective phases that are not equivalent upon a rotation or an interchange of pseudospin states. The sums in question appear in the expressions for the Hamiltonian (4.1) and the chemical potentials (4.4) and (4.5).

When both the SOC term and the interaction term are present in the expressions (4.4) and (4.5) for the chemical potentials, they may be rewritten as two coupled equations second-degree in  $\sqrt{N_0^{\uparrow}}$  and  $\sqrt{N_0^{\downarrow}}$ , respectively, the so-

lutions to which are difficult to handle analytically in generality.<sup>1</sup> Therefore, for the following analysis, the expression (4.1), (4.4) and (4.5) are simplified by means of the following assumptions:

- a) The pseudospin states are treated equally with respect to all input parameters, i.e.

$$\mu^\uparrow = \mu^\downarrow \equiv \mu, \quad \epsilon_{\mathbf{k}_{0i}}^\uparrow = \epsilon_{\mathbf{k}_{0i}}^\downarrow \equiv \epsilon_{\mathbf{k}_{0i}}, \quad U^{\uparrow\uparrow} = U^{\downarrow\downarrow} \equiv \frac{U^{\uparrow\downarrow}}{\alpha} \equiv U; \quad (4.17)$$

and

- b) if  $N_0^\uparrow, N_0^\downarrow \neq 0$ , we *postulate* that

$$N_0^\uparrow = N_0^\downarrow \equiv N_0/2. \quad (4.18)$$

If  $N_0^\uparrow \neq N_0^\downarrow = 0$ , then

$$N_0^\uparrow \equiv N_0, \quad (4.19)$$

and vice versa.

Consequently, if  $N_0^\uparrow, N_0^\downarrow \neq 0$ , the expressions (4.4) and (4.5) are equal, and produce the following expression for  $N_0$ :

$$\frac{N_0}{N_s} = 2f \frac{\epsilon_{\mathbf{k}_{0\ell}} + |s_{\mathbf{k}_{0\ell}}| + \mu}{\left( \sum_{jj'} \sum_{\alpha} \right)''' U^{\uparrow\alpha} \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}} \quad (4.20)$$

where the reader should note that  $\mathbf{k}_{0i}$  has been replaced by  $\mathbf{k}_{0\ell}$  to avoid ambiguity in the ensuing calculations; and either Eq. (4.4) or (4.5) produces

$$\frac{N_0}{N_s} = \frac{\epsilon_0 + \mu}{U} \stackrel{(4.7)}{=} \frac{4t + \mu}{U} \quad (4.21)$$

if  $N_0^\uparrow \neq N_0^\downarrow = 0$  or  $N_0^\downarrow \neq N_0^\uparrow = 0$ , in which case  $|s_{\mathbf{k}_{0\ell}}| = 0$  by condition (3.32), which in turn implies  $\mathbf{k}_{0\ell} = \mathbf{k}_{00} = \mathbf{0}$  and  $f = 1$ . As expected, the

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<sup>1</sup>These coupled equations are nevertheless solvable; using *Maple*, the author is able to invert the expressions (4.4) and (4.5) using the `solve` function in order to obtain expressions for  $N_0^\uparrow$  and  $N_0^\downarrow$ .

<sup>2</sup>This is impossible if  $N_0^\uparrow \neq N_0^\downarrow = 0$  or  $N_0^\downarrow \neq N_0^\uparrow = 0$ , since the expressions (4.4) and (4.5) for  $\mu^\uparrow$  and  $\mu^\downarrow$  depend of the existence of condensed particles in the respective pseudospin states. However, if for instance  $N_0^\downarrow = 0$ , then all dependencies on  $\mu^\downarrow$  in the original Hamiltonian (3.92) cancel, and so  $\mu^\downarrow$  may be neglected, in which case  $\mu^\uparrow \equiv \mu$  implicitly.



solution (4.21) is identical to the single-component solution (2.85). Note that in order to consistently obtain the expression (4.20) from Eq. (4.4) and (4.5), one must have that

$$\begin{aligned} & \left( \sum_{j'j'} \right)''' \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\uparrow + \theta_{\mathbf{k}_{0i'}}^\uparrow) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\ &= \left( \sum_{j'j'} \right)''' \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\downarrow + \theta_{\mathbf{k}_{0i'}}^\downarrow) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}, \end{aligned} \quad (4.22)$$

by equating Eq. (4.4) and (4.5) under the assumption (4.17). If condition (4.22) does *not* hold, then there is a conflict between the assumptions that the chemical potentials are equal, and that there are also equally many condensed particles of either pseudospin state. The Hamiltonian (4.1) may now be rewritten as

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 \\ &\approx -\frac{N_s}{2} \left( \frac{\epsilon_{\mathbf{k}_{0\ell}} + |s_{\mathbf{k}_{0\ell}}| + \mu}{\left( \sum_{j'j'} \sum_{\alpha} \right)'''} U^{\uparrow\alpha} \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \right)^2 \\ &\cdot \left( \sum_{ij'j'} \sum_{\alpha\beta} \right)'''' U^{\alpha\beta} \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}}, \end{aligned} \quad (4.23)$$

if  $N_0^\uparrow, N_0^\downarrow \neq 0$ , by Eq. (4.20); and

$$\mathcal{H} = \mathcal{H}_0 \approx -\frac{N_s}{2U} (4t + \mu)^2 \quad (4.24)$$

if  $N_0^\uparrow \neq N_0^\downarrow = 0$  or  $N_0^\downarrow \neq N_0^\uparrow = 0$ , by Eq. (4.21).

In the following sections, the analysis is continued for each respective phase. The quantitative definition of each phase listed in Tab. 4.1 will be used in conjunction with the list (3.8)–(3.11) of momentum-conserving condensate configurations in order to write out the sums  $\left( \sum_{ij'j'} \sum_{\alpha\beta} \right)''''$  and  $\left( \sum_{j'j'} \sum_{\alpha} \right)''''$ .

## 4.1 The PZ Phase

For the PZ phase, for which  $N_0^\uparrow \neq N_0^\downarrow = 0$  and the condensate momentum magnitude  $k_0 = 0$ —as illustrated in Fig. 4.1a—all calculations have already been performed. The condensate density is

$$\frac{N_0}{N_s} \stackrel{(4.21)}{=} \frac{4t + \mu}{U}, \quad (4.25)$$

and the free energy  $F_{\text{PZ}}$  is

$$F_{\text{PZ}} \stackrel{(4.3),(4.24)}{=} -\frac{N_s}{2U} (4t + \mu)^2. \quad (4.26)$$

$F_{\text{PZ}}$  is independent of the phase  $\theta_0^\uparrow$ , which is therefore arbitrary.

## 4.2 The NZ Phase

For the NZ phase, for which  $N_0^\uparrow = N_0^\downarrow \equiv \frac{N_0}{2} \neq 0$  and the condensate momentum magnitude  $k_0 = 0$ —as illustrated in Fig. 4.1b—the condensate density is

$$\frac{N_0}{N_s} \stackrel{(4.20)}{=} \frac{2}{U} \frac{\epsilon_0 + \mu}{1 + \alpha} = \frac{2}{U} \frac{4t + \mu}{1 + \alpha} \quad (4.27)$$

and the free energy  $F_{\text{NZ}}$  is

$$F_{\text{NZ}} \stackrel{(4.3),(4.23)}{=} -\frac{N_s}{U(1 + \alpha)} (4t + \mu)^2. \quad (4.28)$$

The condition (4.22) is trivially satisfied since

$$\theta_0^\alpha - \theta_0^\alpha - \theta_0^\alpha + \theta_0^\alpha = 0 \quad \forall \alpha. \quad (4.29)$$

$F_{\text{PZ}}$  is independent of the phases  $\theta_0^\uparrow$  and  $\theta_0^\downarrow$ , which are therefore arbitrary.

## 4.3 The PW Phase

For the PW phase, which is illustrated in Fig. 4.1c and defined quantitatively in Tab. 4.1, the condensate density is

$$\frac{N_0}{N_s} \stackrel{(4.20)}{=} \frac{2}{U} \frac{\epsilon_{\mathbf{k}_{01}} + |s_{\mathbf{k}_{01}}| + \mu}{1 + \alpha}, \quad (4.30)$$

and the free energy  $F_{\text{PW}}$  is

$$\begin{aligned}
 F_{\text{PW}} &\stackrel{(4.3),(4.23)}{=} -\frac{N_s}{U(1+\alpha)} (\epsilon_{\mathbf{k}_{01}} + |s_{\mathbf{k}_{01}}| + \mu)^2 \\
 &\stackrel{(4.6),(4.7)}{=} -\frac{N_s}{U(1+\alpha)} \left( 4t \cos(k_0 a) + 2\sqrt{2}\lambda_R |\sin(k_0 a)| + \mu \right)^2,
 \end{aligned} \tag{4.31}$$

Again, the condition (4.22) is trivially satisfied since

$$\theta_{\mathbf{k}_{01}}^\alpha - \theta_{\mathbf{k}_{01}}^\alpha - \theta_{\mathbf{k}_{01}}^\alpha + \theta_{\mathbf{k}_{01}}^\alpha = 0 \quad \forall \alpha, \tag{4.32}$$

and  $F_{\text{PW}}$  is independent of the phases  $\theta_{\mathbf{k}_{01}}^\uparrow$  and  $\theta_{\mathbf{k}_{01}}^\downarrow$ , which are therefore constrained only by Eq. (3.37). In order to determine the remaining variational parameter  $k_0$ ,  $F_{\text{PW}}$  must be minimized with respect to this. The derivative of  $F_{\text{PW}}$  with respect to  $k_0$  is

$$\begin{aligned}
 \frac{\partial F_{\text{PW}}}{\partial k_0} &= -\frac{2N_s}{U(1+\alpha)} \left( 4t \cos(k_0 a) + 2\sqrt{2}\lambda_R |\sin(k_0 a)| + \mu \right) \\
 &\quad \cdot \left( -4ta \sin(k_0 a) + 2\sqrt{2}\lambda_R a \cos(k_0 a) \text{sgn}(\lambda_R \sin(k_0 a)) \right) = 0.
 \end{aligned} \tag{4.33}$$

The quantity  $4t \cos(k_0 a) + 2\sqrt{2}\lambda_R |\sin(k_0 a)| + \mu$  cannot be zero, since this would render the condensate density (4.30) zero, contrary to initial assumptions. Therefore,

$$-4ta \sin(k_0 a) + 2\sqrt{2}\lambda_R^2 a \cos(k_0 a) \text{sgn}(\sin(k_0 a)) = 0, \tag{4.34}$$

which yields

$$k_0 = \frac{1}{a} \arctan \left( \frac{\sqrt{2}\lambda_R}{2t} \right). \tag{4.35}$$

Now, using

$$\cos(\arctan(x)) = \frac{1}{\sqrt{x^2 + 1}}, \quad \sin(\arctan(x)) = \frac{x}{\sqrt{x^2 + 1}}, \tag{4.36}$$

one finds that

$$\begin{aligned}
 \epsilon_{\mathbf{k}_{01}} + |s_{\mathbf{k}_{01}}| &= 4t \cos(k_0 a) + 2\sqrt{2}\lambda_R |\sin(k_0 a)| \\
 &= \frac{4t + \frac{2\lambda_R^2}{t}}{\sqrt{\frac{\lambda_R^2}{2t^2} + 1}} = 4t \sqrt{\frac{\lambda_R^2}{2t^2} + 1},
 \end{aligned} \tag{4.37}$$

from which it follows that the condensate density (4.30) is

$$\frac{N_0}{N_s} = \frac{2}{U} \frac{4t \sqrt{\frac{\lambda_R^2}{2t^2} + 1} + \mu}{1 + \alpha}, \quad (4.38)$$

and that the free energy (4.31) is

$$F_{\text{PW}} = -\frac{N_s}{U(1 + \alpha)} \left( 4t \sqrt{\frac{\lambda_R^2}{2t^2} + 1} + \mu \right)^2. \quad (4.39)$$

The second derivative of  $F_{\text{PW}}$  with respect to  $k_0$ , evaluated at the value (4.35), is

$$\frac{\partial^2 F_{\text{PW}}}{\partial k_0^2} = \frac{4N_s a^2}{U(1 + \alpha)} 4t^2 \sqrt{\frac{\lambda_R^2}{2t^2} + 1} \left( 2 \left( \frac{\lambda_R^2}{2t^2} + 1 \right) + \mu \right) > 0, \quad (4.40)$$

which confirms that the value of  $F_{\text{PW}}$  at this point is a minimum. The other local extrema of  $F_{\text{PW}}$  within the first Brillouin zone occur at  $k_0 = 0$  and  $k_0 = \pm\pi/a$ , at which points  $\sin(k_0 a)$  changes sign. When  $\lambda_R > 0$ , the value of  $F_{\text{PW}}$  evaluated at either of these points is greater than the one presented in Eq. (4.39); thus, we conclude that the expression (4.39) is indeed the global minimum value of  $F_{\text{PW}}$  with respect to  $k_0$ .

## 4.4 The SW Phase

For the SW phase, which is illustrated in Fig. 4.1d and defined quantitatively in Tab. 4.1, upon choosing  $\mathbf{k}_{0\ell} = \mathbf{k}_{01}$ , the left-hand side of condition (4.22) becomes

$$\begin{aligned} & \left( \sum_{j'j'} \right)''' \cos(\theta_{\mathbf{k}_{0j'}}^\dagger - \theta_{\mathbf{k}_{0\ell}}^\dagger - \theta_{\mathbf{k}_{0j}}^\dagger + \theta_{\mathbf{k}_{0j'}}^\dagger) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0j'} + \mathbf{k}_{0j'}} \\ &= \cos(\theta_{\mathbf{k}_{01}}^\dagger - \theta_{\mathbf{k}_{01}}^\dagger - \theta_{\mathbf{k}_{01}}^\dagger + \theta_{\mathbf{k}_{01}}^\dagger) + \cos(\theta_{\mathbf{k}_{03}}^\dagger - \theta_{\mathbf{k}_{01}}^\dagger - \theta_{\mathbf{k}_{03}}^\dagger + \theta_{\mathbf{k}_{01}}^\dagger) \\ & \quad + \cos(\theta_{\mathbf{k}_{01}}^\dagger - \theta_{\mathbf{k}_{01}}^\dagger - \theta_{\mathbf{k}_{03}}^\dagger + \theta_{\mathbf{k}_{03}}^\dagger) = 3, \end{aligned} \quad (4.41)$$

and the right-hand side becomes

$$\begin{aligned}
 & \left( \sum_{j'j'} \right)''' \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\downarrow + \theta_{\mathbf{k}_{0i'}}^\downarrow) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{03}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{03}}^\downarrow) = 3,
 \end{aligned} \tag{4.42}$$

and so condition (4.22) is satisfied. Note that choosing  $\mathbf{k}_{0\ell} = \mathbf{k}_{03}$  would have made no difference; the equations would have been equivalent upon a rotation of  $k$ -space. Furthermore,  $f = 2$ , and the sum in the denominator of the expression (4.20) for the condensate density is

$$\begin{aligned}
 & \left( \sum_{j'j'} \sum_{\alpha} \right)''' U^{\uparrow\alpha} \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\alpha + \theta_{\mathbf{k}_{0i'}}^\alpha) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= U \left( \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) + \cos(\theta_{\mathbf{k}_{03}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) \right. \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{03}}^\uparrow) + \alpha \left( \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \right. \\
 & \quad \left. \left. + \cos(\theta_{\mathbf{k}_{03}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{03}}^\downarrow) \right) \right) \\
 & \stackrel{(4.14)}{=} U(3 + \alpha).
 \end{aligned} \tag{4.43}$$

The condensate density is therefore

$$\frac{N_0}{N_s} \stackrel{(4.20)}{=} \frac{4}{U} \frac{\epsilon_{\mathbf{k}_{01}} + |s_{\mathbf{k}_{01}}| + \mu}{3 + \alpha}. \tag{4.44}$$

The sum in the numerator of the expression (4.23) for the Hamiltonian is

$$\begin{aligned}
 & \left( \sum_{ijj'} \sum_{\alpha\beta} \right)''' U^{\alpha\beta} \cos(\theta_{\mathbf{k}_{0j'}}^\alpha - \theta_{\mathbf{k}_{0i}}^\alpha - \theta_{\mathbf{k}_{0j}}^\beta + \theta_{\mathbf{k}_{0i'}}^\beta) \delta_{\mathbf{k}_{0i} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= U \left( \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) + \cos(\theta_{\mathbf{k}_{03}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) \right. \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{03}}^\uparrow) + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{03}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{03}}^\downarrow) \\
 & \quad + \alpha \left( \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{03}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \right. \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{03}}^\downarrow) + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) \\
 & \quad \left. + \cos(\theta_{\mathbf{k}_{03}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{03}}^\uparrow) \right) \\
 & \quad + (\mathbf{k}_{01} \longleftrightarrow \mathbf{k}_{03}) \\
 &= 4U(3 + \alpha),
 \end{aligned} \tag{4.45}$$

where  $(\mathbf{k}_{01} \longleftrightarrow \mathbf{k}_{03})$  indicates that all preceding terms are effectively repeated, upon an interchange of  $\mathbf{k}_{01}$  and  $\mathbf{k}_{03}$ . The free energy  $F_{\text{SW}}$  is therefore

$$\begin{aligned}
 F_{\text{SW}} & \stackrel{(4.3),(4.23)}{=} - \frac{2N_s (\epsilon_{\mathbf{k}_{01}} + |s_{\mathbf{k}_{01}}| + \mu)^2}{U(3 + \alpha)} \\
 & \stackrel{(4.6),(4.7)}{=} - \frac{2N_s (4t \cos(k_0 a) + 2\sqrt{2}\lambda_R |\sin(k_0 a)| + \mu)^2}{U(3 + \alpha)}.
 \end{aligned} \tag{4.46}$$

Again,  $F_{\text{SW}}$  is independent of the phases  $\theta_{\mathbf{k}_{01}}^\uparrow, \theta_{\mathbf{k}_{01}}^\downarrow, \theta_{\mathbf{k}_{03}}^\uparrow, \theta_{\mathbf{k}_{03}}^\downarrow$ , which are therefore constrained only by Eq. (3.37). The dependency of  $F_{\text{SW}}$  on  $k_0$  is essentially the same as the dependency of  $F_{\text{PW}}$  on  $k_0$ , cf. Eq. (4.31).  $F_{\text{SW}}$  is therefore minimal for

$$k_0 \stackrel{(4.35)}{=} \frac{1}{a} \arctan \left( \frac{\sqrt{2}\lambda_R}{2t} \right). \tag{4.47}$$

The final expression for  $F_{\text{SW}}$  is thus

$$F_{\text{SW}} = - \frac{2N_s \left( 4t \sqrt{\frac{\lambda_R^2}{2t^2} + 1} + \mu \right)^2}{U(3 + \alpha)}. \tag{4.48}$$

## 4.5 The LW Phase

For the LW phase, which is illustrated in Fig. 4.1g and defined quantitatively in Tab. 4.1, the parentheses (...)''' may be omitted from the sums in which they appear, because all four points in  $k$ -space are occupied by the condensate. Upon choosing  $\mathbf{k}_{0\ell} = \mathbf{k}_{01}$ , the left-hand side of condition (4.22) becomes

$$\begin{aligned}
 & \sum_{ji'j'} \cos(\theta_{\mathbf{k}_{0j'}}^\uparrow - \theta_{\mathbf{k}_{0\ell}}^\uparrow - \theta_{\mathbf{k}_{0j}}^\uparrow + \theta_{\mathbf{k}_{0i'}}^\uparrow) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) + \cos(\theta_{\mathbf{k}_{02}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{02}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{03}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) + \cos(\theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{04}}^\uparrow + \theta_{\mathbf{k}_{01}}^\uparrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{02}}^\uparrow + \theta_{\mathbf{k}_{02}}^\uparrow) + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{03}}^\uparrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{04}}^\uparrow + \theta_{\mathbf{k}_{04}}^\uparrow) + \cos(\theta_{\mathbf{k}_{02}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{04}}^\uparrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{04}}^\uparrow - \theta_{\mathbf{k}_{01}}^\uparrow - \theta_{\mathbf{k}_{03}}^\uparrow + \theta_{\mathbf{k}_{02}}^\uparrow) \\
 & \stackrel{(4.11),(4.12),(4.16)}{=} 7 \pm 2,
 \end{aligned} \tag{4.49}$$

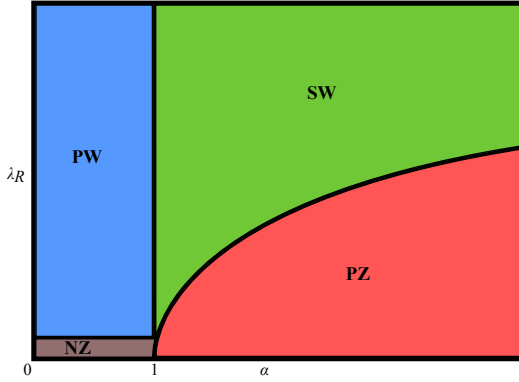
and the right-hand side becomes

$$\begin{aligned}
 & \sum_{ji'j'} \cos(\theta_{\mathbf{k}_{0j'}}^\downarrow - \theta_{\mathbf{k}_{0\ell}}^\downarrow - \theta_{\mathbf{k}_{0j}}^\downarrow + \theta_{\mathbf{k}_{0i'}}^\downarrow) \delta_{\mathbf{k}_{0\ell} + \mathbf{k}_{0j}, \mathbf{k}_{0i'} + \mathbf{k}_{0j'}} \\
 &= \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{02}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{02}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{03}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) + \cos(\theta_{\mathbf{k}_{04}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{04}}^\downarrow + \theta_{\mathbf{k}_{01}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{02}}^\downarrow + \theta_{\mathbf{k}_{02}}^\downarrow) + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{03}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{04}}^\downarrow + \theta_{\mathbf{k}_{04}}^\downarrow) + \cos(\theta_{\mathbf{k}_{02}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{04}}^\downarrow) \\
 & \quad + \cos(\theta_{\mathbf{k}_{04}}^\downarrow - \theta_{\mathbf{k}_{01}}^\downarrow - \theta_{\mathbf{k}_{03}}^\downarrow + \theta_{\mathbf{k}_{02}}^\downarrow) \\
 & \stackrel{(4.11),(4.12),(4.16)}{=} 7 \mp 2,
 \end{aligned} \tag{4.50}$$

and so condition (4.22) is *not* satisfied, meaning there is a conflict between the assumptions that the chemical potentials are equal, and that there is also equally many condensed particles of both pseudospin states. This phase will therefore be discarded for the remainder of this analysis, although the reader should note that this conflict of assumptions does not invalidate this phase; instead, a more thorough analysis of all solutions for  $N_0^\uparrow$  and  $N_0^\downarrow$  upon inverting the expressions (4.4) and (4.5) is required in order to determine whether or not this phase exists.

## 4.6 Phase Diagram

All that remains to be done in order to determine the phases of the condensate—specifically as a function of the interspecies interaction strength  $\alpha$  and the SOC strength  $\lambda_R$ —is to minimize the free energy globally with respect to these input parameters. This is done by determining which phase is associated with the lowest free energy at any given point  $(\alpha, \lambda_R)$ , i.e. by comparing  $F_{\text{PZ}}$ ,  $F_{\text{NZ}}$ ,  $F_{\text{PW}}$  and  $F_{\text{SW}}$ . This procedure produces the following phase diagram:



**Figure 4.2:** Sketch of the phases of the pure condensate as a function of the interspecies interaction strength  $\alpha$  and the SOC strength  $\lambda_R$ ; see Fig. 4.1 for definitions of the phases. The NZ phase region is exaggerated in this sketch, as it occurs only when  $\lambda_R = 0$  when  $k_0$  is approximated as continuous.

This analytically derived phase diagram coincides with the numerical results presented by P. N. Galteland *et al.* in Ref. [45, Fig. 2]. The boundary between the PW and the SW phase is given by  $\alpha = 1$ ,<sup>3</sup> and the boundary between the PZ and the SW phase is given by the expression

$$\lambda_R = \frac{\sqrt{2(4t(\alpha - 1) + \mu(\alpha + 7))(4t + \mu) - 8\sqrt{\mu^2(4t + \mu)^2(\alpha + 3)}}}{8}. \quad (4.51)$$

<sup>3</sup>Observe that this boundary coincides with the condition (3.84) for which the assumption that there are equally many condensed particles of any momenta carried by the condensed particles, for a given pseudospin state, does no longer necessarily hold true.



Note that if the positive sign had been chosen in the expressions (3.38) and (3.39) for the chemical potentials, the expression (4.46) for  $F_{\text{SW}}$  would instead have been

$$\begin{aligned}
 F_{\text{SW}} &= -\frac{2N_s (\epsilon_{\mathbf{k}_{01}} - |s_{\mathbf{k}_{01}}| + \mu)^2}{U(3 + \alpha)} \\
 &\stackrel{(4.6),(4.7)}{=} \frac{2N_s (4t \cos(k_0 a) - 2\sqrt{2}\lambda_R |\sin(k_0 a)| + \mu)^2}{U(3 + \alpha)} \\
 &\stackrel{(4.47)}{=} -\frac{2N_s \left( 4t \left( 1 - \frac{\lambda_R^2}{2t^2} \right) / \sqrt{\frac{\lambda_R^2}{2t^2} + 1} + \mu \right)^2}{U(3 + \alpha)},
 \end{aligned} \tag{4.52}$$

which produces a boundary between the SW and the PZ phase that is not in agreement with the literature, e.g. Ref. [45].

# CHAPTER 5

## *Miscellaneous Discussion*

### 5.1 Impact of Phases

As mentioned in the text preceding Eq. (3.27), the expectation value  $a_{\mathbf{k}_{0i}}^\alpha$  of the condensate operators  $A_{\mathbf{k}_{0i}}^\alpha$  is usually taken to be real and equal to the square root of the corresponding condensate number. This choice was shown indeed not to have any impact on the non-SOC case presented in Sec. 2.6, as well as on the PZ and the NZ phase presented in Sec. 4.1 and 4.2. The phases  $\theta_{\mathbf{k}_{0i}}^\alpha$  defined in Eq. (3.27) *did*, however, have a crucial impact on the PW and the SW phase presented in Sec. 4.3 and 4.4: Because the SOC  $s_{\mathbf{k}}$  is generally complex-valued, the relative differences in the phases— $\theta_{\mathbf{k}_{01}}^\uparrow$  and  $\theta_{\mathbf{k}_{01}}^\downarrow$  for the PW phase, and  $\theta_{\mathbf{k}_{01}}^\uparrow$ ,  $\theta_{\mathbf{k}_{01}}^\downarrow$ ,  $\theta_{\mathbf{k}_{03}}^\uparrow$  and  $\theta_{\mathbf{k}_{03}}^\downarrow$  for the SW phase—were *necessary* in order to render the chemical potentials real-valued, which is the case for *any* condensate configuration for which the SOC contributes to the chemical potentials; cf. the expressions (3.33) and (3.34) for the non-interacting case. The differences in phases are generally fixed by Eq. (3.37), (3.51) and (3.59). In other words, neither the PW phase nor the SW phase would have existed in the absence of the phases  $\theta_{\mathbf{k}_{0i}}^\alpha$ .

### 5.2 Handling Linear Terms in the Hamiltonian

After applying mean field theory to the Hamiltonian (3.20), one is left with a number of terms that are linear in either condensate fluctuations, producing  $\mathcal{H}_{(1)}$ , or in excitation operators, producing  $\mathcal{H}_1$ , which are given by Eq. (3.28) and (3.93), respectively. It was argued that  $\mathcal{H}_{(1)}$  would have to cancel on the basis that the free energy  $F$  had to be minimal with respect to the number of condensed particles, akin to what was done by D. van Oosten *et al.* in Ref. [46], which was handled by deducing appropriate

expressions for the chemical potentials. D. van Oosten *et al.* [46] did not encounter any terms analogous to  $\mathcal{H}_1$ , however. It would seem natural that this contribution to the Hamiltonian would also somehow cancel, in order to ensure a Hamiltonian bounded from below, and the convergence of any appropriate Gaussian integral. A few suggested methods for handling  $\mathcal{H}_1$  are listed below:

- a) Appropriately adjusting the chemical potentials. One may argue that due to the phenomenon of ground state depletion, linear terms in excitation operators would affect the number of condensed particles analogously to condensate fluctuations, and that as such,  $\mathcal{H}_1$  must cancel for the same reason that  $\mathcal{H}_{(1)}$  must cancel, i.e. that  $F$  is assumed to be minimal with respect to the number of condensed particles. Therefore, one might attempt to cancel  $\mathcal{H}_1$  by deducing an appropriate expression for the chemical potentials. However, on its own, adjusting the chemical potentials fails to produce cancellation terms that are linear in excitation operators.
- b) Absorbing the linear terms into the bilinear terms, or “completing the square.” Consider the following toy example:

$$H = \mathbf{A}^\dagger \mathcal{M} \mathbf{A} + \mathbf{X}^\dagger \mathcal{M} \mathbf{A} + \mathbf{A}^\dagger \mathcal{M} \mathbf{X} = (\mathbf{A} + \mathbf{X})^\dagger \mathcal{M} (\mathbf{A} + \mathbf{X}) - \mathbf{X}^\dagger \mathcal{M} \mathbf{X}. \quad (5.1)$$

Here,  $\mathbf{A}$  is a vector of operators,  $\mathcal{M}$  is a matrix with scalar entries, and  $\mathbf{X}$  is a vector with scalar entries. By adding and subtracting the term  $\mathbf{X}^\dagger \mathcal{M} \mathbf{X}$ , the terms linear in  $\mathbf{A}$  and  $\mathbf{A}^\dagger$  were absorbed into the bilinear term by introducing a constant shift  $\mathbf{X}$  to  $\mathbf{A}$ . Identifying  $\mathbf{X}^\dagger \mathcal{M} \mathbf{A} + \mathbf{A}^\dagger \mathcal{M} \mathbf{X}$  as analogous to  $\mathcal{H}_1$ , and  $\mathbf{A}^\dagger \mathcal{M} \mathbf{A}$  as analogous to  $\mathcal{H}_2$ —given by Eq. (3.94)—one may attempt to handle  $\mathcal{H}_1$  in a similar fashion.

- c) A combination of the above. If a constant shift is introduced to the operators, the single-particle terms in Eq. (3.94) produces terms that are linear in excitation operators. This way, an appropriate adjustment of the chemical potentials may produce terms that aid in cancelling  $\mathcal{H}_1$ . However, a naïve application of this shift appears to produce additional terms originating from the single-particle terms, that are linear in excitation operators, but with momentum-dependent coefficients, which therefore cannot be handled by adjusting the chemical potentials.

# CHAPTER 6

## *Summary and Outlook*

This thesis comprises an analytic study of ultracold, synthetically spin-orbit coupled, weakly interacting two-component Bose gases in Bravais lattices. In particular, the method by which D. van Oosten *et al.* deduced expressions for the chemical potentials in the superfluid phase in Ref. [46], was applied and generalized to the spin-orbit coupled case, yielding the mean field expressions (3.87) and (3.88) for the chemical potentials, which may be further simplified provided certain conditions are met, resulting in the expressions (3.89) and (3.90). The general framework developed in Ch. 2 and 3 was applied to a simple example of a pure condensate residing on a square lattice, the results of which coincides with numerical results obtained by P. N. Galteland *et al.* in Ref. [45]. A few intermediate results, equivalents in the literature to which are unbeknownst to both the author and his supervisor, were obtained as well; in particular, many-fold cases were shown to potentially involve terms in the Hamiltonian that are *linear* in excitation operators; cf. Tab. 3.1.

The expressions (3.87) and (3.88), or (3.89) and (3.90), leave much to be explored. In particular, no application of the framework developed in Ch. 3 that included excitations—i.e. including the terms  $\mathcal{H}_1$  and  $\mathcal{H}_2$  in the Hamiltonian (3.91)—was successfully developed by the author, due to difficulties handling the linear terms comprised by  $\mathcal{H}_1$ . A few suggestions for how to handle these terms were presented in Sec. 5.2, though the author invites the reader to search for other methods. Once the linear terms have been handled, the generalized diagonalization procedure presented in Sec. 2.7 may be applied to the Hamiltonian (3.91) in order to obtain quasi-particle energy spectra, which in turn may be used to find an explicit expression for the free energy  $F$  by substituting the appropriate quantities in the general expression (2.104), after which explicit expressions for all variational parameters in terms of the input parameters, as well as the phases of the system, may be deduced by minimization of  $F$  with respect to the variational parameters.

Furthermore, the simple and heavily restricted example presented in Ch.

4, may be explored in more detail. Only solutions for  $N_0^\uparrow$  and  $N_0^\downarrow$  to the coupled equations (3.89) and (3.90) for which  $N_0^\uparrow = N_0^\downarrow$ , were explored, assuming the two pseudospin states were treated equally with respect to all input parameters. There are multiple general solutions to the coupled equations (3.89) and (3.90), that should all be addressed; in particular, one may identify the particular general solutions that reduce to the particular solutions explored in the respective sections 4.1–4.4 upon assuming that the two pseudospin states are treated equally with respect to all input parameters.

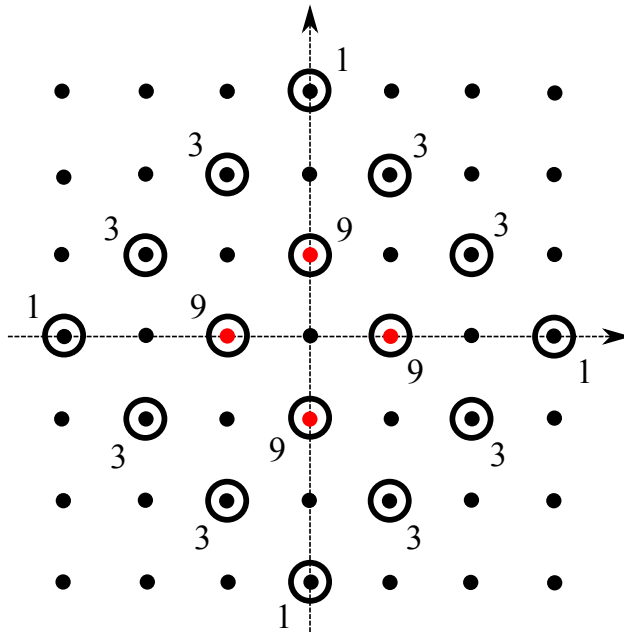
Finally, for cases in which the SOC is non-zero—and, by extension, the pseudohelicity of the bosons is well-defined—it may be of interest to convert all appropriate expressions presented in Ch. 3 to the pseudohelicity basis presented in Eq. (2.67). Intuitively, this may potentially result in simplifications, since the non-diagonality of the Hamiltonian of the spin–orbit coupled, weakly interacting Bose gas, would then only result from perturbations relative to the non-interacting case.

# Appendices

# APPENDIX A

## *Counting Momentum Configurations*

### A.1 A Visualized Iterative Method



**Figure A.1:** A unit square lattice. The red points denote the points that are nearest to the origin. The number by the encircled points indicate the number of ways one may reach that point in three unit steps from the origin.

Counting the number of configurations for case 1–5 in Tab. 3.1 in the four-fold case, may be done by hand by inspecting the unit square lattice

## APPENDIX A. COUNTING MOMENTUM CONFIGURATIONS

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in Fig. A.1. Momentum conservation dictates that when there are at least three condensate particles involved in a two-body scattering event,

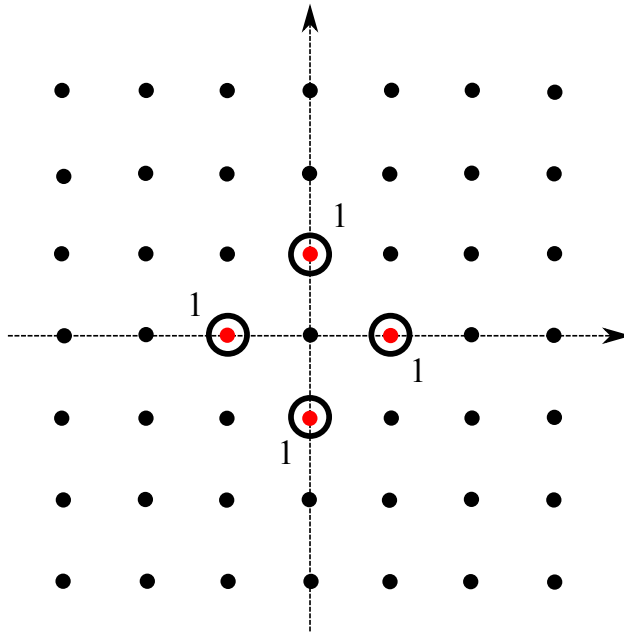
$$\mathbf{k}_{0i} + \mathbf{k}_{0j} = \mathbf{k}_{0i'} + \mathbf{p}', \quad i, j, i' = 1, 2, 3, 4, \quad (\text{A.1})$$

$$\Rightarrow \mathbf{p}' = \mathbf{k}_{0i} + \mathbf{k}_{0j} - \mathbf{k}_{0i'}, \quad (\text{A.2})$$

where the  $\mathbf{k}_{0i}$  are condensate momenta, and  $\mathbf{p}'$  a fourth momentum determined by the above relation. All instances for which  $\mathbf{p}'$  is a condensate momentum correspond to case 1 of Tab. 3.1, while all other instances correspond to either one of case 2–5. By rotating the lattice presented in Fig. 2.3a, scaling it such that all condensate momenta have a magnitude of 1, and neglecting all points that are not reachable by an integral number of vertical and horizontal unit steps from the origin, one is left with the unit square lattice in Fig. A.1. One then recognizes that Eq. (A.2) is equivalent to determining  $\mathbf{p}'$  by moving three unit steps through this lattice; the steps are determined by the value of the indices  $i, j, i'$ . Therefore, the *total* number of configurations for which  $\mathbf{p}'$  is a condensate momentum, is equal to the total number of ways one may reach either of the four encircled red points in Fig. A.1, i.e.  $4 \cdot 9 = 36$ , and conversely, the total number of configurations for which  $\mathbf{p}'$  is *not* a condensate momentum, is equal to the total number of ways one may reach the remaining encircled points, i.e.  $4 \cdot (1 + 3 + 3) = 28$ .

It may be useful to generalize this counting. Consider the same unit square lattice, but this time, only taking *one* unit step from the origin. The corresponding diagram is presented in Fig. A.2.

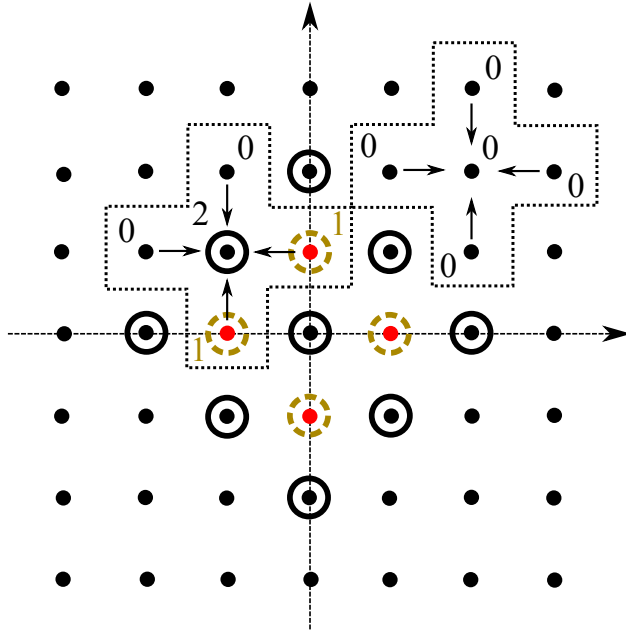




**Figure A.2:** The same situation as illustrated in Fig. A.1, but this time limited to taking one unit step from the origin.

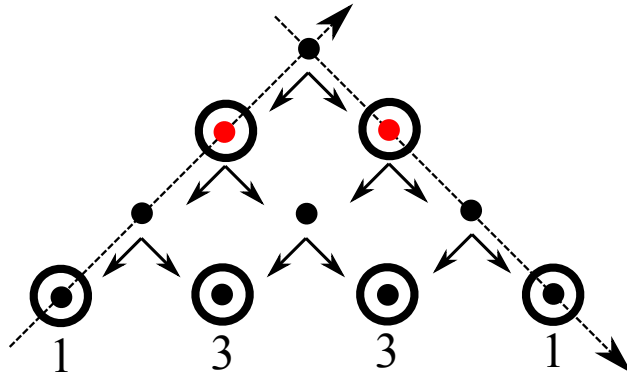
Conversely, the two-step variant is presented in Fig. A.3.





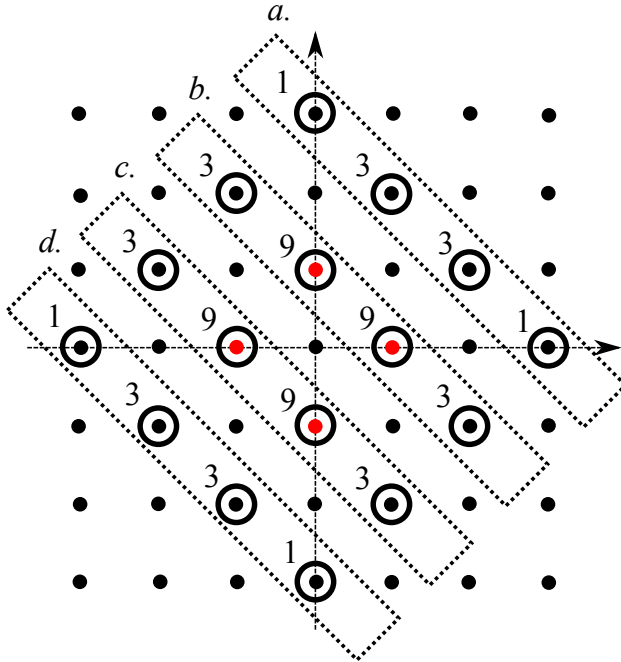
**Figure A.4:** Complementary illustration for Fig. A.3. Instead of counting the number of ways one may reach an arbitrary point by taking two steps from the origin, one may use the one-step case as a starting point. The one-step case is colored in yellow, corresponding to Fig. A.2. Counting the number of ways of reaching an arbitrary point by taking two steps from the origin, is equivalent to counting the number of ways one may reach nearest-neighboring points in one step from the origin.

This counting generalizes to the case of taking  $n$  unit steps from the origin. To count the number of ways of reaching an arbitrary point in the  $n$ -step case, one counts the number of ways of reaching any nearest-neighboring point in  $n - 1$  unit steps from the origin. Now, the relationship between the most distant reachable points and Pascal's triangle is evident by inspection of Fig. A.5.



**Figure A.5:** The rotated fourth quadrant of Fig. A.1. The relationship between the reachable points most distant from the origin, and Pascal's triangle, is evident by inspection. This generalizes to the  $n$ -step case.

For a square lattice, whether or not an arbitrary point is reachable in  $n$  steps alternates depending on whether  $n$  is even or odd, unless the point is too far away from the origin; this pattern may be observed by comparing Fig. A.2, A.3 and A.1 consecutively. This leads to another pattern directly related to Pascal's triangle, illustrated in Fig. A.6.

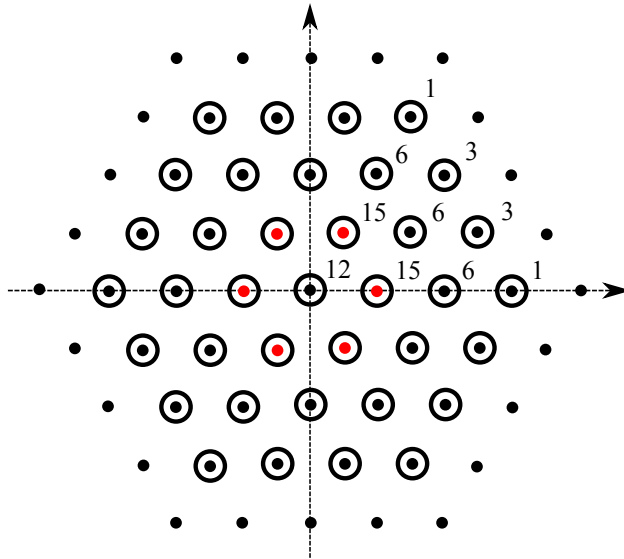


**Figure A.6:** Rows of encircled points in Fig. A.1, labeled *a.*–*d.*. The numbers in row *a.* and *d.* are the entries of the fourth row of Pascal’s triangle, multiplied by 1. The numbers in row *b.* and *c.* are also the entries of the fourth row of Pascal’s triangle, multiplied by 3. Observe that the sequence 1, 3, 3, 1 of multiplicative factors is also the fourth row of Pascal’s triangle. This pattern holds in the  $n$ -step case as well; see for instance Fig. A.3.

The method of counting in the  $n$ -step case presented above may be used to compute the total number of configurations for the equivalents of case 1–5 in Tab. 3.1 for higher order scattering events. For instance, for three-body scattering events, one would consider the 5-step case, and in general, for  $m$ -body scattering events, one would consider the  $(2m - 1)$ -step case, which follows from conservation of momentum.

The above method may also be applied to other lattice geometries, and generalized to other dimensions. See for instance Fig. A.7, in which the number of ways of reaching arbitrary points in three unit steps from the origin on a two-dimensional hexagonal lattice is presented, computed using the iterative method presented in Fig. A.4. Note that the pattern of multiplicative

factors that was present in the case of a square lattice—cf. Fig. A.6—is no longer present for this geometry. This case corresponds to two-body scattering events on a two-dimensional lattice geometry for which condensed particles may carry any of six possible momenta.



**Figure A.7:** The hexagonal equivalent to what is presented in Fig. A.1. The number of ways in which an arbitrary point may be reached by taking three unit steps from the origin, was computed using the iterative method presented in Fig. A.4. Only one of six sections are numbered in the diagram; the symmetry dictates that these numbers are the same for every other section as well.

## A.2 Combinatorial Expressions

In combinatorics, the stepwise process described in the previous section is formally known as a *lattice walk*. The lattice points are referred to as *nodes*, and labeled e.g.  $(a, b)$  on a square lattice, corresponding to the point that is  $a \in \mathbb{Z}$  horizontal and  $b \in \mathbb{Z}$  vertical steps away from the origin  $(0, 0)$  in Fig. A.1. Derivations of the expressions for the number of ways of reaching a specific node in  $n$  steps from the origin, are presented by S. Hollos in Ref. [62], for the special cases of one-, two- and three-dimensional cubic lattices.

## APPENDIX A. COUNTING MOMENTUM CONFIGURATIONS

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The final expressions are presented in Tab. A.1.

**Table A.1:** Lattice walk expressions

$D$	Node	$N_n$
1	$a$	$\binom{2\ell+a}{\ell}$
2	$(a, b)$	$\binom{2\ell+a+b}{\ell} \binom{2\ell+a+b}{\ell+a}$
3	$(a, b, c)$	$\binom{2\ell+a+b+c}{\ell} \sum_{k=0}^{\ell} \binom{\ell}{k} \binom{\ell+a+b+c}{k+b+c} \binom{2k+b+c}{k+b}$

Table of expressions for the number of ways  $N_n$  one may reach a specific node on a  $D$ -dimensional cubic lattice in  $n$  steps from the origin, provided  $\ell \geq 0$ ; otherwise,  $N_n = 0$ . The expressions are due to S. Hollos [62]. Here,  $a, b, c \in \mathbb{Z}$ , and  $\ell, k$  are non-negative integers. The quantity  $\ell$  is the total number of steps in all negative directions in the lattice—e.g. in the  $-\mathbf{x}$  and  $-\mathbf{y}$  direction on a square lattice—and is related to  $n$  via the relation  $n = 2\ell + a$ ,  $n = 2\ell + a + b$  and  $n = 2\ell + a + b + c$  in one, two and three dimensions, respectively.

# *Bibliography*

- [1] J. Linder and A. Sudbø, Phys. Rev. A **79**, 063610 (2009).
- [2] J. O. Andersen, *Introduction to Statistical Mechanics* (Akademika forlag, Trondheim, 2012).
- [3] S. N. Bose, Z. Phys. **26**, 178 (1924).
- [4] M. Planck, Verhandl. Dtsch. phys. Ges. **2**, 237 (1900).
- [5] A. Einstein, Ann. Phys. **322**, 132 (1905).
- [6] *The Nobel Prize in Physics 1921* (Nobel Media AB 2014, [https://www.nobelprize.org/nobel\\_prizes/physics/laureates/1921/](https://www.nobelprize.org/nobel_prizes/physics/laureates/1921/), access date 13/8/2018).
- [7] A. Einstein, Sitzungsber. Preuss. Akad. Wiss. 1924 **22**, 261 (1924).
- [8] A. Einstein, Sitzungsber. Preuss. Akad. Wiss. 1925 **1**, 3 (1925).
- [9] P. Kapitza, Nature **141**, 74 (1938).
- [10] J. F. Allen and A. D. Misener, Nature **142**, 643 (1938).
- [11] F. London, Nature **141**, 643 (1938).
- [12] L. D. Landau, Phys. Rev. **60**, 356 (1941).
- [13] *The Nobel Prize in Physics 1962* (Nobel Media AB 2014, [https://www.nobelprize.org/nobel\\_prizes/physics/laureates/1962/](https://www.nobelprize.org/nobel_prizes/physics/laureates/1962/), access date 13/8/2018).
- [14] L. P. Pitaevskii, *Bose–Einstein Condensation* (Clarendon Press, Oxford, 2003).
- [15] C. J. Pethick and H. Smith, *Bose–Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2001).
- [16] V. L. Ginzburg, ChemPhysChem **5**, 930 (2004).
- [17] *The Nobel Prize in Physics 1972* (Nobel Media AB 2014, [https://www.nobelprize.org/nobel\\_prizes/physics/laureates/1972/](https://www.nobelprize.org/nobel_prizes/physics/laureates/1972/), access date 13/8/2018).



## BIBLIOGRAPHY

---

- [18] *The Nobel Prize in Physics 2003* (Nobel Media AB 2014, [https://www.nobelprize.org/nobel\\_prizes/physics/laureates/2003/](https://www.nobelprize.org/nobel_prizes/physics/laureates/2003/), access date 13/8/2018).
- [19] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 5221 (1995).
- [20] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999).
- [21] A. J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001).
- [22] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995).
- [23] K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [24] *The Nobel Prize in Physics 2001* (Nobel Media AB 2014, [https://www.nobelprize.org/nobel\\_prizes/physics/laureates/2001/](https://www.nobelprize.org/nobel_prizes/physics/laureates/2001/), access date 13/8/2018).
- [25] E. A. Cornell and C. E. Wieman, *Rev. Mod. Phys.* **74**, 875 (2002).
- [26] W. Ketterle, *Rev. Mod. Phys.* **74**, 1131 (2002).
- [27] O. Morsch and M. Oberthaler, *Rev. Mod. Phys.* **78**, 179 (2006).
- [28] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- [29] R. Grimm, M. Weidemüller, and Y. B. Ovchinnikov, *Adv. Atom. Mol. Opt. Phys.* **42**, 95 (2000).
- [30] I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).
- [31] D. Jaksch, C. Bruder, J. Cirac, C. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- [32] J. Mun, P. Medley, G. K. Campbell, L. G. Marcassa, D. E. Pritchard, and W. Ketterle, *Phys. Rev. Lett.* **99**, 150604 (2007).

## BIBLIOGRAPHY

---

- [33] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, and W. Ketterle, *Phys. Rev. Lett.* **80**, 2027 (1998).
- [34] J. H. Denschlag, J. E. Simsarian, H. Häffner, C. McKenzie, A. Browaeys, D. Cho, K. Helmerson, S. L. Rolston, and W. D. Phillips, *J. Phys. B* **35**, 3095 (2002).
- [35] K. Jiménez-García, R. L. Compton, Y.-J. Lin, W. D. Phillips, J. V. Porto, and I. B. Spielman, *Phys. Rev. Lett.* **105**, 110401 (2010).
- [36] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, *Nature* **415**, 39 (2002).
- [37] D. Jaksch, *Contemp. Phys.* **45**, 367 (2004).
- [38] J. Gu, Y.-P. Zhang, Z.-D. Li, and J.-Q. Liang, *Phys. Lett. A* **335**, 310 (2005).
- [39] X. P. Liu, *Phys. Rev. A* **76**, 053615 (2007).
- [40] Y.-J. Lin, K. Jiménez-García, and I. B. Spielman, *Nature* **471**, 83 (2011).
- [41] J. Higbie and D. M. Stamper-Kurn, *Phys. Rev. Lett.* **88**, 090401 (2002).
- [42] Z. Wu, L. Zhang, W. Sun, X.-T. Xu, B.-Z. Wang, S.-C. Ji, Y. Deng, S. Chen, X.-J. Liu, and J.-W. Pan, *Science* **354**, 6308 (2016).
- [43] V. Galitski and I. B. Spielman, *Nature* **494**, 49 (2013).
- [44] K. Jiménez-García, L. J. LeBlanc, R. A. Williams, M. C. Beeler, C. Qu, M. Gong, C. Zhang, and I. B. Spielman, *Phys. Rev. Lett.* **114**, 125301 (2015).
- [45] P. N. Galteland and A. Sudbø, *Phys. Rev. B* **94**, 054510 (2016).
- [46] D. van Oosten, P. van der Straten, and H. T. C. Stoof, *Phys. Rev. A* **63**, 053601 (2001).
- [47] S. Solli, Master's thesis, Norwegian University of Science and Technology, 2017.
- [48] Janssønn, A. T. G. (project report, December 2017).

## BIBLIOGRAPHY

---

- [49] D. Griffiths, *Introduction to Elementary Particles* (Wiley-VCH, Weinheim, 2008).
- [50] P. C. Hemmer, *Kvantemekanikk* (Tapir Akademisk Forlag, Trondheim, 2005).
- [51] A. Manchon, H. C. Koo, J. Nitta, S. M. Frolov, and R. A. Duine, *Nature Materials* **14**, 871 (2015).
- [52] S. B. Sjømark, Master's thesis, Norwegian University of Science and Technology, 2016.
- [53] C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 226801 (2005).
- [54] H. Bruus and K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics* (Oxford University Press, Oxford, 2004).
- [55] J. P. Sethna, *Statistical Mechanics: Entropy, Order Parameters and Complexity* (Oxford University Press, Oxford, 2006).
- [56] N. N. Bogoliubov, *J. Phys. (Moscow)* **11**, 23 (1947).
- [57] N. N. Bogoliubov, *Nuovo Cimento* **7**, 794 (1958).
- [58] C. Tsallis, *J. Math. Phys.* **19**, 277 (1978).
- [59] J. L. van Hemmen, *Z. Phys. B* **38**, 271 (1980).
- [60] S. T. H. Hartman, Master's thesis, Norwegian University of Science and Technology, 2018.
- [61] D. Toniolo and J. Linder, *Phys. Rev. A* **89**, 061605 (2014).
- [62] S. Hollos, *Walks on Infinite Lattices* (<http://www.exstrom.com/math/lattice/inflatwalks.pdf>, access date 13/8/2018, 2007).