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Josephson current through the flat Bloch band of a sawtooth lattice

Master’s Thesis
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We investigate numerically the effects of interactions on the transport properties through a sawtooth lattice with a flat band. The goal is to assess the experimental feasibility of observing the supercurrent through the flat band in the ultracold quantum gas experiment of the ETH Zürich lithium lab. We study the equilibrium Josephson effect of sawtooth lattice between two superconducting leads. The sawtooth lattice with interactions is modeled using a tight-binding Hubbard model. The used tight-binding model parameters correspond to an optical potential realizable in an ultracold gas experiment by means of the Digital Mirror Device that the ETH group uses. The interactions on the systems are considered at the mean-field level. The superconducting order parameters and mean particle densities in the sawtooth ladder are calculated self-consistently using a Bogoliubov-de Gennes scheme. The quantum transport software Kwant was used in the numerical calculations.

In the numerical studies, we characterize the dependence of the critical Josephson current through a sawtooth lattice on various system energy scales, both in the interacting and the non-interacting case. We observe finite Josephson current at the flat band at finite interaction strengths. By tuning boundary states and the flat band state to be degenerate, substantial increase in the flat band current is observed. The superconducting critical temperature within the considered range of interactions are of order a few nK. It is smaller than the temperatures of the considered experimental setup by one order of magnitude. Thus, the considered setup is not adequate to measure the flat band critical Josephson current. However, by tuning parameters and developing a proper experimental setup, measuring the critical Josephson current is possible in principle.

Foreword

This work was carried out from June to December 2018, while I was working at the Quantum Dynamics group at Aalto University. I would like to thank Academy Professor Päivi Törmä for the opportunity to participate in this interesting project and giving profound advice along the way. I thank Dr. Sebastiano Peotta for being my instructor. His persistence on answering my questions, providing ideas, and helping me along the way was essential in completing this thesis. I also thank other members of the Quantum Dynamics group for discussions and help. I thank Dr. Pablo Burset and Prof. Christian Flindt for useful discussions related to the Josephson effect. My gratitude also goes to Prof. Tilman Esslinger and his Lithium team at ETH Zürich, Mr. Martin Lebrat, Mr. Samuel Häusler, Mr. Philipp Fabritius, Mr. Jeffrey Mohan, Dr. Laura Corman, and a former member Dr. Dominik Husmann for sharing details regarding to their two-terminal transport experiment for lithium-6.

This master’s thesis marks the end of an era in my life. Finally, after six and half years of various excursions within a plethora of academic subjects and other (more or less) well-planned deviations from the beaten track, this work concludes my basic studies. At this point, I think it is now appropriate to look back and reminisce on how I got interested in physics and how the interest developed.

It all started back in the fall 2007, when I was 14 year old. Back then, I had thought about many options for my career, like being a historian or an author, but frankly I had not found a proper interest. Then, my aunt gave me a book on the history of natural sciences. Despite my initial prejudices against the subject, I read the book and enjoyed it. Unexpectedly, the book caught my attention to the peculiarities of physics, especially relativity. However, the rather general level of detail of the book would not satisfy my curiosity: I wanted to know what was behind all these phenomena. Thus, I began my first project in physics: I decided to learn the general relativity within the following two years and then be done with physics. To achieve the goal, I began to learn mathematics and physics on my own as a hobby. I used some high school books that I found from the attic of my grandparent’s house, Wikipedia articles and so on.

By the time I got to high school, I had learned that the project wasn’t as easy as I originally thought. I had taught myself some necessary methods like calculus, simple matrix calculations, and simple special relativity. However, I was still far from grasping the general relativity. Realizing this didn’t make me stop but instead I got much more eager. The amount of work that I had spent learning physics and mathematics had induced severe sunk cost fallacy. By the suggestion of my high school physics teacher, I began to read the Feynman Lectures on Physics. I completed the first two volumes during high school. In addition to basic physics, I learned from it to appreciate the value of understanding instead of trusting authorities and memorizing things. In other words, the connections between facts turned out to be more important than the...
facts themselves. Even up to this day I cannot use or remember formulas, methods, or concepts that I haven’t derived or understood myself.

Anyway, suddenly the two-odd year project turned into a longer one and my focus had become quite a bit wider. I decided to apply to university to study physics and began my studies in the Fall 2012. Then, finally on my fourth year of studies I had a course on the general relativity and learned to understand its basic phenomena. Thus, my first physics project was complete. Despite my original plan to leave physics after accomplishing the feat, I realized that I couldn’t anymore let go of the kick involved in doing physics and solving related problems. Now, after a couple of years from that point, I’m still doing physics as is demonstrated by this work and plan to carry on to doctoral studies.

I would like to thank my parents Eeva and Ari, my brother Kalle, and my friends for their support. Especially, I thank my friends Toni and Sofia for many useful physics and metaphysics discussions that have helped me a lot the last couple of years. Also, I thank my high school physics teacher Antti Savinainen for the encouragement all those years ago and pointing me to the right direction. Finally, I would like to thank my aunt Raija for giving that book on the history of natural sciences all those years ago.

I think that once in a while, usually after lots of hard work, it is nice to put things to context and remember that in the end we are studying only a small part of the nature’s vast tapestry. Instead of discouragement, I think this thought establishes that there is also importance to other aspects in life. After all, it is sometimes nice to go back to the basics and enjoy the world instead of being overly analytical about it. I end this Foreword to a related quote that has stuck in my head since I first read it from the Feynman Lectures on Physics (Volume I, Lecture 3, "The Relation of Physics to Other Sciences"):  

A poet once said, "The whole universe is in a glass of wine." We will probably never know in what sense he meant that, for poets do not write to be understood. But it is true that if we look at a glass of wine closely enough we see the entire universe. There are the things of physics: the twisting liquid which evaporates depending on the wind and weather, the reflections in the glass, and our imagination adds the atoms. The glass is a distillation of the Earth’s rocks, and in its composition we see the secrets of the universe’s age, and the evolution of stars. What strange arrays of chemicals are in the wine? How did they come to be? There are the ferments, the enzymes, the substrates, and the products. There in wine is found the great generalization: all life is fermentation. Nobody can discover the chemistry of wine without discovering, as did Louis Pasteur, the cause of much disease. How vivid is the claret, pressing its existence into the consciousness that watches it! If our small minds, for some convenience, divide this glass of wine, this universe, into parts — physics, biology, geology, astronomy, psychology, and so on — remember that nature does not know it! So let us put it all back together, not forgetting ultimately what it is for. Let it give us one more final pleasure: drink it and forget it all!

In Otaniemi, January 24, 2019

Ville Pyykkönen
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Chapter 1

Introduction

Symmetry principles are at the heart of quantum mechanics. For instance, in the condensed matter physics perspective, the discrete translational symmetry of a lattice has implications on the possible eigenstates of the system Hamiltonian. The famous Bloch's theorem implies that the single particle eigenstates of a lattice system are labeled by the quasimomentum, which is the conserved quantum number arising from the discrete translational symmetry [1]. In the limit of a macroscopic lattice system, the energies of the eigenstates form smooth curves with respect to the quasimomentum. These curves are known as Bloch bands or, simply, bands. For each quasimomentum value, there are usually multiple eigenstates with different energies, that is, a lattice system usually has multiple bands. The collection of the bands, known collectively as the band structure, contains all the information about the possible quantum states of the independent particles in the system.

The systems in condensed matter physics often involve competing energy scales, typically the kinetic Fermi energy and the Coulomb interaction energy. However, there exists lattice systems that have flat Bloch bands in their band structure in which the kinetic energy vanishes. These bands, also simply known as flat bands, are defined as being either very narrow compared to the separation to other bands or completely degenerate. In a flat band, the group velocity, which measures the particle velocity is thus either very small or zero. It follows that particle transport in the non-interacting single particle picture is forbidden and the particles are localized. As the kinetic energy is not anymore competing for being the dominating energy scale, any other introduced energy scale dominates the behavior of the particles in a flat band. For this reason, flat bands offer a way to study strongly correlated phenomena in a novel way [2].

The quest for high temperature or even room temperature superconductivity is of interest due to the scientific goal of understanding the phenomenon and for technological reasons. It has been postulated that lattice systems with flat bands could offer a route to room temperature superconductivity [3, 4]. As in the non-interacting limit the particles at the flat band are localized, the question arises whether a flat band can carry a supercurrent. To answer this question, it turns out to be sufficient to show whether or not the system has a non-zero superfluid weight [5, 6]. It has been shown that superfluid
weight on a flat band is proportional to the integral of quantum metric over a Brillouin zone and the interaction strength between particles [7]. Furthermore, in the same article, it was shown that the quantum metric is given a low limit by the Chern number, which is a topological invariant of the flat band Bloch function. Thus, flat bands with non-zero Chern number have superfluid weight directly proportional to the interaction strength between particles. Also, for instance the Lieb lattice on which flat bands have zero Chern number, the superfluid weight is shown to be proportional to the interaction strength [8]. Thus, in the light of the theoretical evidence, the attractive interactions should make a flat band able to carry a supercurrent: the superconductivity should be well-posed phenomenon at the flat band, given that the superfluid weight is finite.

The above results on flat band superconductivity lack experimental verification. A possible platform for the experimental realization would be an ultracold quantum gas experiment. Ultracold gas experiments are a highly tunable platform to study quantum many-body phenomena involving lattice systems within and beyond solid state physics [9]. For instance, an ultracold gas experiment for studies of transport phenomena is located at ETH Zürich Lithium lab, which is described in Refs. [10, 11]. In the setup, a scattering region is placed between two reservoirs of neutral fermionic Lithium-6 atoms. Thus, it is a basic two terminal setup, which is used to measure the transport properties of the scattering region. Interactions can be imposed on the quantum system and reservoirs to study superconductivity.

In the experimental study, one has to focus on an effect in which the superconducting current through a flat band could be observed. Such phenomenon is the Josephson effect, which is a prominent transport phenomenon observed in junctions that comprises two superconductors and a scattering region that works as a link between them, namely a Josephson junction [12]. In the Josephson effect, a supercurrent is observed in the scattering region. The effect is caused either by a voltage bias or a phase bias, and it is called the AC and DC Josephson effect, respectively. In the latter case, the phase bias means a superconducting phase difference between the two superconductors. A superconductor has macroscopic wavefunction, which is described by an amplitude and a phase. The superconductors react to a spatially changing phase by a current that is proportional to the phase gradient. The Josephson current through a flat band could be in principle observed in a flat band system placed between two superconductors.

Perhaps the simplest lattice system with a flat band is the sawtooth lattice. Ref. [13] proposes a way to realize the sawtooth lattice in ultracold atom gas experiments. The band structure of an infinite sawtooth lattice comprises a dispersive band and a flat band. It has been shown that with interaction strengths above a certain threshold, the superfluid weight of the half-filled flat band is higher than the superfluid weight of the half-filled dispersive band [14]. Thus, we expect that above the interaction strength threshold, the observed maximal Josephson current in the sawtooth lattice should be larger for the flat band than for the dispersive band. Therefore, the observed Josephson current at the flat band is expected to be significant.

In this project, we investigate numerically the effects of interactions on transport through a sawtooth lattice with a flat band. The goal is to assess the experimental feasi-
bility of observing the supercurrent through the flat band. Specifically, we study whether the observation is possible with the experimental setup at the ETH Zürich Lithium lab. We also pursue possible experimental signatures of the flat band in the system. Our basic strategy is to study numerically the behavior of a finite piece of the sawtooth lattice between two superconductors. We model the system using a tight-binding Hubbard model. The interactions on the systems are treated on mean-field level within the framework of the Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity [15]. In order to calculate the the DC Josephson effect in the system, we utilize the Bogoliubov-de Gennes approach to mean field theory [16, 17]. Importantly, the order parameters and mean particle densities in the sawtooth ladder are calculated self-consistently, as in Ref [18]. Finite temperatures can also be considered within the framework. The quantum transport software Kwant was used in the numerical calculations [19].

The structure of the thesis is the following. In chapter 2 we give the theoretical and experimental background and goals of this work in more detail. The chapter 3 introduces the theoretical methods. The results are presented in chapter 4. The chapter 5 discusses the results and concludes the thesis.
Chapter 2

Background and Goals

In this chapter, we introduce the essential background that motivates this thesis at a general level. We give a brief introduction to the superconductivity and the Josephson effect. Secondly, we introduce the experimental setup of the ETH group, which can be used to directly probe the transport properties of various lattice systems. Thirdly, we give a brief introduction to the physics of the flat bands. Finally, in the context of the background given, we describe the goals of the thesis.

2.1 Superconductivity and Josephson effect

Superconducting phase is a state of matter that is characterized by vanishing resistance and the expulsion of magnetic field, also known as the Meissner effect. The superconductivity was discovered by H.K. Onnes in 1911 in mercury below the temperature of 4.2 K [20]. The temperature below which a material is superconducting is known as its critical temperature. The Meissner effect was discovered in 1933 by W. Meissner and R. Ochsenfeld [21]. Another peculiar effect of superconductivity is the quantization of magnetic flux through superconducting rings as was predicted by London [22] and experimentally confirmed by Deaver and Fairbanks [23] and independently by Doll and Nábauer [24].

The basic microscopical theoretical understanding of superconductivity was established by Bardeen, Cooper, and Schrieffer in 1957 [15]. This theory is known as the BCS theory after the authors. The theory explains superconductivity as a superfluid of bosonic Cooper pairs that condense in the superconducting ground state. The binding energy of a Cooper pair gives an essential energy scale for the theory, known as the superconducting gap, pair potential, or order parameter. The critical temperature is related to the superconducting gap. Earlier phenomenological theories of the superconductivity include the London theory [25] that successfully explains the Meissner effect, and the Ginzburg-Landau theory [26].

Having a finite order parameter, or pair potential is not sufficient for superconductivity. The necessary and sufficient condition for the superconductivity is that the so-called
superfluid weight is finite \([5, 6]\). The superfluid weight \(D_s\) is defined as a suitable limit of current-current correlators, or equivalently as the proportional constant between the increase of free energy of the system per volume and the momentum of a Cooper pair squared:

\[
\frac{\Delta F}{V} = \sum_{ij} D_{s,i} p_i p_j,
\]

(2.1)

where \(\Delta F\) is the change in the free energy, \(V\) is the volume of the system and \(p_i, p_j\) are the \(i\)th and \(j\)th component of the momentum of a Cooper pair \(p = \nabla \phi\), where \(\phi\) is the superconducting phase. The superfluid weight is in general a second order tensor, that is, the relation might be dependent on the direction due to possible anisotropy of the system. By a qualitative comparison to the usual kinetic energy \(E\) formula for \(N\) particles in volume \(V\)

\[
\frac{E}{V} = \frac{np^2}{2m}
\]

(2.2)

where \(n = N/V\) is the particle density, we can identify \(D_s = n_s/2m\), where \(n_s\) is the number density of the Cooper pairs in the superfluid and \(m\) is the effective mass of the Cooper pairs. Thus, roughly speaking, if \(D_s = 0\), there are no Cooper pairs or the effective mass is infinite. Either way, there cannot be superconductivity as there are either no carriers or they cannot move as they are localized. On the other hand, finite superfluid weight implies both non-zero carrier density and finite effective mass for the Cooper pairs, implying that the system is superconducting.

The superconductors that are understood in terms of the BCS theory are known as conventional superconductors. In contrast, the superconductors that cannot be explained by the BCS theory are known as unconventional superconductors. Unconventional superconductivity is an active field of research. The first found unconventional superconductor is a lanthanum-based cuprate perovskite material with critical temperature of 35 K by Bednorz and Müller in 1986 [27], which at the time had significantly higher critical temperature than the other known superconductors. It was the first of the so-called high-temperature superconductors. Later on, superconductors with higher critical temperatures have been found. For instance, Wu et al. [28] found that yttrium-based cuprate perovskite has critical temperature of 92 K, which makes it possible to cool the material to the superconducting state by liquid nitrogen. Many ceramic superconductors possess even higher critical temperatures, up to 133 K. Interestingly, unconventional superconductivity was observed in twisted bilayer graphene with magic angle 1.1° with the critical temperature of 1.7 K [29]. The flat bands formed in the twisted bilayer graphene at the magic angle are postulated to be important [30]. A theory that would explain unconventional superconductors exhaustively has not yet been developed (as of 2018). The long term goal of the superconductor research is to reach room-temperature superconductivity, in which the critical temperature is above 273.15 K or 0 °C.

The highest achieved critical temperature at the moment is 203 K which is achieved in \(\text{H}_2\text{S}\) at the extreme pressure of 150 GPa [31]. However, they declare that it is explainable by conventional superconductivity. The conventional superconductor with highest
known critical temperature at normal pressure is magnesium diboride MgB₂ with critical temperature of 39 K, which was found in 2001 by Nagamatsu et al. [32].

The superconducting state is peculiar as it is quantum mechanically coherent over macroscopic distances since the ground state is described by a single wave-function with a well-defined uniform amplitude and phase. If the phase is forced to vary by a magnetic field, impurity or other effect, and the effects are not too drastic, the way that system reaches a thermodynamic equilibrium is to introduce a current. The current is related to the superconducting phase gradient. This is the case since exciting particles from the ground state is not energetically feasible due to the superconducting gap if the external perturbation is not too big, that is, the phase gradient is small. Importantly, as the system is in thermodynamic equilibrium, the introduced current does no dissipate. Thus, it is called a supercurrent.

An experimentally important way to introduce variation in the superconducting phase is to introduce inhomogeneity to the system. For instance, when two superconductors are connected by an insulator, a normal metal, or by some other structure capable of transport, a supercurrent can flow between the superconductors even without voltage between the superconductors, even if the middle region is not a superconductor. This occurs when the two connected superconductors have different superconducting phases. This phenomenon is called the Josephson effect after B.D. Josephson who first theoretically predicted the effect [12]. Also, such junction is called a Josephson junction and the supercurrent through the junction is often called the Josephson current. A Josephson junction is illustrated in the Fig. 2.1. For weak links, the current phase relation (CPR) is of the form \[ I = I_c \sin \phi, \] where \( I_c \) is called the critical current and \( \phi \) is the superconducting phase difference, that is, \( \phi = \phi_L - \phi_R \), where \( \phi_L, \phi_R \) are the superconducting phases of left and right superconductor, respectively. The phenomenon is related to tunneling of Cooper pairs from a superconductor to another. As this phenomenon occurs at equilibrium, there is no dissipation even in the non-superconducting part of the system. The phenomenon in which constant current arises from the a superconducting phase difference is called the DC Josephson effect. There is also the AC Josephson effect in which an alternating current arises in the junction when a constant voltage is applied. The frequency of the current is dependent on the voltage, so the AC effect acts as a voltage-frequency converter.

2.2 Ultracold atom gas experiments and mesoscopic physics

Ultracold quantum gases offer a highly tunable platform to study many-body quantum systems. In addition to studying phenomena of dilute quantum gases, with ultracold atom gases one can simulate solid state systems, realize tight-binding models and study strongly correlated systems beyond solid state physics. The ultracold gas differs from other cold gases by the fact that the Boltzmann statistics break and the quantum statistics become important. The field of ultracold gases began with the first realizations of a Bose-Einstein condensate in a gas of rubidium-87 atoms by E. Cornell, C. Wieman et al. [34] and in gas of sodium-23 by W. Ketterle et al [35]. Importantly, the AC and DC
Josephson effects have been observed in a ultracold atom gas experiment, both with bosons [36–38] and fermions [39].

Mesoscopic physics has been of central interest in condensed matter physics since 1980’s. As the name of the field indicates, the mesoscopic physics consists of phenomena that land in between microscopic and macroscopic scales: from the size of a couple of atoms up to micrometre scale. This scale is interesting as current technology is capable of manufacturing devices and controlling systems of this scale. The size of such systems are below electron phase-relaxation length. Thus, quantum mechanical effects are apparent in mesoscopic physics. On one hand, understanding the physics of this region is important for being able to utilize the phenomena in technology. On the other hand, controlled mesoscopic systems offer a direct testing ground for quantum mechanical models of condensed matter physics.

Ultracold atom gas experiments provide a prominent platform for simulating physics of the mesoscopic scale. Especially, the usual mesoscopic setup comprising of a system of interest connected to two or more particle reservoirs can be realized in the ultracold gas context. This is done by connecting two atom reservoirs with a modifiable narrow constriction. Importantly, the constriction can be designed to realize lattice models of condensed matter physics. This offers a direct test of physics of many condensed matter models that are yet to see a realization in the solid state context. In particular, also bosonic systems can be realized.

In the scope of this thesis, the ultracold gas setup of the Lithium lab of Quantum Optics Group at ETH Zurich is of interest. The setup is presented for instance in Refs. [10, 11]. A sketch of the system is presented in the Figure 2.2. The setup consists of
two reservoirs of $^6$Li atoms at the typical absolute temperature of 67 nK that are in the lowest and the third lowest hyperfine states. The considered isotope of the Lithium atom is a fermion; it behaves in this case as a spin-1/2 particle due to being in exactly two different hyperfine states. A quantum wire is imposed in between the reservoirs using two orthogonal laser beams. The Gaussian envelopes of the crossing beams have characteristic sizes of 9.1 μm vertically (see figure 2.2) and 30 μm horizontally, setting the characteristic sizes of the constriction. The reservoirs act as a source and a drain for current through the quantum wire. A mesoscopic lattice can be superimposed on the quantum wire as an optical lattice using a Digital Micromirror Device (DMD). Importantly, the number of imprinted barriers and their positions can be controlled freely. Also, it is in principle possible to realize more complicated tight-binding systems, such as ones with flat bands, in between the reservoirs.

Interactions between the neutral lithium-6 atoms can be introduced using Feshbach resonances [11, 40]. Importantly, by using attractive interactions, the regions near the ends of the optical lattice imprinted in the quantum wire can be tuned to superfluid, that is, superconductivity can be introduced to system [11]. The interaction parameter can be tuned quite freely. Also, the chemical potentials on the reservoirs and on the optical lattice can be separately controlled using an attractive Gaussian beam, called the gate beam.
A benchmark for mesoscopic physics experiments is given by the quantized conductance of a ballistic conductor, connected by leads to two reservoirs [41]. It is one of the first mesoscopic effects studied. The conductance of a single channel in the conductor is given in units determined solely by elementary constants: $2e^2/h$, where $e$ is the charge of the carrier, $h$ is the Planck’s constant and the factor of 2 corresponds to two spin states of an electron. Thus, by increasing the chemical potential difference of the two reservoirs, more and more channels open: the conductance increases in discrete manner. This result has been also reproduced within neutral ultracold atoms by the ETH group [10]. There instead of electrical current, they consider particle current so the conductance quantum turned out to be $2/h$ or $1/h$, depending on whether they consider both hyperfine states or only single one. The fact that the typical mesoscopic phenomena studied in solid state can also be realized with the ultracold gases gives assurance that the setup is suitable for our purposes.

Other achievements of the ETH Lithium lab include showing that the band insulator state in a 1D chain lattice system is still an insulator for strong interactions in a 1D chain lattice system, hinting at presence of a Luther-Emery liquid [11].

The optical lattices offer much freedom in designing the lattice. For instance, realizable systems include a sawtooth lattice and a zigzag lattice [13]. Importantly for the current work, the sawtooth lattice can be tuned so that it contains a flat Bloch band in its band structure. However, possible noise and imperfections in realization of the lattice might be an issue. The sawtooth is one of the simplest lattice structures containing a flat band. The flat band physics and the sawtooth lattice are introduced in the next section.

### 2.3 Flat band physics and sawtooth lattice

In order to understand the concept of a flat band, let us review the basic concepts of the band structure of a lattice system. The following short review of the band structure is based on Ref. [1]. Lattice systems are one of the central concepts in condensed matter physics. Their inherent discrete translational symmetry has direct implications on possible energy levels of particles in the lattice. The effects of the symmetry are encapsulated in the famous Bloch’s theorem. The theorem is the following

**Theorem 1** (Bloch’s theorem). Let $\mathbf{a}_1, \ldots, \mathbf{a}_m$ be the basis vectors of a Bravais lattice and $\mathbf{T} = n_1 \mathbf{a}_1 + \cdots + n_m \mathbf{a}_m$ where $n_i$ are integers, be any translation vector in the lattice. Let $V(\mathbf{r})$ be a periodic potential such that $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{T})$ for all lattice translations $\mathbf{T}$ in the Bravais lattice. Let us consider a particle under the influence of the periodic potential with the Hamiltonian $\hat{H} = \frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})$. The eigenstates of the Hamiltonian $\hat{H}$ can be chosen to be of form

$$\psi(\mathbf{r}) = e^{i\mathbf{q} \cdot \mathbf{r}} u(\mathbf{r})$$

where $\mathbf{q}$ is called quasimomentum and $u(\mathbf{r})$ is a function with the same periodicity as the potential $V(\mathbf{r})$, that is, $u(\mathbf{r}) = u(\mathbf{r} + \mathbf{T})$ for all lattice translations $\mathbf{T}$. In other words, the eigenstates can be written as a product of a plane wave and a function with the periodicity of the underlying lattice. Furthermore, the plane waves have to follow the boundary conditions of the system.
A direct implication of the theorem is that the eigenstates of the Hamiltonian of the lattice system are characterized by quasimomentum, which is the conserved quantum number related to the discrete translational symmetry of the system. The quasimomentum is analogous to momentum that arises from continuous translational invariance of a system, hence its name. However, in a lattice system the momentum is not a good quantum number because the system does not have full continuous translational invariance and, therefore, the momentum is not conserved in general.

If the system is macroscopic, the possible values of quasimomentum are quasicontinuous. The energies of lattice system Hamiltonian eigenstates vary continuously with the quasimomentum, forming the so-called Bloch band or simply a band. A Bloch band is given by the plane wave characterized by the quasimomentum and a periodic function $u(r)$ determined from the Schrödinger equation. Usually, the periodic function $u(r)$ in the Bloch's theorem is not unique. On the contrary, many such functions satisfy the Schrödinger equation, in general with different eigenenergies. There is a Bloch band for each such periodic function, giving rise to the band structure of the lattice system. Thus, the Bloch bands are characterized by a band index $n$ and are of form $E = E_n(q)$ where the quasimomentum $q$ acts as a variable. It can be shown (see for instance the Appendix E in Ref. [1]) that the velocity $v_n(q)$ of particle lattice system on a Bloch band with band index $n$ is given by the group velocity

$$v_n(q) = \frac{1}{\hbar} \nabla_q E_n(q),$$

where $\nabla_q$ denotes gradient with respect to the quasimomentum $q$. It is noteworthy that in a perfect crystal, independent particles move indefinitely with a constant velocity.

A flat Bloch band in a band structure of a lattice system is defined as being dispersionless, being highly degenerate, or having small bandwidth compared to its separation from other bands. Thus, as its name indicates, the band as pictured in energy-quasimomentum space is flat. A direct consequence of the flatness is that the group velocity of non-interacting particles in it is either very small or vanishes. As stated above, the group velocity is the measure of how fast wave-packets or, in this case, particles move in the system. Thus, for the flat bands, the particle transport is forbidden; the single particle eigenstates related to the band are localized. As bandwidth is ruled out as an energy scale in a flat band, any other introduced energy scale is dominating. Any perturbations to the system, like interaction or disorder, might turn the flat band to dispersive. Then, the dispersive behavior is qualitatively dependent on the nature of the perturbations. Thus, flat bands are expected to produce interesting phenomena when interactions or disorder are introduced to the system.

One of the most important and also the first examples of flat bands appearing in condensed matter physics are the Landau levels, the degenerate energy levels of an electron in a magnetic field corresponding to the classical cyclotron trajectories. Their role was essential in the first observations of the quantum Hall effect that were made in two-dimensional electronic gases in strong magnetic fields. For instance, such gas is formed in the insertion layer of a MOSFET transistor, which provided the setup of the first observation of the quantum Hall effect by Klitzing, Gorda, and Pepper [42].
mechanism of the effect is explained for instance in Ref. [41] and is briefly the following. Firstly, the flat banded Landau levels in the 2D electron gas forbid electron transport in the bulk, forcing it to the edges, where the confinement effects lead to dispersive edge states. As the magnetic field separates the different directions of the current to opposite edges of the gas, no backscattering occurs: the edge states are perfect quantum channels with conductance of one conductance quantum $e^2/h$, as given by Landauer formula. It is noteworthy that usually the Landau levels do not have the usual spin degeneracy due to the magnetic field induced Zeeman splitting. The number of such states per edge is determined by the number of filled Landau states $v$. Thus, the total Hall conductance is $\sigma_H = ve^2/h$, explaining the integer quantum Hall effect.

The first lattice system to be theoretically shown to contain flat bands in its unperturbed lattice structure was the dice lattice followed shortly by the Lieb lattice [2]. The Lieb lattice and its variants have been used to study flat band ferromagnetism and ferromagnetism in the Hubbard model [43–45]. The flat banded lattice model at the focus of the present study is the sawtooth lattice. Other examples of flat banded systems include kagome lattice, diamond ladder, stub lattice and a checkerboard lattice [2]. The flat band can either be a property of the system caused by its symmetry, or can result of parameter tuning. Flat banded systems can be realized for instance in electronic systems including superconducting wire networks, photonic systems, and in ultracold atom optical lattices introduced above [2].

In order to show a concrete example of a lattice system with a flat band let us introduce the sawtooth lattice. The sawtooth lattice is a quasi-1D lattice comprised of a unit cell of two lattice sites or orbitals as sketched as a graph in the figure 2.3. The orbitals of a unit cell are labeled as $A$ and $B$. Its Hamiltonian (without interactions) is

$$
\hat{H} = \sum_i \left[ \epsilon_A \hat{c}^\dagger_{A,i,0} \hat{c}_{A,i,0} + \epsilon_B \hat{c}^\dagger_{B,i,0} \hat{c}_{B,i,0} + t_{A,B} (\hat{c}^\dagger_{A,i,0} \hat{c}_{B,i,0} + \text{h.c.}) \\
+ t_{A,B} (\hat{c}^\dagger_{A,i+1,0} \hat{c}_{B,i,0} + \text{h.c.}) + t_A (\hat{c}^\dagger_{A,i+1,0} \hat{c}_{A,i,0} + \text{h.c.}) \right],
$$

(2.5)

where the lattice sites are denoted by index $i$, $\sigma$ denotes the spins of the particles, h.c. denotes the Hermitian conjugate, the on-site energies of the model are labeled as $\epsilon_A$ and $\epsilon_B$, respectively and the hopping parameter from $A$ to $A$ is labeled as $t_A$ and from $A$ to $B$ as $t_{AB}$. The hopping between adjacent $B$ sites is forbidden.

It can be shown that the sawtooth lattice has a flat Bloch band if the on-site energies are equal $\epsilon_A = \epsilon_B$ and for hopping parameters it holds $t_{AB} = \sqrt{2}t_A$ (see Appendix A for details). The band structure of the sawtooth lattice for the case $t_A = -1, t_{AB} = -\sqrt{2}$ and $\epsilon_A = \epsilon_B = 1$ is shown in the Fig. 2.4. It is seen that the sawtooth lattice has a dispersive band and a flat band.

The flat band is caused by destructive interference of different paths of the particles. Thus, a basis for the flat band states is formed by a set of localized eigenfunctions. On a sawtooth lattice, the localized states are $V$ shaped as shown in Fig. 2.5. For the flat band localized states, it is conventional to give the sign of the wave function at the sites of the state. The signs illustrate the destructive interference on the neighboring sites where the
wavefunction vanishes. It is noteworthy that the localized states are not orthogonal as they overlap on single sites. A corresponding orthonormal basis is given by so-called maximally localized Wannier functions, which are certain real space functions of lattice site index, Fourier transformed from the Bloch functions [46]. In the case of a flat banded system, they are similar to the localized states but have exponentially decaying tails, which make the functions orthonormal.

Even though flat band is a single particle property, it has implications on correlated many-particle physics. In the flat band limit, the critical temperature $T_c$ of a superconducting phase given by the BCS theory has been shown to be linearly dependent on the interaction strength $T_c \propto V_c$ [3, 4]. This is in contrast to the dispersive band BCS theory result $T_c \propto \exp \left( \frac{1}{\sqrt{g(E_F)}} \right)$, where $g(E_F)$ is the density of states at the Fermi energy. The flat band density of states is diverging, so systems with flat bands might lead to high-temperature superconductivity. For instance, for high critical temperature cuprates it has been shown that its CuO$_2$ planes have a Lieb lattice structure with a flat band [47]. However, as flat band is dispersionless in non-interacting case, it is important to show that it can indeed carry a supercurrent when in a superconducting state. To this end, it has been shown that the superfluid weight of a flat band is proportional to the integral of quantum metric over a Brillouin zone, that is, the physically unique values of the quasimomenta, and the interaction strength [7]. Also, in the same article it is shown that the quantum metric is bounded by the Chern number. The quantum metric is a second order tensor that measures the infinitesimal Bures distances between continuously parameterized quantum states [48]. The Chern number is an integer invariant related to the topology of a quantum state [48]. In the quantum Hall effect, the Chern number plays the role of the integer that quantizes the Hall conductivity; the quantum
Figure 2.4: Band structure of a sawtooth lattice for parameters $t_A = -1$, $t_{AB} = -\sqrt{2}$, $\epsilon_A = \epsilon_B = 1$.

Hall effect is as robust as it is because its roots are in the topological properties of the Bloch wavefunction [49]. Also, it has been shown the superfluid weight is bounded from below by the absolute value of Berry curvature, that is, finite Berry curvature is a sufficient condition for superfluidity in interacting systems [50]. The Berry phase is a phase gathered when a quantum state is varied a whole closed cycle in a parametrized space; the Berry curvature is related to the line integral giving the phase through the Stokes’ theorem: it is the pseudovector field that gives the Berry phase when its curl is integrated over a plane enclosed by the closed cycle [48]. Also, lattice systems with zero Chern number can have finite superfluid weight as is the case for instance for the Lieb lattice [8]. For the case of a sawtooth lattice, it has been shown that above a certain finite interaction strength the superfluid weight of the system when the flat band is half-filled dominates the superfluid weight of the case of half-filling of the dispersive band [14]. Interestingly, it has been shown that for certain 1D lattice systems consisting solely of flat bands, under interactions single particles are localized but preformed pairs may carry finite current [51]. Recently, it has been shown that the effective mass of a bound state of a two-body problem is determined by band structure invariants [52]. This result establishes that the Cooper pairs on a flat band can have finite effective mass defined at the two-body problem level.

The theoretical results on the flat band superfluid weight $D_s$ indicate that interactions should make transport through a flat band possible. However, this remains to be exper-
\[ |\psi_{N,\sigma}\rangle = (\sqrt{2}\hat{c}^\dagger_{A,N,\sigma} - \hat{c}^\dagger_{B,N,\sigma} - \hat{c}^{\dagger}_{B,N-1,\sigma}) |0\rangle \]

Figure 2.5: The V form of the localized states of the flat band in the sawtooth lattice. Such state can be formed at any of such V shaped region of the lattice. Both the exact form and the sign notation of the localized state are given.

Experimental verified. Ultracold gas experiments are a potential basis for the experimental realization due to their tunability. The contribution of this thesis is to provide numerical data on feasibility of such a experimental realization and generally characterize the system. We study a finite portion of the sawtooth lattice between two superconducting leads and calculate the Josephson current through it. We consider the interactions on mean-field level and calculate the related superconducting ground state of the system using the self-consistent Bogoliubov-de Gennes method. In order to understand the interacting case, we study first the non-interacting case. We evaluate the interacting results first at zero temperature and finally introduce finite temperature.
Chapter 3

Theory and methods

In this chapter, we introduce our theoretical and numerical tools. We discuss the model for sawtooth lattice, Bogoliubov-de Gennes theory for the lattice system, and evaluating the parameters of the theory self-consistently. For the self-consistent method, we discuss the methods used for ensuring and speeding up the convergence.

3.1 Sawtooth lattice model

In the previous chapter, we introduced the sawtooth lattice and its tight-binding model. In this section, we introduce another way to simulate the sawtooth lattice: as a potential that emulates a possible optical potential in an ultracold gas experiment. Finally, we discuss how from such experimentally realistic potential it is possible to extract the tight-binding parameters. The reason to consider such a model in this thesis is to verify that the tight-binding model gives experimentally relevant results that are qualitatively right. In practice, we compare the potential model to the tight-binding model with the experimentally realistic parameters.

An example of a realistic potential that can be imprinted in the ultracold gas experiment using a DMD as in Ref. [11] is shown in Fig. 3.1. The potential is one the models considered in Antti Ranni’s master thesis [53]. In order to do calculations with the experimental potential, the Laplacian in the Schrödinger equation is discretized. The obtained discrete Hamiltonian is

\[ \hat{H} = \sum_{\sigma} \left( 4t + V(x_i, y_i) \right) \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma} - \sum_{(ij)} t \hat{c}^\dagger_{i} \hat{c}_{j}, \]  

where \( x_i \) and \( y_i \) are the \( x \) and \( y \) components of the position vector of the site \( i \), \( t = \frac{N^2}{2ma^2} \), where \( m \) is the mass of considered particles. The potential is of form

\[ V(x, y) = V_{\text{DMD}}(x, y) + V_{\text{trap}}(x) + V_{\text{step}}(y) \]  

where \( V_{\text{DMD}} \) represents the sawtooth lattice that can be printed experimentally by the digital mirror device (DMD), \( V_{\text{trap}} \) is a harmonic confinement potential in transverse
direction to confine particles to the sawtooth lattice, and $V_{\text{step}}$ is a step potential to give a baseline for the DMD potential. The harmonic confinement potential is of form

$$V_{\text{trap}}(x) = \frac{1}{2} m \omega_x^2 x^2, \quad \omega_x = \frac{\hbar}{ml_x^2}$$ (3.3)

where $l_x$ is the length scale of the harmonic confinement. The step potential is of form

$$V_{\text{step}}(y) = \frac{-V_0}{1 + \exp(-(y+y')/l_{\text{step}}) + \exp((y-y')/l_{\text{step}})}$$ (3.4)

where $y'$ determines the position of the edge of the step and $l_{\text{step}}$ is the length of the step. The obtained model is basically of tight-binding type square lattice model with on-site energies and hoppings.

To give a concrete example of the DMD potential, let us describe the example potential shown in the Fig. 3.1. Other components of the potential are as described above. The
DMD potential, $V_{\text{DMD}}$ is given by

\[
V_{\text{DMD}}(x, y) = V_0 \left[ \sum_n f \left( x + d_x, y - \left(2n + \frac{1}{2}\right) d_y \right) + \sum_n f(x - d_x), y - \left(2n - \frac{1}{2}d_y\right) \right] + V_1 \sum_n f(x, y - n d_y),
\]

(3.5)

where

\[
f(x, y) = \exp \left( -\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} \right)
\]

(3.6)
is a Gaussian potential. The set of indices $n$ determines the exact length (in unit cells) and position of the lattice. The parameters $V_0$ and $V_1$ are controlling the depths of the wells and $\sigma_x, \sigma_y$ their sizes. The positional parameters $d_x$ and $d_y$ give the separation of the wells and also the periodicity of the sawtooth lattice.

In this thesis, for computational simplicity we consider the sawtooth lattice as a tight-binding model instead of an experimentally realistic potential. The tight-binding model should be suitable if the Gaussian wells in the potential are deep enough so that only the lowest bound state in the well is relevant. In order to establish this, we perform non-interacting transmission calculations on both models and compare the results. These are carried by the software package Kwant that utilizes efficient graph theory based methods to do wavefunction matching between leads and the system [19]. The software also provides an interface to assemble tight-binding Hamiltonians.

In order to get the two models to be as similar as possible, we use tight-binding parameters extracted from the experimentally realistic potential. The extraction is done by calculating overlaps and local energies of maximally localized Wannier functions of the full system [14]. The parameters used in this study are given in the Results chapter.

### 3.2 BCS Theory of a generic lattice

In this section, we consider the theory of superconductivity of fermionic particles on a generic lattice. The original theory by Bardeen, Cooper and Schrieffer (BCS) [15] utilizes an ansatz for the ground state and a variational approach. We follow here a method that is more like the equivalent approach by Bogoliubov et al. [16]. Instead of a variational ansatz and the related free-energy minimization procedure, we obtain the BCS ground state by diagonalizing the related Bogoliubov-de Gennes Hamiltonian and occupying different states according to the Fermi-Dirac distribution function. Thus, from the diagonalization one obtains expressions for the mean values of the observables in the ground state. Specifically, we derive formulas for average particle number, pairing potential, and current in the system.
3.2.1 BCS Hamiltonian

Let the lattice have $N$ sites labeled by $i \in \{1, 2, \ldots, N\}$. The Hamiltonian of the lattice system is a Fermi-Hubbard Hamiltonian, including on-site energies, hopping amplitudes between sites and on-site interaction of particles of opposite spins. On a site there cannot be two particles with same spin due to Pauli exclusion principle, so this kind of interaction term between particles with same spin vanishes automatically. The (grand canonical) Hamiltonian of the system is

$$\hat{H} = \sum_{i, \sigma} (\epsilon_{i\sigma} - \mu_i) \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - \sum_{i, \sigma, j, \sigma'} t_{i\sigma, j\sigma'} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} - \sum_i V_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} (3.7)$$

where $\sigma, \sigma'$ denote spins $\{\uparrow, \downarrow\}$ and $i, j$ are site indices. Also, $\epsilon_{i\sigma}, \mu_i, t_{i\sigma, j\sigma'}, U_i$ are on-site energies, chemical potentials, hopping matrix and interaction energies, respectively. The operators $\hat{c}_{i\sigma}^\dagger, \hat{c}_{i\sigma}$ create and annihilate, respectively, a particle with spin $\sigma$ to/from site $i$. The first term of the Hamiltonian contains the on-site energy, including the chemical potential. The second term contains various hopping terms. The third term includes the on-site interactions. The sign of the term is chosen to be negative as we are considering attractive interactions in this thesis. Thus, the attractive interactions have $V > 0$. We have discarded interactions between particles at other sites but these could be easily added to the Hamiltonian if some extended Fermi-Hubbard model would be of interest. For convenience, let us write the Hamiltonian as a sum of single particle Hamiltonian at site $i$

$$\hat{H} = \sum_{ij} \hat{H}_{0, ij} + \hat{H}_i = \sum_{ij} \sum_{\sigma, \sigma'} \left( \delta_{ij} \delta_{\sigma \sigma'} (\epsilon_{i\sigma} - \mu_i) - t_{i\sigma, j\sigma'} \right) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} - \sum_i V_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} (3.8)$$

where we have denoted $\hat{H}_{0, ij} = \sum_{\sigma, \sigma'} (\delta_{ij} \delta_{\sigma \sigma'} (\epsilon_{i\sigma} - \mu_i) - t_{i\sigma, j\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}$ the single particle Hamiltonian and $\hat{H}_i$ the interaction part, involving two particles.

In general, such Hamiltonian is hard to treat exactly. To make progress, we restrict the scope to mean field description of the problem. In the mean field approximation, instead of direct correlations we consider each particle coupled to the mean densities of other particles. The interaction Hamiltonian $\hat{H}_i$ becomes (see Appendix for details)

$$\hat{H}_i \approx \hat{H}_i^{MF} = -\sum_i V_i \left( \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \right) \text{Pairing terms}$$

$$+ \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \text{Hartree terms}$$

$$- \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} - \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger + \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \text{Fock terms}$$

(3.9)

where we have identified the terms of Hartree-Fock approximation and the pairing terms.

In this thesis, we consider the pairing terms and Hartree terms. We assume that the Fock terms vanish because no magnetism in the vicinity of the system is considered.
Without the magnetic field, the system is time-reversal invariant. Thus, we have $t_{i\sigma,i\sigma'} = t_{j\sigma',j\sigma}$. Also, without a magnetic field, we have $\langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \rangle = \langle \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \rangle$. We also denote $\Delta_i = -V_i \langle \hat{c}_{i\uparrow} \hat{c}_{i\uparrow} \rangle$ and $\bar{n}_{i\sigma} = \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \rangle$. The mean field interaction term can be thus written as

$$
\hat{H}^{\text{MF}} = \sum_i \left( \Delta_i^* \hat{c}_{i\uparrow} \hat{c}_{i\uparrow} + \Delta_i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}^\dagger - V_i \bar{n}_{i\uparrow} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - V_i \bar{n}_{i\downarrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow} + \frac{|\Delta_i|^2}{V_i} + V_i \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} \right) \quad (3.10)
$$

We call the whole mean-field Hamiltonian the BCS Hamiltonian and write it in the form

$$
\hat{H}_{\text{BCS}} \equiv \sum_{ij} \hat{H}_{\phi_{ij}} + \hat{H}^{\text{MF}} = \sum_{ij} \left[ \sum_{\sigma,\sigma'} (\delta_{ij} \delta_{\sigma\sigma'} (e_{i\sigma} - \mu_i - V_i \bar{n}_{i\sigma}) - t_{i\sigma,j\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} \right]
$$

$$
+ \delta_{ij} \left( \Delta_i^* \hat{c}_{i\uparrow} \hat{c}_{i\uparrow} + \Delta_i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}^\dagger + \frac{|\Delta_i|^2}{V_i} + V_i \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} \right) \quad (3.11)
$$

where $\bar{c}$ denotes spin opposite to $\sigma$. We moved the Hartree terms to the on-site terms as both contain particle number operators. Let us define $\bar{\mu}_{i\sigma} = \mu_i + V_i \bar{n}_{i\sigma}$.

It is useful to write the BCS Hamiltonian in an equivalent matrix form, also known as the Nambu form:

$$
\hat{H}_{\text{BCS}} = \sum_{ij} \begin{bmatrix} \hat{c}_{i\uparrow}^\dagger & \hat{c}_{i\downarrow}^\dagger \\
\hat{c}_{i\downarrow} & \hat{c}_{i\uparrow} \end{bmatrix} \begin{bmatrix} \delta_{ij} (e_i - \bar{\mu}_i) - t_{i\uparrow,j\uparrow} & \delta_{ij} \Delta_i^* \\
\delta_{ij} \Delta_i & -\delta_{ij} (e_i + \bar{\mu}_i) + t_{i\downarrow,j\downarrow} \end{bmatrix} \begin{bmatrix} \hat{c}_{j\uparrow}^\dagger \\
\hat{c}_{j\downarrow} \end{bmatrix}
$$

$$
+ \sum_i \left( e_{ii} - \bar{\mu}_i + \frac{|\Delta_i|^2}{V_i} + V_i \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} \right) \quad (3.12)
$$

The additional terms in the constant energy part are due to changing order of operators using the fermionic commutation relations. The pairs of up-spin annihilation and down-spin creation operators are called Nambu spinors and they form the Nambu space.

The constant terms are usually discarded in the following discussions as they only change the zero of the absolute energy scale. However, these can be of importance in self-consistent calculations of ground-state energy.

### 3.2.2 Canonical transformation – Bogoliubov-de Gennes theory

The BCS Hamiltonian is quadratic so it should diagonalizable. In other words, it is possible to represent the Hamiltonian as a sum of decoupled quasiparticles. This is desirable as independent single quasi-particle states of the system can be occupied according to the Fermi-Dirac statistics to form the ground state. The ground state observables can then be calculated easily.

Diagonalizing the Hamiltonian is done by a canonical transformation called a Bogoliubov transformation. In other words, the system is transformed into a new set of
creation and destruction operators $\hat{\gamma}_{ne}^\dagger, \hat{\gamma}_{ne}$ that fulfill the fermionic anticommutation relations and renders the Hamiltonian to the form

$$\hat{H} = \hat{\gamma}^\dagger D \hat{\gamma} + E_0 \tag{3.13}$$

where $\hat{\gamma}$ is a vector of the new operators, $D$ is a diagonal matrix and $E_0$ collects the energy constants.

The Bogoliubov transformation of the Hamiltonian in the Nambu form can be done directly by diagonalizing the matrix that represented in the block form is

$$\mathcal{H}_{BdG,ij} \equiv \begin{bmatrix} \delta_{ij}(e_{i\uparrow} - \mu_{i\uparrow}) - t_{i\uparrow,i\uparrow} & \delta_{ij}\Delta_i^* \\ \delta_{ij}\Delta_i & -\delta_{ij}(e_{i\downarrow} - \mu_{i\downarrow}) + t_{i\downarrow,i\downarrow} \end{bmatrix}. \tag{3.14}$$

We call this matrix Bogoliubov-de Gennes Hamiltonian. We may use a standard linear algebra result to write

$$\mathcal{H}_{BdG} = S D S^{-1} \tag{3.15}$$

where $S$ is a matrix with normalized eigenvectors of $\mathcal{H}$ as columns and $D$ is a diagonal matrix with the eigenvalues of $\mathcal{H}$ in corresponding order. The matrix $S$ is unitary as $\mathcal{H}_{BdG}$ is Hermitian. We can write the matrix part of the BCS Hamiltonian as

$$\hat{H}_{BCS} = \hat{\xi}^\dagger \mathcal{H}_{BdG} \hat{\xi} + E_0 = \hat{\xi}^\dagger S D S^{-1} \hat{\xi} + E_0 = \hat{\gamma}^\dagger D \hat{\gamma} + E_0 \tag{3.16}$$

where we denote $\hat{\xi} \equiv |\hat{\xi}_{\uparrow\uparrow}, \hat{\xi}_{\downarrow\downarrow}, \ldots, \hat{\xi}_{\uparrow\downarrow}, \hat{\xi}_{\downarrow\uparrow}|$, $\hat{\gamma} \equiv S^{-1} \hat{\xi}$, and by $E_0$ the constant terms. This is the diagonalized form of the BCS Hamiltonian. The quasiparticles introduced by the operators $\hat{\gamma} = S^{-1} \hat{\xi}$ and its hermitian conjugate are called Bogoliubov quasiparticles.

The symmetry between up and down spins has implications on the eigenvectors and eigenvalues of the Hamiltonian. In this work we assume such symmetry. However, up until this point this has not made any difference except when discarding the Fock terms. If the spins are symmetric we have $e_{i\uparrow} = e_{i\downarrow}$. Also, if there is no spin-orbit coupling, we have $t_{i\uparrow,i\downarrow} = t_{i\downarrow,i\uparrow}$. If there would be a magnetic field, the symmetry would be broken. Thus, we assume that there is no magnetic field and the average densities of the up-spin and down-spin particles are equal, that is, $n_{i\uparrow} = n_{i\downarrow}$. It follows that $\mu_{i\uparrow} = \mu_{i\downarrow}$. Compiling these properties in notation, we may denote $e_i \equiv e_{i\uparrow} = e_{i\downarrow}$, $t_{ij} \equiv t_{i\uparrow,j\uparrow} = t_{i\downarrow,j\downarrow}$ and $\mu_i \equiv \mu_{i\uparrow} = \mu_{i\downarrow}$. The spin symmetry renders the Bogoliubov-de Gennes Hamiltonian into

$$\mathcal{H}_{BdG,ij} = \begin{bmatrix} \delta_{ij}(e_i - \mu_i) - t_{ij} & \delta_{ij}\Delta_i^* \\ \delta_{ij}\Delta_i & -\delta_{ij}(e_i - \mu_i) + t_{ij} \end{bmatrix}. \tag{3.17}$$

The Hamiltonian has now the following similarity transform: the Hamiltonian is similar to itself with a minus sign. The transformation is implemented by the following operation

$$M = C \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \tag{3.18}$$

where $C$ represents the complex conjugate with properties $Ca = a^*C, C^2 = 1$. Its inverse is readily seen to be

$$M^{-1} = C \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{3.19}$$
We observe for matrix $A$ of similar kind as the blocks of the Hamiltonian are that

$$MAM^{-1} = C \begin{bmatrix} 0 & a^* \\ 1 & -a \end{bmatrix} C \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = C \begin{bmatrix} a & b^* \\ b & -a \end{bmatrix} = -A .$$

(3.20)

Let us introduce a matrix

$$M_{ij} = C \begin{bmatrix} 0 & -\delta_{ij} \\ \delta_{ij} & 0 \end{bmatrix} .$$

(3.21)

Using the matrix, we can write the BCS Hamiltonian also as

$$\hat{H}_{\text{BCS}} = -\hat{c}^\dagger M \hat{H}_{BdG} M^{-1}\hat{c} + E_0 .$$

(3.22)

From this form it is seen that if $\gamma = S^{-1}\hat{c}$ is a vector of quasiparticle operators of the system, then so is $S^{-1}M^{-1}\hat{c}$. This is because we have by using the obtained result that

$$\hat{H}_{\text{BCS}} = -\hat{c}^\dagger M \hat{H}_{BdG} M^{-1}\hat{c} + E_0 = -\hat{c}^\dagger M S D S^{-1} M^{-1}\hat{c} + E_0 .$$

(3.23)

Thus, if the matrix $S$ is substituted by the matrix $MS$ and $D$ with $-D$, we obtain another diagonalized form of the BCS Hamiltonian. Also, $S^{-1}M^{-1}\hat{c}$ would be the corresponding quasiparticle vector. Similarly we obtain that if a vector $v$ is an eigenvector of the system $\hat{H}_{BdG} v = E v$ then also $M^{-1}v$ is with the opposite eigenvalue $-E$. This is because if $\hat{H}_{BdG} v = E v$, then $M \hat{H}_{BdG} M^{-1} v = -E v$ or $\hat{H}_{BdG} M^{-1} v = -E M^{-1} v$. In conclusion, we have shown that for the spin symmetric case the eigenvalues come in pairs of positive and negative energies, related to the swap of up-spin and down-spin particles.

The diagonalization of $\hat{H}_{BdG}$ is equivalent to solving the eigenvalue problem

$$\hat{H}_{BdG} v = E v .$$

(3.24)

This is called Bogoliubov-de Gennes (BdG) equation. There are $2N$ eigenvalues and eigenvectors of the equation, where $N$ is the number of lattice sites. The factor of 2 comes from the two possible spins of a particle at a lattice site. We have shown that the eigenvalues and eigenvectors come in related pairs of positive and negative energies. Let $S$ be a matrix with the eigenvectors of $\hat{H}_{BdG}$ as columns. The eigenvectors are of length $2N$ and we assume that they are normalized. The matrix $S$ is unitary as the normalized eigenvectors of a Hermitian matrix related to different eigenvalues are orthonormal. Further, let us assume that the vectors in the matrix are ordered from left to right as pairs of eigenvectors with the same absolute eigenvalue, in the increasing order of the common absolute eigenvalue of the pair.

Let us define the matrices $u$ and $v$ as odd and even rows, respectively, of the columns of the matrix $S$ related to positive eigenvalues. Thus, each eigenvector is formed of $N$ pairs $(u_{in}, v_{in})$ corresponding to the lattice sites, $u_{in}$ being related to up-spin and $v_{in}$ to down spin particles. More specifically, $u_{in}, v_{in}$ are the $2(i-1)$th and $2i-1$th elements, respectively of the eigenvector with eigenvalue $(+1)E_n$.

Using the matrices $u$ and $v$, let us now define the notation for the quasiparticle operators. Due to the fact that eigenvectors come in related pairs, we want that similar
correspondence is visible in the quasiparticle operators. We introduce a spin label for the quasiparticle operators. The operators arise from operating with $S$ on the vector $\hat{c}$ and are

\[ \hat{\gamma}_n^\uparrow = \sum_i \left( u_{i,n}^* \hat{c}_{i}^\uparrow + v_{i,n}^* \hat{c}_{i}^\downarrow \right) \]
\[ \hat{\gamma}_n^\downarrow = \sum_i \left( v_{i,n} \hat{c}_{i}^\uparrow - u_{i,n} \hat{c}_{i}^\downarrow \right) \]

(3.25)

where the complex conjugates are due to the inverse of a unitary matrix being its Hermitian conjugate. It is worth a note that that up spin and down spin coefficients are related through the operator $M$. The size of the matrices $u$ and $v$ are $(N, N)$ where $N$ is the number of lattice sites. Thus, there are $N$ pairs of $\gamma$ annihilation (or creation) operators similarly as there are $N$ pairs of particle annihilation (creation) operators. We find that the quasiparticle operators fulfill the fermion commutation relations that require

\[ \sum_i \left( |u_{i,n}|^2 + |v_{i,n}|^2 \right) = 1 \]

(3.26)

as is the case due to unitarity.

Due to the unitarity of the matrix $S$, we can readily invert it to obtain particle creation and annihilation operators in terms of the quasiparticles. The result is given by taking transpose and complex conjugation of the matrix $S$ and expressing the results in terms of matrices $u$ and $v$. We have

\[ \hat{c}_{i}^\uparrow = \sum_n \left( u_{i,n} \hat{\gamma}_n^\uparrow + v_{i,n} \hat{\gamma}_n^\downarrow \right) \]
\[ \hat{c}_{i}^\downarrow = \sum_n \left( v_{i,n} \hat{\gamma}_n^\uparrow - u_{i,n} \hat{\gamma}_n^\downarrow \right) \]

(3.27)

### 3.2.3 Particle number and pairing potential

Central observables in the BCS theory are the pairing potential and local particle number. Let us derive formulas for their expectation values in the ground state for later use. This can be done by using the Bogoliubov transformed operators. We use the fact that the quasiparticles are independent and follow the Fermi-Dirac distribution, that is, the density matrix is diagonal in the energy space for them. For the order parameter we obtain

\[ \Delta_l = -V_l \langle \hat{c}_{i}^\downarrow \hat{c}_{i}^\uparrow \rangle \]
\[ = -V_l \sum_{nm} \left( v_{i,n}^* \hat{\gamma}_n^\downarrow \hat{\gamma}_m^\uparrow - u_{i,n} \hat{\gamma}_m^\uparrow \hat{\gamma}_n^\downarrow \right) \]
\[ = -V_l \sum_{nm} \left( v_{i,n}^* u_{i,m} \langle \hat{\gamma}_n^\downarrow \hat{\gamma}_m^\uparrow \rangle + v_{i,n}^* v_{i,m} \langle \hat{\gamma}_n^\downarrow \hat{\gamma}_m^\uparrow \rangle - u_{i,n} u_{i,m} \langle \hat{\gamma}_n^\uparrow \hat{\gamma}_m^\downarrow \rangle - u_{i,n} v_{i,m} \langle \hat{\gamma}_n^\downarrow \hat{\gamma}_m^\uparrow \rangle \right) \]

(3.28)
As Bogoliubov quasiparticles are independent, we find \( \langle \hat{\phi}^\dagger_{n\uparrow} \hat{\phi}_{n\downarrow} \rangle = \langle \hat{\gamma}_{n\uparrow} \hat{\gamma}_{n\downarrow} \rangle = 0 \). The particles follow Fermi-Dirac statistics so we have

\[
\langle \hat{\gamma}^\dagger_{n\sigma} \hat{\gamma}_{m\sigma} \rangle = \frac{\delta_{nm}}{e^{\frac{E_n}{k_B T}} + 1},
\]

and

\[
\langle \hat{\gamma}_{n\sigma} \hat{\gamma}^\dagger_{m\sigma} \rangle = 1 - \frac{\delta_{nm}}{e^{\frac{E_n}{k_B T}} + 1}.
\]

Thus, we find

\[
\Delta_i = -V_i \sum_n \left( u_{i,n}^* u_{i,n} \frac{1}{e^{\frac{E_n}{k_B T}} + 1} - u_{i,n} v_{i,n}^* \left( 1 - \frac{1}{e^{\frac{E_n}{k_B T}} + 1} \right) \right)
\]

\[
= -V_i \sum_n \frac{v_{i,n}^* u_{i,n}}{1 + e^{\frac{E_n}{k_B T}}}
\]

\[
= V_i \sum_n u_{i,n} v_{i,n}^* \tanh \left( \frac{E_n}{2k_B T} \right)
\]

The mean particle number at a site can be evaluated similarly:

\[
\langle \hat{\epsilon}^\dagger_{i\sigma} \hat{\epsilon}_{i\sigma} \rangle = \sum_{nm} \left( \langle u_{i,n}^* \hat{\phi}^\dagger_{n\uparrow} \pm v_{i,n} \hat{\gamma}_{n\downarrow} \rangle \left( u_{i,n} \hat{\gamma}_{n\uparrow} \pm v_{i,n}^* \hat{\phi}_{n\downarrow} \right) \right)
\]

where + is for up-spin and - is for down-spin particles. The result is

\[
\langle \hat{\epsilon}^\dagger_{i\sigma} \hat{\epsilon}_{i\sigma} \rangle = \sum_n \left( \frac{|u_{i,n}|^2}{e^{\frac{E_n}{k_B T}} + 1} + \frac{|v_{i,n}|^2}{e^{\frac{E_n}{k_B T}} + 1} \right)
\]

where we used the fact that

\[
1 - \frac{1}{e^a + 1} = \frac{e^a}{e^a + 1} = \frac{1}{e^{-a} + 1}.
\]

Here we see directly the correspondence of \( u \) to positive energy states and correspondence of \( v \) to negative energy states. It is also noted that as expected, the particle number is symmetric for up and down spin cases.

### 3.2.4 Current operator and expectation value

The current from the site \( j \) to the site \( i \) of a lattice system, denoted as \( I_{ij} \), is defined as the number of particles that flow from the site \( j \) to the site \( i \) in a unit time. The unit of the current is number of particles in a unit of time, for instance 1/s. We have that \( I_{ij} = -I_{ji} \). The current \( I_{ij} \) is positive if the net flow is from the site \( j \) to \( i \) and vice versa.
When the particle number is conserved, the continuity equations states that

\[
\frac{dn_i}{dt} = \sum_j I_{ij}, \quad (3.35)
\]

where the sum is over other sites in the system. In other words, if the particle number at the site \(i\) changes over time, the particles flow to the site/from the site to the other sites as current. Thus, the particle number in the whole system is a constant: no particle is created or lost spontaneously. However, it is seen from the BCS Hamiltonian that in general the particle number is not conserved: the pairing terms in the mean-field approximation either destroys or creates two particles of opposite spins. To take this fact into account, we must add another term to the continuity equation, \(K_i\) which measures the number of particles created in this way in a unit time. Accordingly, a negative value of \(K_i\) implies that the number of particles at the site \(i\) decreases in time. Thus, the overall continuity equation is

\[
\frac{dn_i}{dt} = \sum_j I_{ij} + K_i. \quad (3.36)
\]

The current operators \(\hat{I}_{ij}\) and particle creation rate operators \(\hat{K}_i\) can be defined by adopting the continuity equation for the operators

\[
\frac{d\hat{n}_i}{dt} = \sum_j \hat{I}_{ij} + \hat{K}_i. \quad (3.37)
\]

To evaluate the operators, we may utilize the Heisenberg equation of motion for the particle number operator

\[
\frac{d\hat{n}_i}{dt} = \frac{i}{\hbar} [\hat{N}_{\text{BCS}}, \hat{n}_i] + \frac{\partial \hat{n}_i}{\partial t}. \quad (3.38)
\]

The current operator is (see Appendix for details)

\[
\hat{I}_{ij} = \frac{i}{\hbar} \sum_\sigma t_{ij}(-\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma} \hat{c}_{i\sigma}) \quad (3.39)
\]

and the particle creation rate operator is

\[
\hat{K}_i = \frac{i}{\hbar} \left(\Delta_i^* \hat{c}_{i\uparrow} \hat{c}_{i\uparrow}^\dagger - \Delta_i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}\right) \quad (3.40)
\]

The expectation value of the operators are

\[
I_{ij} = \frac{i}{\hbar} \sum_\sigma t_{ij} \left(-\langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}\rangle + \langle \hat{c}_{j\sigma} \hat{c}_{i\sigma}\rangle\right) \quad (3.41)
\]

\[
K_i = \frac{i}{\hbar} \left(\Delta_i^* \langle \hat{c}_{i\uparrow} \hat{c}_{i\uparrow}\rangle - \Delta_i \langle \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}\rangle\right). \quad (3.42)
\]
For a generic complex number $c$ we have $\text{Im}(c) = -\frac{i}{2}(c - c^*)$ so we can write

$$I_{i,j} = \frac{2}{\hbar} \sum_{\sigma} t_{i,j} \text{Im} \left( \langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle \right)$$

(3.43)

$$K_i = -\frac{2}{\hbar} \text{Im} \left( \Delta_i^* \langle \hat{c}_{i\uparrow} \hat{c}_{i\uparrow}^\dagger \rangle \right).$$

(3.44)

For a system with spin exchange symmetry, the sum over the spins results in a factor of two to the results.

As discussed earlier, in general the particle number might not be conserved. However, if we solve pair potentials $\Delta_i$ self-consistently, as introduced below, we have that $\Delta_i = -V_i (\langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle^* + \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle)$ so we have

$$\text{Im} \left( \Delta_i^* \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle^* \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle \right) = \text{Im} \left( -V_i (\langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle^2 \right) = 0$$

(3.45)

where we used the fact that modulus squared and the interaction strength $V_i$ are real. Thus, for self-consistently calculated regions, we find

$$K_i = 0$$

(3.46)

which conserves charge. On the other hand, by setting a non-self-consistent order parameter $\Delta$ we may introduce current sources and sinks to system. This is the key to consider a Josephson current in a closed system.

The remaining task is to write the hopping operator expectation values using the Bogoliubov quasiparticle expectation values. Similarly as before, we calculate

$$\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle = \sum_{nm} \left( \left( u_{i,n}^* \gamma_{n\uparrow}^\dagger \pm v_{i,n} \gamma_{n\downarrow}^\dagger \right) \left( u_{j,n} \gamma_{n\downarrow} \pm v_{j,n}^* \gamma_{n\uparrow} \right) \right)$$

(3.47)

which leads to

$$\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle = \sum_n \left( \frac{u_{i,n}^* u_{j,n}}{e^{\frac{\Delta_n}{k_B T}} + 1} + \frac{v_{i,n} v_{j,n}^*}{e^{-\frac{\Delta_n}{k_B T}} + 1} \right),$$

(3.48)

which can be input to the current expectation value formula to obtain the Bogoliubov-de Gennes scheme prediction.

### 3.3 Self-consistent determination of parameters

In this thesis, we evaluate the Josephson current through the sawtooth lattice with interactions. This is done in practice by considering a finite portion of sawtooth lattice in between two superconducting leads. For the leads, it is sufficient to impose constant order parameters. As in our analysis the leads are considered to be finite, that is, the system is closed, non-self-consistent order parameters are needed to introduce a finite current. The Josephson current can be introduced by having the same absolute order parameter $\Delta_L$ for the two leads but with different phases introduced by factors $\exp(i\phi_1)$
and \( \exp(i\phi_z) \) for left and right leads, respectively. The phase difference causes the equilibrium Josephson current. However, to obtain the effects of interactions of the sawtooth lattice on the Josephson current, the Hartree term and pairing terms in the sawtooth lattice have to determined, given the interaction strength in it. The self-consistent method is a way of accomplishing this goal.

The order parameter and occupation numbers, that is, the Hartree term at each of the lattice sites are a priori unknown. Thus, a part of the solution for finite interactions is to evaluate these parameters. There are a couple of different methods for achieve this goal. As the BdG equations describe the ground state properties of the system one could consider the equivalent problem of minimization of the free energy of the system. The minimization could be done directly by various algorithms. However, usually the problem is set in seemingly different but, in principle, equivalent language: as a fixed point problem of the unknown parameters. The basic principle behind this approach is that, given some guess for the parameters, one can input them to the Hamiltonian and diagonalize it to obtain new values for the same parameters. If the unknown parameters are collected in the vector \( \mathbf{X} \), we can write for the output parameters \( \mathbf{X}' = f(\mathcal{H}_{\text{BdG}}(\mathbf{X})) \), where \( \mathcal{H}_{\text{BdG}}(\mathbf{X}) \) is the BdG Hamiltonian with parameters \( \mathbf{X} \) and \( f \) denotes the function that takes in the Hamiltonian and outputs the parameters using the equations that give the occupation number and order parameter in the system from the eigenvectors and eigenenergies, Eqs. (3.33) and (3.31). Repeating this procedure with the obtained values, one establishes an iterative algorithm to calculate these parameters.

To clarify that the self-consistent solution is in fact a fixed-point form, let us write the method in a bit different language. Let us define \( F(\mathbf{X}) \equiv f(\mathcal{H}_{\text{BdG}}(\mathbf{X})) \). Using this notation, the self-consistent method is to solve the fixed-point equation \( F(\mathbf{X}) = \mathbf{X} \). In the most basic form of the algorithm, the solution is obtained iteratively \( \mathbf{X}_{n+1} = F(\mathbf{X}_n) \). The iteration is ended when \( |\mathbf{X}_{n+1} - \mathbf{X}_n| < \delta \) for some small tolerance \( \delta > 0 \).

The conditions of convergence for the self-consistent method are generally not clear. It might suffer from slow convergence or have oscillating or diverging solutions in its basic form. In the context of density functional theory, which addresses a similar problem of evaluating unknown density parameters, it is the case that the solution might be oscillatory in such a way that the iteration has two separately converging sub-sequences that do not converge to the proper solution [54]. Many methods have been developed to circumvent these issues. We consider a couple of different methods, which are described below.

Various mixing methods are often used to ensure and to speed-up the self-consistent convergence. The mixing methods mix previous iterates with the newest iteration to obtain a balanced solution. The simplest mixing algorithm mixes the current and the previous values in the following manner:

\[
\mathbf{X}_{n+1} = (1 - \alpha)\mathbf{X}_n + \alpha F(\mathbf{X}_n),
\]

where \( 0 < \alpha \leq 1 \) is the mixing parameter giving the proportion of new and previous iterates in the new value. For the following discussions, it is useful to define a function
\( G(X) \equiv F(X) - X \) and write

\[
X_{n+1} = X_n + \alpha G(X_n) .
\] (3.50)

If the parameter vector in the mixing algorithm converges, it is readily seen that the same fixed point equation is fulfilled. It has been shown that for a proper initial guess for the vector \( X \) and a small enough mixing parameter \( \alpha \), the iteration converges to a unique value which corresponds to a minimum in the free energy [54]. However, the solution might be a local minimum instead of the global one. One approach to achieve the global minimum is to perform the self-consistent iteration with various initial guesses and choose the obtained solution with the least energy.

The problem with the simple mixing iteration is that, as the new solution is only partly given by the function \( F \), the convergence can still be slow even though it converges. Also, one has to choose the mixing parameter by hand via testing, which is time consuming for practical tasks. Here we consider two solutions to these problems by introducing the DIIS (direct inversion in the iterative subspace) method, which is also known as the Pulay mixing [55] or the Anderson method [56], and the Broyden method [57]. The methods have distinct advantages. In practice, it is an empirical task to find which method is the most suitable. In the following, we present these algorithms briefly.

The Pulay mixing method is a generalization of the simple mixing introduced above. It utilizes the \( M \) previous iterations to form optimized density vectors and residual vectors in the spanned subspace. These optimal vectors are then mixed as in the simple mixing. The method assumes that the residuals are linear in the density vectors, that is, one can consider the residual vectors in the same subspace as the density vectors. The method finds the density vectors in the space that correspond to residual vectors minimizing the Euclidean norm, as is the target in fixed-point iteration. In other words, if a new minimal residual vector is obtained in the subspace formed by the \( M + 1 \) subsequent residuals, then the corresponding optimal density vector is obtained by some weights in the space of previous \( M + 1 \) density vectors \( X \). The Pulay mixing converges faster and is more robust against divergence problems than the simple linear mixing.

The update formula for the Pulay mixing is given by

\[
X_{n+1} = X_n + \alpha G(X_n) - (\Delta X_n + \alpha \Delta G_n)(\Delta G_n^T \Delta G_n)^{-1} \Delta G_n^T G(X_n) .
\] (3.51)

where \( (\Delta X_n)_{ij} \equiv X_{n-M+j,i} - X_{n-M+j-1,i} \) where \( X_{ij} \) is the \( i \)th component of the vector \( X_j \) of \( j \)th iterate, and the residual difference matrix \( (\Delta G_n)_{ij} \equiv G(X_{n-M+j})_i - G(X_{n-M+j-1})_i \) where \( G(X_n)_i \) is the \( i \)th component of the residual vector \( G(X_n) \). For the derivation of the formula, see Appendix. It has been shown that in certain cases using the Pulay mixing only at at some iterations periodically and otherwise using the simple mixing algorithm makes convergence faster [58]. This method is called the Periodic Pulay mixing. Choosing the hyperparameters for the iterations is an empirical task.

The Broyden method is essentially a quasi-Newton method, which updates both the density vector and the Jacobian matrix. Thus, it is called a secant method. It makes the same assumption as the Pulay mixing that the residual vectors can be expanded in linear order of the density vectors. However, instead of minimizing the Euclidean norm of the
residual, the method minimizes the norm of the difference of the Jacobian iterate. The Broyden method update formulae are

\[
X_{n+1} = X_n - J_n^{-1} G(X_n)
\]

\[
J_{n+1} = J_n + \frac{\Delta G_n \Delta X_n^T - J_n \Delta X_n \Delta X_n^T}{\Delta X_n \Delta X_n^T}.
\]

The Jacobian update in this form has the disadvantage that, in order to update \(X\), the Jacobian must be inverted. To solve this problem, we can use the Sherman-Morrison formula to write

\[
J_{n+1}^{-1} = J_n^{-1} + \frac{\Delta X_n - J_n^{-1} \Delta G_n}{\Delta X_n^T J_n^{-1} \Delta G_n} \Delta X_n^T J_n^{-1},
\]

Derivations of these formulae are shown in the Appendix.

As a note, one could derive another Broyden type method for the inverse Jacobian by demanding instead that \(\|J_{n+1}^{-1} - J_n^{-1}\|_F\) is minimized with the constraint \(J_{n+1}^{-1} \Delta G_n = \Delta X_n\). This leads to the update formula (see the Appendix for details)

\[
J_{n+1}^{-1} = J_n^{-1} + \frac{\Delta X_n \Delta G_n^T - J_n^{-1} \Delta G_n \Delta G_n^T}{\Delta G_n^T \Delta G_n},
\]

which has the same form as Eq. D.19 but the roles of \(\Delta G_n\) and \(\Delta X_n\) have changed, which follows from the symmetry of the terms. The method would actually have the advantage to have less algebraic operators to evaluate. However, which method is the best in practice is determined by the use case.

### 3.4 Quantum Dot – methods in practice

As a way of introducing background physics and demonstrating the Josephson current calculation method in a simple case, we consider a quantum dot coupled to two superconducting leads. In the present context, a quantum dot is a system consisting of a single energy level. In many lattice systems, single levels are separated enough that locally in the parameter space with energies nearby the level they behave similarly as a single level system. Therefore, in understanding more complicated systems, studying single quantum levels give some insight. To keep the matter simple, we study the case in which the particles in the quantum dot are not interacting. However, in order to see the Josephson effect, we assume interaction in the leads: the lead pairing terms are finite.

The Hamiltonian of the quantum dot is

\[
\hat{H}_{\text{QD}} = \sum_{\sigma} (\epsilon_{\sigma} - \mu) \hat{c}_{\text{QD},\sigma}^\dagger \hat{c}_{\text{QD},\sigma}
\]

where \(\mu\) is the chemical potential, \(\hat{c}_{\text{QD},\sigma}, \hat{c}_{\text{QD},\sigma}^\dagger\) are the single site quantum dot destruction and creation operators, \(\epsilon_{\sigma}\) is the energy level of the dot that is sometimes called the gate voltage referring to its nature similar to the chemical potential level that is in experiments.
Figure 3.2: The tight-binding model for a quantum dot (blue) connected to two leads (red). The on-site energy of the quantum dot $e_{QD}$ and the hopping amplitude between the dot and the leads $t_C$ are shown. The leads are shown only as two sites but they are arbitrarily long. They continue in similar fashion as shown. The lead hopping amplitude parameter is denoted by $t_l$. The chemical potential $\mu$ determines the reference energy level. In order to highlight the Josephson junction structure, boxes are drawn around the leads (red) and the dot (cyan).

used to control the dot. In general, the energy level may by spin-dependent, for instance if the system is in a magnetic field that introduces Zeeman splitting. However, we assume that the system has symmetry between up and down spins and so $\epsilon_L = \epsilon_\uparrow$. The total Hamiltonian of the considered system is

$$\hat{H} = \hat{H}_{QD} + \hat{H}_{L,1} + \hat{H}_{L,2} + \hat{H}_{coupling}$$

(3.56)

where $\hat{H}_{L,1}$ and $\hat{H}_{L,2}$ are the Hamiltonians of the leads and the $\hat{H}_{coupling}$ is the coupling between the leads and the quantum dot. The model is illustrated in Fig. 3.2. In this study, the superconducting leads are discretized 1D leads that have the Hamiltonian

$$\hat{H}_L = \sum_{i\sigma} \left( (2t_l - \mu) \hat{c}^{\dagger}_{L,i,\sigma} \hat{c}_{L,i,\sigma} - t_l \hat{c}^{\dagger}_{L,i+1,\sigma} \hat{c}_{L,i,\sigma} + \text{h.c.} \right)$$

$$+ \Delta_L \hat{c}^{\dagger}_{L,i,\uparrow} \hat{c}^{\dagger}_{L,i,\downarrow} + \Delta_L \hat{c}_{L,i,\uparrow} \hat{c}_{L,i,\downarrow}$$

(3.57)

where $\mu$ is the chemical potential, $\hat{c}_{L,i,\sigma}, \hat{c}^{\dagger}_{L,i,\sigma}$ are the lead destruction and creation operators for site $i$ and spin $\sigma$ and $t_l = \frac{\hbar}{2m}$ is the lead hopping amplitude where $a$ is the spacing between the lattice sites in the leads, and $\Delta_L$ is the superconducting pairing potential in the lead. In principle, the leads are semi-infinite but for superconducting calculations, we truncate the leads to a certain length. Also, for a semi-infinite lead, the dispersion is $E(k) = \epsilon_L + 2t_l \cos(k)$, $k \in [0, \pi]$ and so the density of states in leads is $\rho_L(E) = \frac{1}{\pi t_L} \frac{1}{\sqrt{1 - \left( \frac{E - \epsilon_L}{2t_L} \right)^2}}$ [41]. In the wide lead approximation, $t \gg |\epsilon_L - E/2|$, we have $\rho_L(E) = \frac{1}{2\pi t_L}$, which is is reasonable as there are two modes in the leads and the bandwidth is $2t_L$. The dot-lead coupling Hamiltonian is

$$\hat{H}_{coupling} = -t_C \sum_{\sigma} \left( \hat{c}^{\dagger}_{QD,\sigma} \hat{c}_{L,1,\sigma} + \text{h.c.} + \hat{c}^{\dagger}_{QD,\sigma} \hat{c}_{L,2,\sigma} + \text{h.c.} \right)$$

(3.58)
where \( \hat{c}_{l_1, \sigma} \) and \( \hat{c}_{l_2, \sigma} \) are the destruction operators for the sites nearest to the dot of the leads 1 and 2, respectively, and \( t_C \) is called the lead-system contact hopping amplitude.

Let us review some properties of superconducting equilibrium Josephson current through a quantum dot. A full review on which the following is based on can be found in Ref. \[59\]. Another review that also considers the non-equilibrium case is Ref. \[60\]. First of all, Fermi’s golden rule gives the tunneling rate from the quantum dot to a lead as \( \Gamma = 2\pi \rho_l t_C^2 \) where \( \rho_l \) is the density of states in the leads. Now, let us consider two cases: the energy level of the dot is much larger than the tunneling rate \( |e|/\Gamma \gg 1 \) and vice versa \( |e|/\Gamma \ll 1 \). In the first case, the dependence of the Josephson current from the left lead \( L_1 \) to the dot (or from dot to the right lead \( L_2 \)) on the superconducting phase difference of the leads \( \phi_l = \phi_{l_1} - \phi_{l_2} \) is

\[
I_{L_1} = \Delta_l \sin(\phi_l) \left( \frac{\Gamma}{e} \right)^2, \quad \frac{|e|}{\Gamma} \gg 1. \tag{3.59}
\]

Thus, the current phase relation (CPR) is sinusoidal, as it is for the weak link in a traditional Josephson junction. The \( \Gamma^2 \) dependence also makes sense, since the current is proportional to the rate that particle goes through the system, first from a lead to the quantum dot then back to the lead. On the other hand, for the case \( |e|/\Gamma \ll 1 \) we have two asymptotic cases depending on the relative sizes of the superconducting order parameter \( \Delta_l \):

\[
I_{L_1} = \frac{\sin(\phi)}{2\sqrt{\left( \frac{\phi}{\pi} \right)^2 + \cos^2(\phi/2)}} \times \begin{cases} \Delta & \text{for } \frac{\phi}{\pi} \ll 1, \frac{|e|}{\Gamma} \ll 1 \\ \Gamma & \text{for } \frac{\phi}{\pi} \gg 1, \frac{|e|}{\Gamma} \ll 1. \end{cases} \tag{3.60}
\]

In the case \( e = 0 \) we find that the current phase relation is

\[
I_C \propto 1 - \frac{\sin(\phi)}{2 |\cos(\phi/2)|} = \frac{\sin(\phi/2) \cos(\phi/2)}{|\cos(\phi/2)|} = \begin{cases} \sin(\phi/2) & \text{for } 0 \leq \phi \leq \pi \\ -\sin(\phi/2) & \text{for } \pi < \phi \leq 2\pi. \end{cases} \tag{3.61}
\]

Thus, the CPR looks like having half of the phase difference and the relation changes sign abruptly at \( \phi = \pi \). When the energy of the quantum dot \( e \) is small, then the contact between the leads is as strong as possible. Also, instead of \( \Gamma^2 \) the dependence is on \( \Gamma \) until saturation with constant \( \Delta \). The \( \sin(\phi/2) \) dependence of the critical current is indication of strong coupling between the leads.

To see whether we can observe the presented behavior with our considered methods we performed the Josephson current calculations on the quantum dot. This example also illustrates the calculations in practice. To be specific, we considered a system on which the lead hopping parameter is \( t_l = 30 \text{ kHz} \) and the energy level of the quantum dot is \( e = 400 \text{ Hz} \) in reference to our energy zero. The temperature is set to \( T = 0 \text{ K} \). We perform a parameter sweep on both contact hopping amplitude \( t_C \) and the superconducting order parameter \( \Delta_l \) in the leads.

Firstly, we fix the wanted contact hopping amplitude \( t_C \) and the superconducting lead order parameter \( \Delta_l \) and perform a chemical potential sweep around the energy level
of the quantum dot. For each value of the chemical potential, we evaluate the CPR by using the Bogoliubov-de Gennes method described in the Section 3.2 for the system with leads truncated to \( L = 20 \) sites. This is done in practice by varying the superconducting phase difference between the leads from \( \phi = 0 \) to \( \phi = 2\pi \) and evaluating the current at each point. The superconducting phase difference is imposed by setting the order parameter of the left lead to be \( \Delta_L \exp(i\phi) \) and the order parameter of the right lead to \( \Delta_R \).

It is worth a note that the effect of changing the chemical potential is the same as moving the energy level of the quantum dot \( \epsilon \). This is the case because the chemical potential defines the basic energy reference point for a fermionic grand canonical system. It follows that, if the energies of the most energetic particles, that is, the chemical potential is the same as the energy level of a system, it is equivalent to say that the energy of the level is zero. We have chosen to vary the chemical potential instead of the energy levels because the chemical potential is a more robust property of the system, indicating the energy of the most energetic electrons. Also, due to the contact between the system and the leads, the effective energy level is changed from the value \( \epsilon \) in general, so the direct physical meaning of \( \epsilon \) in the system is vague.

A couple of examples of CPRs for parameters \( \Delta_L = 2 \) kHz and \( t_C = 1.5 \) kHz for different chemical potentials \( \mu \) of the system are shown in Fig. 3.3. As indicated above, the effective energy level of the quantum dot is different from \( \epsilon \). The level in this case is found to be \( \epsilon_{\text{eff}} = 277.2 \) Hz. When the chemical potential \( \mu \) is tuned to this level, the quantum dot behavior of \( \epsilon = 0 \) is observed, that is, the phase dependence is \( I \propto \sin(\phi/2) \) with a sign change at \( \phi = \pi \). When the chemical potential is smaller, we see that gradually the CPR shifts to the large \( \epsilon \) case of \( I \propto \sin(\phi) \), as given by the theory.

Secondly, we determine the critical Josephson current for each chemical potential. The critical Josephson current is defined as the maximum observed current when the phase difference is varied. Thus, it can be extracted from the CPR. The extracted critical currents for the chemical potential sweep for \( \Delta_L = 411 \) Hz and a couple of \( t_C \) are shown in the Fig. 3.4. It is seen that corresponding to the energy level of the quantum dot there is a peak in the critical Josephson current amplitude. This phenomenon, which is called resonant tunneling, is related to the fact that there is a quasi-bounded state in the dot available that amplifies the current when the chemical potential is tuned to resonance with it.

We are interested in the critical Josephson currents at the peaks as these values give information related to the states or energy levels that cause the peaks. Thus, thirdly in the analysis, we determine the maximal critical currents of the peaks as a function of the chemical potential, which is known as the peak critical current. In the case of the quantum dot, we are interested in how the peak critical Josephson current is dependent on the contact hopping amplitude \( t_C \) and the lead pairing potential \( \Delta_L \). We performed these analyses and the results are collected in Figs. 3.5, 3.6. The results are according to the theory: the observed \( t_C \) dependence is quadratic and the \( \Delta_L \) dependence for small values is linear. We do not observe the saturation of \( t_C \) dependence as we do not consider high enough \( t_C \). We did not study the large \( \epsilon \) behavior.
Figure 3.3: The current phase relation of quantum dot with $\epsilon = 0.4$ kHz couple to two leads with contact hopping amplitude $t_C = 1.5$ kHz and $\Delta_L = 2$ kHz for various chemical potentials $\mu$. The contact to the lead alters the effective energy level of the quantum dot, which is for this case found to be 277.2 Hz. For the related chemical potential, the system behaves as predicted for $\epsilon = 0$. For lower chemical potential or, equivalently, larger gate voltage $\epsilon$, the behavior approaches the usual $\sin(\phi)$ form.

Figure 3.4: Critical current and the normal state transmission probability through the quantum dot versus chemical potential of the system. The lead pairing potential amplitude is set to 411 Hz. It is seen that there is a resonance peak in the energy spectrum corresponding to the energy level both in the transmission probability and critical Josephson current. Also the effect of varying contact hopping amplitude $t_C$ is illustrated.
Figure 3.5: The dependence of the peak critical Josephson current on the contact hopping amplitude $t_C$ of the quantum dot for different pairing potentials of the leads $\Delta_L$. The theory form $I_c \propto \Gamma \propto t_C^2$ is fitted to the data points and shows agreement. The dependence is observed to be parabolic. Also, in the limit $t_C \to 0$, the tangent is flat, in line with the theoretical prediction. The current increases with respect to $\Delta_L$ up to a limit.

Figure 3.6: The dependence of the maximal peak critical Josephson current on the lead pairing potential $\Delta_L$ for different contact hopping amplitudes $t_C$ of the quantum dot. The theory form $I_c \propto \Delta_L$ is seen when $\Delta_L$ is small. For high $\Delta_L$, the current saturates and the dependence vanishes.
Chapter 4

Results

In this chapter, we present the numerical simulations performed and their results. Firstly, we show that the tight-binding model and the full optical potential model give qualitatively the same results regarding to the transmission probability, that is, in non-interacting conductance. Secondly, for reference, we consider the behavior of the system without interactions on the sawtooth lattice. We introduce interactions in leads but the sawtooth lattice is kept non-interacting. Thirdly, we introduce the interactions on the sawtooth lattice and consider its effect. Fourthly, a boundary potential is introduced to study its effects on the flat band current. Finally, the finite temperature results are given. In this chapter Planck’s constant is set to $\hbar = 1$. Thus, all the energies are expressed in units of frequency, hertz (Hz). The unit of current is not affected by this choice. The unit is $1/s$. These are typical units in the ultracold gas experiments due to their very low energies.

4.1 Comparison of transmission obtained by tight binding and by a realistic potential

In order to verify that the tight-binding model presented in the Methods section is sufficiently realistic for further studies of the sawtooth lattice, we performed the non-interacting transmission calculations on it as were done in Antti Ranni’s master thesis Ref. [53] for the realistic potential. The temperature of the system is kept at $T = 0$ K. The transmission calculations on the sawtooth lattice tight-binding model have been carried out by the software package Kwant [19].

The tight-binding Hamiltonian of the sawtooth lattice with N unit cells is as showed in the methods section

$$\hat{H} = \hat{H}_{\text{sawtooth}} + \hat{H}_{l_1} + \hat{H}_{l_2} + \hat{H}_{\text{contact}}$$

(4.1)

where $\hat{H}_{\text{sawtooth}}$ is the Hamiltonian for the sawtooth, $\hat{H}_{l_1}, \hat{H}_{l_2}$ are the lead Hamiltonians similar to the ones consider in the quantum dot case (Section 3.4), and $\hat{H}_{\text{contact}}$ is the contact Hamiltonian between the leads and the sawtooth lattice. A graph of the model
Figure 4.1: Graph of tight-binding model considered in the calculations. Example with 4 side wells is shown, but the model can be of arbitrary length. One-dimensional discretized leads with hopping parameter of 30 kHz are connected to both sides of the system. The system hopping amplitudes and on-site energies are labeled for an example of sites; the parameters are the same for all A and B type sites and hopping amplitudes between them. The hopping amplitude between the sawtooth lattice and the leads is denoted $t_C$. The red lattice sites denote that similar one-dimensional lattice lead goes on infinitely long.

used is shown in Fig. 4.1. For the sawtooth lattice, the Hamiltonian is

$$\hat{H}_{\text{sawtooth}} = \sum_{i, \sigma} \left( \epsilon_A \hat{c}_{A,i\sigma}^\dagger \hat{c}_{A,i\sigma} + \epsilon_B \hat{c}_{B,i\sigma}^\dagger \hat{c}_{B,i\sigma} \\
+ t_{AB} (\hat{c}_{B,i\sigma}^\dagger \hat{c}_{A,i\sigma}) + \text{h.c.} \\
+ t_{AB} (\hat{c}_{A,i+1\sigma}^\dagger \hat{c}_{B,i\sigma}) + \text{h.c.} \\
+ t_A (\hat{c}_{A,i+1\sigma}^\dagger \hat{c}_{A,i\sigma}) + \text{h.c.} \right) \\
+ \sum_{\sigma} \epsilon_A \hat{c}_{A,N+1\sigma}^\dagger \hat{c}_{A,N+1\sigma}$$

(4.2)

where the final term takes into account the fact that when the sawtooth lattice is truncated, a single site of type A is left in the end that does not have a corresponding B site. The lead Hamiltonians are same as in the quantum dot case, but in this case without pairing terms

$$\hat{H}_{L_1} = \sum_{i, \sigma} (2t_L - \mu) \hat{c}_{L_1,i\sigma}^\dagger \hat{c}_{L_1,i\sigma} - t_L (\hat{c}_{L_1,i+1\sigma}^\dagger \hat{c}_{L_1,i\sigma} + \text{h.c.})$$

(4.3)

$$\hat{H}_{L_2} = \sum_{i, \sigma} (2t_L - \mu) \hat{c}_{L_2,i\sigma}^\dagger \hat{c}_{L_2,i\sigma} - t_L (\hat{c}_{L_2,i+1\sigma}^\dagger \hat{c}_{L_2,i\sigma} + \text{h.c.})$$

(4.4)

where the lead site indexing increases away from the sawtooth lattice. Finally, the contact Hamiltonian is

$$\hat{H}_{\text{contact}} = -t_C \left( \hat{c}_{L_1,1\sigma}^\dagger \hat{c}_{A,1\sigma} + \text{h.c.} + \hat{c}_{L_2,1\sigma}^\dagger \hat{c}_{A,N+1\sigma} + \text{h.c.} \right)$$

(4.5)

where the indexing of the sites of the sawtooth lattice is as in Fig. 4.1.
The tight binding parameters were extracted from the potential model and are given in the Table 4.1. The lead hopping amplitude is set to $t_L = 30$ kHz and the contact hopping amplitude is $t_C = 0.05$ kHz. The ratio $t_{AB}/t_A$ is rather close to the wanted ratio $\sqrt{2}$ the relative error being 0.3%. In the calculation of a realistic potential a step potential of 40 kHz is added. Thus, we add 40 kHz to the $e_A$, $e_B$. Also, we assume that $t_B = 0$. In order to make the flat band visible as is the case in the potential calculations by Antti Ranni, we break the flat band condition a bit by using $t_{AB} = 1.35 t_A$.

As discussed in the Chapter 3, a way to study the sawtooth lattice is to discretize the continuum Hamiltonian using finite-difference approximation. The Hamiltonian can then be written as

$$\hat{H}_{\text{sawtooth}} = \sum_{\sigma} \left( -\frac{\hbar^2}{2m_{L,i}a^2} + V_{x,i\sigma} \right) \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + \frac{\hbar^2}{2m_{L,i}a^2} \sum_{\langle i,j \rangle} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \quad (4.6)$$

where $V(x, y)$ is a potential, $m_{L,i}$ is the atomic mass of lithium-6 isotope, $a$ is the discretization length in the square lattice, and $\langle i, j \rangle$ denotes nearest neighboring sites. The realistic potential tries to capture the experimental setup. In the following $y$ direction is along the sawtooth lattice and $x$ is perpendicular in the plane of the lattice. The realistic potential is constructed by three different components as described in the Chapter 3

$$V(x, y) = V_{DMD}(x, y) + V_t(x) + V_{\text{step}}(y), \quad (4.7)$$

where $V_{\text{DMD}}(x, y)$ simulates the digital mirror device (DMD) potential in the ultracold gas experiment optical potential, $V_t$ is a trapping potential, and $V_{\text{step}}$ is step potential. The potential is imprinted on a square lattice that discretizes a plane. The sites on which potential is over 75 kHz are discarded in the analysis. The exact form of the potential terms are given in Eqs. (3.3), (3.4), and (3.5). The simulation used parameters (see the exact for the potential terms for details) presented in the Table 4.2.

The results for the calculations for 2, 3, and 4 side wells, that is, sawtooth spikes are shown in the figures 4.2, 4.3, and 4.4 for both tight binding and the realistic potential.

Table 4.1: Tight binding parameters corresponding to a realistic sawtooth lattice potential.

<table>
<thead>
<tr>
<th>$t_A/h$ (kHz)</th>
<th>$t_B/h$ (kHz)</th>
<th>$t_{AB}$ (kHz)</th>
<th>$e_A/h$ (kHz)</th>
<th>$e_B/h$ (kHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.271</td>
<td>0.032</td>
<td>0.382</td>
<td>-22.186</td>
<td>-22.180</td>
</tr>
</tbody>
</table>

Table 4.2: The parameters of the sawtooth lattice potential used in simulations. The parameters are defined in Eqs. (3.3), (3.4), and (3.5).

<table>
<thead>
<tr>
<th>$d_x$</th>
<th>$d_y$</th>
<th>$l_x$</th>
<th>$l_{\text{step}}$</th>
<th>$\sigma_x$</th>
<th>$\sigma_y$</th>
<th>$V_0$</th>
<th>$V_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.547 $\mu$m</td>
<td>1.5 $\mu$m</td>
<td>0.75 $\mu$m</td>
<td>0.10 $\mu$m</td>
<td>0.63 $\mu$m</td>
<td>0.40 $\mu$m</td>
<td>-40 kHz</td>
<td>-32.28 kHz</td>
</tr>
</tbody>
</table>
calculations. It is noteworthy that the energy scale of the peaks is different for the different calculations and the calculated peaks are so narrow that the finite discretization of energy causes huge error in the exact height of the transmission peaks. Thus, we can only read and compare the relative positions of the peaks in the figures. We also calculated the eigenvalues of the finite portion of the sawtooth lattice without the leads, that is, only the Hamiltonian $\hat{H}_{\text{sawtooth}}$. The results are collected in the table 4.3.

Table 4.3: Eigenvalues of the closed sawtooth lattice tight binding systems. Energies are in units of kHz.

<table>
<thead>
<tr>
<th>Side wells</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
<th>$E_7$</th>
<th>$E_8$</th>
<th>$E_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>17.15</td>
<td>17.63</td>
<td>18.33</td>
<td>18.36</td>
<td>18.52</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>17.07</td>
<td>17.40</td>
<td>17.79</td>
<td>18.35</td>
<td>18.35</td>
<td>18.51</td>
<td>18.53</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>17.03</td>
<td>17.27</td>
<td>17.56</td>
<td>17.87</td>
<td>18.35</td>
<td>18.35</td>
<td>18.51</td>
<td>18.52</td>
<td>18.53</td>
</tr>
</tbody>
</table>

It is seen that with both approaches we obtain corresponding peaks. The types of the peaks were verified by determining how the wave functions appear on the lattice. Examples of the different kinds of eigenstates truncated sawtooth lattice with 3 side wells are given in Fig. 4.5. There are as many peaks related to the sawtooth lattice dispersive band as there are side wells. These are the states with the smallest energy. There are also two so-called boundary states corresponding to the edges of the sawtooth lattice of energy $18.3 - 18.4$ kHz. The number of flat-band states is one less than the number of side wells as there are as many different V shaped localized states. They all have energy $\epsilon_A - 2t_A$ which is approximately 18.5 kHz. The total number of states is the same as the number of sites in the sawtooth lattice tight-binding model.

These different types of states can be recognized from both tight binding calculations and the potential calculations. Their positions are not exactly the same which is expected as the tight binding makes approximations. Also boundary states and flat band states are in different order in energy for the two calculations. The reason for this behavior is unknown at the moment. However, general agreement on the important details, that is the relative energies of the conductive band states and the flat band is observed.
Figure 4.2: Transmission vs. energy for two side wells in tight binding sawtooth model (upper) and calculation with realistic potential (lower). The eigenvalues are shown in the lower figure as red lines. The realistic potential calculation is taken from Antti Rannii’s Master Thesis [53].
Figure 4.3: Transmission vs. energy for three side wells in tight binding sawtooth model (upper) and calculation with realistic potential (lower). The eigenvalues are shown in the lower figure as red lines. The realistic potential calculation is taken from Antti Ranni’s Master Thesis [53].
Figure 4.4: Transmission vs. energy for three side wells in tight binding sawtooth model (upper) and calculation with realistic potential (lower). The eigenvalues are shown in the lower figure as red lines. The realistic potential calculation is taken from Antti Ranni’s Master Thesis [53].
Figure 4.5: Examples of wavefunction of different kinds of states of the sawtooth lattice. The size of the circle around a lattice site is proportional to the absolute square of the wavefunction. The dispersive state (left) has finite contributions at all sites. The boundary state (center) is a superposition of two boundary states: it has significant contributions at the boundary sites and exponentially decaying contributions in the middle. The flat band state (right) seen is a superposition of two V shaped localized states. As there are no contribution at the boundaries for the flat band case, the particles in the corresponding non-interacting open system with leads would be localized to the sawtooth lattice and there would be no transport.
4.2 Josephson current in non-interacting sawtooth lattice

In order to establish physical understanding, we performed the Josephson current calculation for the non-interacting sawtooth lattice. Thus, in contrast to the transmission calculations of the previous section, we introduce interactions to the leads in terms of pairing potentials. The Hamiltonian of the sawtooth is the same as in the study of normal state transport Eq. (4.1) except we have superconductivity in the leads as in the Quantum Dot case (Section 3.4)

\[
\hat{H}_L = \sum_{i,\sigma} \left( (2t_L - \mu) \hat{c}^\dagger_{L,i,\sigma} \hat{c}_{L,i,\sigma} - t_L \{ \hat{c}^\dagger_{L,i+1,\sigma} \hat{c}_{L,i,\sigma} + \text{h.c.} \} \\
+ \Delta_L \hat{c}^\dagger_{L,i,\uparrow} \hat{c}^\dagger_{L,i,\downarrow} + \Delta_L^* \hat{c}_{L,i,\uparrow} \hat{c}_{L,i,\downarrow} \right),
\]

(4.8)

where \( L \) is either \( L_1 \) or \( L_2 \), \( t_L \) is the hopping amplitude in the leads, \( \mu \) is the chemical potential, and \( \Delta_L \) is the pairing potential of the lead. The calculations are performed similarly as with the Quantum Dot: we vary the chemical potential \( \mu \) of the system through the relevant energies of the sawtooth lattice determined in the previous section and evaluate the CPR for each point. The phase difference \( \Delta \phi = \phi_{L_1} - \phi_{L_2} \) is introduced to the leads \( L_1 \) and \( L_2 \) by multiplying the order parameter of lead \( L_1 \) by \( \exp(i\Delta \phi) \) and keeping the phase of the right lead fixed. The critical Josephson current is defined as the maximum current with respect to the superconducting phase difference \( \phi \).

The chemical potential sweep can be performed for various combinations of system parameters. We consider the effect of the lead pairing potential \( \Delta_L \) amplitude, the lead sawtooth lattice contact hopping amplitude \( t_C \) and the length of the sawtooth lattice on the peak critical Josephson current of the dispersive state and the boundary state. The temperature is kept at \( T = 0 \) K. The leads are truncated to 20 sites. The hopping amplitudes and on-site energies are as given in Table 4.1, except we add a step potential of 40 kHz to the on-site energies of the sawtooth lattice. We consider the sawtooth lattice with three unit cells in other than the length dependence analysis. Examples of critical Josephson current against the chemical potential and the comparison to normal state transmission calculations is shown in Fig. 4.6. It is seen that critical Josephson current peaks correspond to the transmission peaks. Thus, the states of the sawtooth lattice also carry the current in this case. Boundary states are also visible in the Josephson current spectrum. Importantly, the flat band is not visible. Thus, without interactions in the sawtooth lattice, the flat band states are localized within the numerical accuracy.

The dependence of peak critical Josephson current in the dispersive state and the boundary state on the lead pairing potential \( \Delta_L \) and the contact hopping amplitude \( t_C \) are shown in Figs. 4.7,4.8, 4.9,4.10. The dependencies for the dispersive state look very similar to the corresponding dependencies on the quantum dot with single quantum level. Thus, in the non-interacting case, the dispersive peaks can be considered as independent levels within the considered parameter regions. For the boundary state, the results are not as clear and no such conclusions can be drawn. The current through the boundary state is due to overlap of wavefunctions that decay exponentially from the
edge. Thus, for small contact hopping amplitude values the large Quantum Dot energy level behavior is relevant. Indeed, for small $\Delta_I$ we observe linear behavior. However, for larger amplitudes the behavior is more complicated. The behavior is somewhere in between the different asymptotic regions of the considered Quantum Dot case.

We performed also the test on the length-dependence of the critical Josephson current at the peaks. For the dispersive band peaks, the peak with largest magnitude is picked. The results are shown in the Figs. 4.11, 4.12. For the dispersive state current, the dependence of critical current is found out to be $I_C \propto L^{-0.74}$ where $L$ is the number of unit cells. However, no theoretical explanation is yet found for this dependence. On the other hand, the boundary state critical Josephson current decays exponentially, which is the same behavior as observed in Ref. [53].
Figure 4.6: Critical Josephson current and transmission probability through the non-interacting sawtooth lattice with 3 side wells against chemical potential / energy for a set of contact hopping potentials $t_C$ and lead pair potentials $\Delta_L$. In the upper figure $t_C$ is varied and $\Delta_L$ is kept at constant 0.82 kHz. Similarly, in the lower figure $\Delta_L$ is varied and $t_C$ is kept at constant 1388 kHz. It is seen that to each critical Josephson current peak corresponds to a transmission peak. Also, increasing both considered parameters increases the maximal currents in dispersive band but reduces the boundary state contribution. The flat band is not visible.
Figure 4.7: The dependence of the maximal peak dispersive state critical Josephson current on the contact hopping amplitude $t_{C}$ for different lead pair potentials $\Delta_{L}$ on the non-interacting sawtooth lattice with 3 unit cells. Also the quadratic fit is shown and the corresponding behavior is observed. Thus, the dispersive state peak considered behaves in this regard as an independent quantum level.

Figure 4.8: The dependence of the maximal peak dispersive state critical Josephson current on the lead pair potential $\Delta_{L}$ for different contact hopping amplitudes $t_{C}$s on the sawtooth lattice with 3 unit cells. For small $\Delta_{L}$, linear behavior is observed. For larger values, the dependence saturates. This is in line with the single Quantum Dot case.
Figure 4.9: The dependence of the peak boundary state critical Josephson current on the contact hopping amplitude $t_C$ for different $\Delta_L$ s on the non-interacting sawtooth lattice with 3 unit cells. The exact dependencies are hard to tell from the data.

Figure 4.10: The dependence of the peak boundary state critical Josephson current on the lead pair potential $\Delta_L$ for different $t_C$ s on the non-interacting sawtooth lattice with 3 unit cells. The dependence seems to linear at first and then saturate. This could be explained with the behavior of the Quantum Dot when the energy of the level is large compared to the hopping.
Figure 4.11: The length dependence of dispersive state critical Josephson current for $\Delta_l = 2$ kHz and $t_C = 2$ kHz. The points are observed to follow a curve of form $I_C \propto L^{-0.74}$, where $L$ is the number of unit cells.

Figure 4.12: The length dependence of boundary state critical Josephson current for $\Delta_l = 2$ kHz and $t_C = 2$ kHz. The points are observed to follow an exponential decay that is in line with behavior found in Ref. [53].
4.3 Josephson current in interacting sawtooth lattice

In this section, we present the present the results on the effects of the interactions on sawtooth lattice Josephson current carrying properties. Importantly, we characterize the dependence of flat band current on the interactions. The central result is the observed flat band current in contrast to the sawtooth lattice without interactions. Firstly, we determine the interaction strength dependence of the flat band current. Secondly, we illustrate the dependence of the flat band current on the lead sawtooth contact hopping amplitude $t_c$, the lead absolute pair potential $\Delta_i$, and the length of the sawtooth lattice. Finally, we present the interaction strength dependence of the dispersive and boundary state currents and the dispersive state length dependence. The effect of the interactions on the length dependence of dispersive state is considered in order to see whether the peculiar negative power law found in the non-interacting case persists.

The interactions are included to the sawtooth lattice on mean-field level self-consistently. The Hamiltonian of the sawtooth lattice is

\[
\hat{H}_{\text{sawtooth}} = \sum_{i, \sigma} \left[ (\epsilon_A - \mu_{A,i}) \hat{c}_{A, i \sigma}^\dagger \hat{c}_{A, i \sigma} + (\epsilon_B - \mu_{B,i}) \hat{c}_{B, i \sigma}^\dagger \hat{c}_{B, i \sigma} + \Delta_{A,i} \hat{c}_{A, i \uparrow}^\dagger \hat{c}_{A, i \downarrow} + \Delta_{B,i} \hat{c}_{B, i \uparrow}^\dagger \hat{c}_{B, i \downarrow} + h.c. \right]
\]

\[
+ t_{AB} (\hat{c}_{B, i \uparrow}^\dagger \hat{c}_{A, i \downarrow}) + h.c.
\]

\[
+ t_{AB} (\hat{c}_{A, i + 1 \uparrow}^\dagger \hat{c}_{B, i \downarrow}) + h.c.
\]

\[
+ t_A (\hat{c}_{A, i + 1 \sigma}^\dagger \hat{c}_{A, i \sigma}) + h.c.
\]

\[
+ \sum_{i} \epsilon_A \hat{c}_{\sigma, A, i}^\dagger \hat{c}_{A, i+1 \sigma}^\dagger \hat{c}_{A, N+i \sigma}.
\]

(4.9)

It is the same as for the non-interacting case but, in addition, we have pair potentials $\Delta_{A,i}, \Delta_{B,i}$ and the chemical potential $\mu$ is modified by the Hartree terms to $\mu_{A,i}, \mu_{B,i}$. The contact Hamiltonian and the lead Hamiltonian are the same as in the last section. As presented in the Methods chapter, we calculate the pair potentials and Hartree terms self-consistently. Otherwise, the analysis is the same. The interaction strength in the sawtooth lattice $V_S$ appears implicitly in the Hamiltonian as it is part of the equations for self-consistent parameters.

Using the basic fixed point iteration form of the self-consistent iteration directly is found to be rather slow or leads to oscillating solutions. Especially, at flat band energies there are difficulties in this respect. Thus we applied both Broyden method and periodic Pulay mixing to assure the convergence and make it faster. Broyden method seems to be faster in time but is found not to always converge. Thus, we run Broyden method for a preset number of iterations and move to the periodic Pulay mixing method which always is found to converge. By testing, it was found that that the best length of the memory of the Pulay mixing is 3 previous steps and the best period of applying the Pulay mixing was 2, that is, it is applied on every other iterations. It is demanded that the mean square sum error of the unknown parameters is at maximum 50 ppm. This
leads to the accuracy of current between 1-10% in the tested cases, depending on the parameter region. The number of required iterations increases for larger interactions. For a flat band, the convergence requires in the order of 5000-7000 iterations for the worst cases considered. The number increases rapidly with increasing interaction strength, perhaps indicating that the mean field approximation breaks.

To illustrate the effect of interactions, Fig. 4.13 shows the critical current versus chemical potential of the system for a couple of interaction strengths. The most notable difference to the non-interacting case is that there is a new peak related to the flat band in the current spectrum that does not appear in the transmission spectrum. Also, the interaction moves the positions of the peaks due to the Hartree term being an effective chemical potential. The dispersive peaks and the flat band peaks also grow with interaction. The dependence of the flat band current on the interaction strength is shown in Fig. 4.14 and is found to be linear with interactions larger than 100 Hz and non-linear at the lowest interactions. The linear dependence is according to the expectation. The interaction dependence for small interaction strength is not understood. The deviation might be due numerical error. At the large interaction strength, there is small deviation from the linear line but it is within the accuracy of the analysis. On the other hand, for large interaction strengths we expect deviations as the flat band begins to mix with other bands and the validity of the mean field approximation is worse.

The $t_C$ and $\Delta t$ dependencies of the flat band peaks for a single value of the interaction strength are shown in Figs. 4.15 and 4.16. The observed behavior is in line with the single
Quantum Dot case. For the largest considered values of the contact hopping amplitude, we observe that the quadratic behavior is lost. However, also for the single Quantum Dot, if $\Gamma/\Delta \gg 1$, the dependence on $t_C$ vanishes. The considered interaction strength is below the energy separation of the flat band and other bands, so significant mixing of the bands is not yet observed. Thus, in this sense the interactions seem to turn the flat band into a single level system.

The interaction strength dependence of the Josephson current through the dispersive band and the boundary state are shown in Figs. 4.17 and 4.18, respectively. For the dispersive band, the dependence is linear above $V_S = 100 \text{ Hz}$ within the accuracy of the analysis. Thus, its behavior is similar as for the flat band in this sense. However, the slope is significantly smaller. The boundary state current interaction strength dependence for this choice of parameters is found to be non-linear and have a minimum at around $V_S = 200 \text{ Hz}$. This behavior is not presently understood.

The sawtooth lattice length dependence of the critical current in the flat band and the dispersive band, respectively, for the interacting case are shown in the Figs. 4.19 and 4.20. The flat band critical Josephson current dependence shows that actually the current is not dependent on the length when $L > 3$. The dispersive state critical Josephson current dependence on length is similar to the non-interacting case. We find that the power law for the length dependence of the dispersive band current remains. However, the exponent $a$ on the $L^{-a}$ dependence decreases for increasing interaction. The boundary state dependence could not be obtained with the present numerical accuracy due to errors in small amplitude currents; the Josephson current amplitude in the boundary state vanishes rapidly as the length is increased.
Figure 4.15: The dependence of the peak flat band state critical Josephson current on the contact hopping amplitude $t_C$ for $V_S = 300$ Hz for the sawtooth lattice with 3 unit cells. The behavior is in line with the single Quantum Dot case. For the largest considered values, we observe that the quadratic behavior is lost. However, also for the single Quantum Dot, if $\Gamma/\Delta \gg 1$, the dependence on $t_C$ vanishes.

Figure 4.16: The dependence of the peak flat band state critical Josephson current on the lead pair potential $\Delta_L$ for $V_S = 300$ Hz and $t_C = 1500$ Hz on the sawtooth lattice with 3 unit cells. The behavior is in accordance with the single Quantum Dot case.
Figure 4.17: Interaction strength dependence of the dispersive state current for $t_C = 1000$ and $\Delta_l = 2000$. The dependence is linear above $V_3 = 100$ Hz.

Figure 4.18: Interaction strength dependence of the boundary state current for $t_C = 1000$ and $\Delta_l = 2000$. 
Figure 4.19: The length dependence of the flat band state critical Josephson current for \( \Delta_L = 2 \text{ kHz} \) and \( t_C = 2 \text{ kHz} \). The flat band current is observed to be independent of length after the length of 4 unit cells.

Figure 4.20: The length dependence of dispersive state critical Josephson current for various interaction strengths for \( t_C = 2 \text{ kHz} \) and \( \Delta_L = 2 \text{ kHz} \). The points are observed to follow a curve of form \( I_C \propto L^{-\alpha} \), where \( L \) is the number of unit cells. The \( \alpha \) for these cases are found to be (0.745, 0.715, 0.687, 0.658) in the order of increasing interaction.
4.4 Boundary potential

In the previous section, it is seen that introducing interactions to the system gives rise to critical Josephson current peak corresponding to the flat band state. However, the current is rather small in comparison to the dispersive band peak current even for the largest considered interaction, which is in the order of the band gap between the flat band and the dispersive band. In the theoretical discussions we expected that the flat band current would be significant because actually the superfluid weight is the largest for the larger energy part of the considered interaction spectrum [14]. Based on the observation that the boundary state is like a flat band localized state shown in Figs. 2.5 and 4.5 but has one site taken away as the lattice is truncated, we made a hypothesis that the small observed flat band current is due to the energy mismatch between the boundary state and the flat band state. Thus, our hypothesis implies that by bringing the flat band state and boundary state to same energy would increase the current substantially.

To test the hypothesis, we modify the Hamiltonian to add a new term to the Hamiltonian. For the boundary sites of the sawtooth lattice, we add a constant boundary potential term $V_B$:

$$\hat{V}_B = \sum_\sigma V_B (\hat{c}_{A_{1 \sigma}}^\dagger \hat{c}_{A_{1 \sigma}} + \hat{c}_{A_{N+1 \sigma}}^\dagger \hat{c}_{A_{N+1 \sigma}})$$

(4.10)

where site $A_{1}$ is the leftmost and the site $A_{N+1}$ is the rightmost site of the truncated sawtooth lattice. The effect of this boundary state energy on the critical Josephson current peak positions and heights is illustrated in the figure 4.21. It is seen that the hypothesis is right, the flat band critical Josephson current peak is increased substantially. Dispersive state critical current value is smaller. Interestingly, the boundary state current goes to very small value near the flat band energy but there is a small but finite current when the boundary state energy is above the flat band energy. The boundary states for the cases $V_B = 0$ Hz and the resonance case $V_B = 260$ Hz are shown in Fig. 4.22. Also, it is seen that the boundary potential moves the position of the dispersive states and the boundary states but keeps the flat band state roughly at the same energy. This is the case as the flat band states are localized to the sawtooth lattice with wavefunction zero at the boundary sites as seen in Fig. 4.5. On the other hand, as the dispersive band states are non-zero at the boundary sites, their energy also increases.

The behavior of the flat band peak critical Josephson current versus the boundary potential $V_B$ is illustrated in the Fig. 4.23. It is seen that the current is maximal at certain values of $V_B$ and goes down when $V_B$ is increased after that. The maximum is observed when the flat band state energy and the boundary state energy become degenerate. The critical flat band current dependence on resonance boundary potential $V_B$ is presented in the Fig. 4.24. The dependence is observed to be linear, similarly as in the case of $V_B = 0$ Hz. The magnitude of the flat band critical Josephson current is an order of magnitude higher.

The $V_B$ dependence of the dispersive state current is shown in the Fig. 4.25, and is found to be decreasing roughly linearly in the considered region for both interacting and non-interacting cases. This is probably due to the boundary potentials $V_B$ acting as
Figure 4.21: The critical Josephson current versus chemical potential for various boundary potentials for the interacting (above) and non-interacting (below) cases. It is seen that the flat band state position remain the same but the boundary state and dispersive state positions move in both cases. In the interacting case, the flat band peak current increases substantially. Other state peak currents decrease. Peculiarly, the boundary state current vanishes at the energy of flat band also for the non-interacting case but has small value above it.

potential barriers. Also in the non-interacting case, potential barriers reduce the current. In the interacting case, the boundary state peak is not visible with every value of $V_B$, so we do not show the $V_B$ dependence of the boundary state Josephson current as it is
Figure 4.22: The boundary states for cases $V_B = 0$ Hz (left) and $V_B = 260$ Hz (right). The latter case corresponds to the flat band current resonance, that is, the largest observed flat band current while the boundary potential $V_B$ is varied. It is seen that for the latter case, the boundary state is localized to the edges when in the case $V_B = 0$ Hz, the boundary state has finite but small amplitude also in the bulk.

Figure 4.23: The critical Josephson current at flat band versus boundary potential $V_B$ for different interaction strengths. It is seen that the current value is maximal around $V_B = 250$ Hz and after that it begins to decrease. The value is correspondent to the case in which the flat band state and boundary state become degenerate in energy.

hidden by the flat band peak while in resonance.
Figure 4.24: The dependence of critical Josephson current at flat band at boundary potential resonance on the interaction strength. The dependence is found to be linear as in the case $V_B = 0$ Hz.
Figure 4.25: The dependence of dispersive state critical Josephson current on the boundary potential $V_B$ for interacting (upper) and non-interacting (lower) case. Qualitatively, the same behavior is seen for both cases. For the interacting case, the other parameters are $t_C = 1$ kHz and $\Delta_I = 2$ kHz. For the non-interacting case $t_C = 2$ kHz and $\Delta_I = 2$ kHz.
4.5 Finite temperature

In this section, we present the behavior of critical Josephson current at the dispersive and the flat band of the sawtooth lattice at finite temperatures. We consider also the behavior of superconducting order parameter, that is, the pair potential at the second A type site from left, as shown in Fig. 4.1. Specifically, we consider the case in which the boundary potential introduced in the previous section is tuned such that the flat band and the boundary state are degenerate and the flat band current is maximal. Also, in the other respects, the sawtooth lattice system is the same as considered in the previous section.

The dispersive band critical current and order parameter dependence on temperature are shown in Figs. 4.26, 4.27. Correspondingly, the flat band band critical current and order parameter dependence on temperature are shown in Figs. 4.28, 4.29. The lead pair potential is $\Delta_L = 2$ kHz, the lead-system hopping amplitude is $t_C = 1$ kHz, and the boundary potential $V_B = 260$ Hz in these tests. Parameter sweep on the parameters is not performed. Flat band current is seen to dominate the dispersive band current for all considered temperatures. It is observed that the order parameter and the critical Josephson current goes to zero smoothly instead of suddenly as would be case for thermodynamic limit. This is the case because we consider a system of finite size. Thus, the behavior of a strict phase transition is not observed. However, from the shape of the curve it is possible to estimate the point of the phase transition. We consider the threshold to be when the current goes to less than 1 1/s or at which the slope goes to zero. It is seen that for both dispersive band and the flat band, the peak critical Josephson current vanishes at same temperature as the order parameter, indicating that this is the critical temperature above which superconductivity is lost. The flat band superconductivity is seen to be more persistent than the dispersive band superconductivity, having critical temperatures of 2-4 nK for considered interaction strengths compared to critical temperatures 1-2 nK of dispersive band. Thus, there is a factor of 2 difference in the critical temperatures. The Josephson current and the order parameter are seen to vanish at the same temperature for both cases. The figures demonstrate the behavior that is seen earlier in the text, namely that at the zero temperature the dispersive band current is weakly dependent on the interaction strength whereas for the flat band the dependence is strong.
Figure 4.26: The peak critical Josephson current dependence on temperature for the dispersive band. The current vanishes below measurable amplitude around 1-2 nK, depending on the interaction strength.

Figure 4.27: The pair potential, that is, the superconducting order parameter at an A site of the sawtooth lattice at the conditions of peak critical Josephson current versus temperature for the dispersive band. The order parameter vanishes below measurable amplitude around 1-2 nK, depending on the interaction strength.
Figure 4.28: The peak critical Josephson current dependence on temperature for the flat band. The current vanishes below measurable amplitude around 2-4 nK, depending on the interaction strength.

Figure 4.29: The pair potential, that is, the superconducting order parameter at an A site of the sawtooth lattice at the conditions of peak critical Josephson current versus temperature for the flat band band. The order parameter vanishes around 2-4 nK, depending on the interaction strength, indicating that the superconductivity is lost.
Chapter 5

Discussion and Conclusions

In this chapter, we discuss the results in the context of the goals presented in the Chapters 1 and 2. Finally, we briefly summarize the results.

The goal of the thesis is to investigate qualitative behavior of the sawtooth lattice with a flat band with experimentally realistic parameters. For simplicity, we considered a tight-binding model of the sawtooth lattice instead of a realistic full potential. This choice is computationally simpler and should capture the interesting physics. This is the case as the goal of optical lattices in an ultracold gas experiment is to simulate the physics of a tight-binding model. If the experimental potential model would give significantly differing results, the flat band behavior could be altered.

In order to demonstrate that the optical potential captures the tight-binding model behavior of the sawtooth lattice and that our tight-binding parameters are experimentally realistic, we compared tight-binding non-interacting normal state transmission calculations to the similar calculations performed on a realistic potential. Qualitative agreement is observed at experimentally observable transmission levels. We observe the same number of transmission resonances or peaks related to the dispersive state and the boundary state. We also observe the flat band as it is made slightly non-flat in the analysis. This was the case as the flat band of the realistic potential is also slightly non-flat. A notable difference between the tight-binding and optical potential approaches is that the order of flat band state peak and the boundary state peak in energy is different. This difference is presently not understood fully, but is probably due to roughness at the boundary of the optical potential, which is not present in the considered tight-binding model. Also, the absolute energy scale is different for the two cases due to difference in contact between the leads and the sawtooth lattice. However, the zero point of the energy scale of the energy levels is arbitrary and does not affect the physics per se. This is due to the fact that the chemical potential of the system is modifiable: the same is not true for the tunneling, that is, hopping amplitudes.

Secondly, we studied the Josephson current through the non-interacting sawtooth lattice between to superconducting leads. This was done in order to understand the basic behavior of the system. The critical Josephson current was calculated through the relevant energy levels of the system by sweeping the chemical potential. We observe
critical Josephson current resonance peaks near the energy levels, that is, the transmission resonances in the non-interacting case. The observation is in line with the single quantum dot case considered in the Section 3.4 as a reference case. This behavior is confirmed by characterizing the behavior of peak critical Josephson current values under the change of contact tunneling amplitude between the leads and the system and the lead order parameter. We observe that for the dispersive state, the dependence on the contact hopping between the system and the leads is quadratic. The dependence on the lead order parameter is linear for small parameter and then saturates. These properties are in line with the behavior of quantum dot near the resonance, that is, when the impurity vanishes. Thus, we can understand the dispersive state peaks as single energy levels in the non-interacting limit. The boundary state results are more messy and harder to compare with the quantum dot case. However, for small lead pair potential values the behavior can be related to the quantum dot case for which the energy of the dot is larger than the tunneling rate.

Thirdly, we studied the interacting sawtooth lattice. Important difference with respect to the case of the non-interacting sawtooth lattice case is that we also observe a peak in the system nearby the energy levels related to the flat band state. The flat band peak critical Josephson current is observed to behave linearly on the interaction strength, which is according to the theoretical prediction. The observation of the flat band current was one of the targets of this thesis. Thus, this is one of the main results of the thesis. The critical current peaks related to the dispersive state and the boundary states are observed as in the non-interacting case. However, their positions are shifted in comparison to the non-interacting case as the Hartree term behaves as an equivalent chemical potential. Also, the height and width of the dispersive peaks are increased. Also, the dispersive state current increases linearly on the interaction strength. The boundary state Josephson current behavior with respect to the interaction strength is more complicated: initially the current drops, it achieves a minimum and begins to rise. This behavior is not understood at the moment.

We also studied the contact hopping amplitude and the lead order parameter dependence of the critical Josephson current through the flat band. The dependence on the contact hopping value is for small values quadratic, then it is roughly linear, and for the largest observed values we see that it begins to saturate. This is in line with the quantum dot behavior as for high values of the hopping amplitude the dependence should also saturate. We did not observe this for the dispersive state probably because we did not consider high enough values. The dependence of the flat band current on the order parameter in the leads is also in accordance to the Quantum Dot case. Thus, we observe that the flat band state behaves in these respects similarly to the quantum dot case when the interactions are turned on.

We studied also the dependence of peak critical Josephson current on the length of the sawtooth lattice. It is observed that the flat band state current does not dependent on the length of the system. Thus, it seems that the flat band states form a strong link between the leads. For the dispersive state, in the non-interacting case the dependence follows a power law $I_C \propto L^{-0.74}$, where $I_C$ is the critical current at the dispersive peak.
and \( L \) is the length of the sawtooth lattice in unit cells. The power law for the dispersive peaks remains in with interactions. The exponent changes from \(-0.74\) to \(-0.68\) for when interaction strength is increased from 0 Hz to 400 Hz. This behavior is not well-understood yet and requires further investigation. For the boundary state, we observe exponential decay in the critical current when the length is increased. This is in line with the picture that the boundary state transport is due to finite overlap of the boundary states formed at the boundaries of the sawtooth lattice and the leads, which decay exponentially with respect to the distance from the corresponding boundary site.

The observed flat band current is small in comparison to the dispersive state current for the investigated parameters. However, we expected that the flat band current should be more prominent based on the large contribution on the superfluid weight from the flat band. In order to understand this, we consider the hypothesis that the smallness of the current is caused by the boundary state and the flat band state being at different energies. The hypothesis is based on the observation that the boundary state is like a localized flat band state but is perturbed by the truncation of the system and thus is shifted in energy. We test this hypothesis by introducing a boundary potential to the system, that is, finite potential at the boundary sites of the sawtooth lattice. Increasing the boundary potential increases the boundary state and dispersive band state energies but the flat band energy remains approximately intact. We observe that the flat band current increases significantly when the flat band state and the boundary state are degenerate, that is, at the resonance. When the boundary state is tuned above the flat band state energy, the observed current decreases. Also, based on the non-interacting analysis of the boundary state current, the increase is not explained by simply adding the currents of the two contributions. The observed flat band current is increased by at least an order of magnitude. The dependence of the flat band current on the interaction strength is linear. The dispersive state current is reduced by the addition of the boundary potential. Thus, the flat band current dominates at the considered parameter range.

Finally, we considered the temperature dependence of the current in the boundary resonance case. We saw that the dispersive state current vanishes at 1-2 nK at interaction strengths 200 – 400 Hz. Similarly, the order parameter vanishes at the same temperature. Correspondingly, the flat band current vanishes at 2-4 nK for the same interaction strength variation. Also, the superconductivity in the sawtooth lattice portion of the system is lost at the same temperature, as implied by the vanishing order parameter. The flat band current is seen to dominate the dispersive state current in all temperature ranges. The flat band state is seen to be more robust against temperature than the dispersive state.

In comparison to the obtained critical temperatures, the experimental temperature at the ETH Zürich Lithium lab setup, being 60-70 nK, is larger by a factor of 20-40. Based on this observation, we may draw a conclusion that measuring the Josephson current in the system with the considered parameters is not feasible within the present experimental capability. In order to measure the effect, either the experimental temperature has to be decreased or the system itself has to be designed differently. In the end, probably both actions are required because the difference between the experimental temperature and
the found critical temperature is so high.

There are several ways to alternate the system considered in this thesis in order to make the flat band behavior experimentally observable. One way would be to investigate the same system with larger hopping amplitudes between the sawtooth lattice wells. However, the tight-binding approximation breaks when the single well orbitals overlap too much: also the farther orbitals overlap and, if the overlaps are too big, the prominence of single well orbitals is lost. This would indicate that the tight-binding model from which the flat band arises is not valid anymore and the flat band behavior would be lost to some extend. Also, another possibility is to consider the non-equilibrium transport through the system, that is, setting different chemical potentials for the two leads. Non-equilibrium transport is present in the form of the AC Josephson effect if the leads are superconducting or, above the lead critical temperature, as normal state transport through an interacting system. Simulations are required to determine whether the flat band effect is prominent enough to be experimentally observed in these cases.

In conclusion for the given discussion, in the simulations we found that the Josephson current through the flat band of a sawtooth lattice is finite and is in principle observable. Furthermore, the flat band Josephson current dominates the Josephson current through the other bands of the system when the boundary states and the flat band state are tuned to resonance by a boundary potential barrier between the sawtooth lattice and the leads. These promising results are the main findings of this thesis. However, in the finite temperature simulations we found that the critical current is one order of magnitude smaller than the present experimental temperature in the ETH Zürich Lithium lab ultracold gas experiment. Thus, based on the simulations, the Josephson effect through the system is not observable with the considered experimental setup. Further investigations are needed to see whether or not the situation is the same, if the system is designed differently.

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Bibliography


Appendix A

Flat band condition of a Sawtooth ladder

In this appendix chapter, we consider the tight-binding model of a sawtooth lattice and show that it can have a flat band structure when parameters are set right. The sawtooth lattice comprises unit cells containing two sites where the second is at 60° angle at distance $a$ from the first with respect to a horizontal line. The unit cells are on a straight line at the intervals of the lattice constant $a$. Let us denote the sites in a unit cell by A and B. The unit cells are labeled by an index $i$; for instance, $A_i$ is the A site of unit cell $i$. Let us assume that there are $N$ unit cells.

The tight-binding model assumes that the overall wave function $|\psi\rangle$ is a combination of single-site wave functions $|\psi_{A_i}\rangle$ and $|\psi_{B_i}\rangle$. Furthermore, the Hamiltonian can be written as

$$\hat{H} = \sum_{ij} H_{ij} |i\rangle \langle j|$$  \hspace{1cm} (A.1)

where $|i\rangle$ are the single site states and $H_{ij} = \langle i|\hat{H}|j\rangle$ is the Hamiltonian matrix. The Schrödinger equation is

$$\hat{H} |\psi\rangle = E |\psi\rangle.$$  \hspace{1cm} (A.2)

It can be represented by a matrix equation in the given basis

$$\begin{bmatrix} H_{A_1A_1} & H_{A_1B_1} & \cdots & H_{A_1A_N} & H_{A_1B_N} \\ H_{B_1A_1} & H_{B_1B_1} & \cdots & H_{B_1A_N} & H_{B_1B_N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ H_{A_NA_1} & H_{A_NB_1} & \cdots & H_{A_NB_N} & H_{A_NB_N} \\ H_{B_NB_1} & H_{B_NB_2} & \cdots & H_{B_NB_N} & H_{B_NB_N} \end{bmatrix} \begin{bmatrix} c_{A_1} \\ c_{B_1} \\ \vdots \\ c_{A_{N}} \\ c_{B_{N}} \end{bmatrix} = E \begin{bmatrix} c_{A_1} \\ c_{B_1} \\ \vdots \\ c_{A_N} \\ c_{B_N} \end{bmatrix}$$  \hspace{1cm} (A.3)

where $c_n$ are the coefficients of single site states. The indexing goes as $A_1, B_1, A_2, B_2, \ldots, A_N, B_N$. Let us assume that at $A$ sites the energy is $c_A$ and at $B$ sites $c_B$, that is, $H_{A_iA_i} = c_A$ and $H_{B_iB_i} = c_B$ for all $i \in \{1, 2, \ldots, N\}$. Also, we assume that only the tunneling between neighbouring sites is significant: we label the elements as $H_{A_iA_{i+1}} = H_{A_{i+1}A_i} = t$ for the
adjacents A sites, \( H_{B_i, B_{i+1}} = H_{B_{i+1}, B_i} = t'' \) for the adjacents B sites and \( H_{A_i, B_i} = H_{B_i, A_i} = H_{A_i, B_{i-1}} = H_{B_{i-1}, A_i} = t' \) for neighbouring \( A \) and \( B \) sites. All the other terms are zero. We also assume periodic boundary conditions.

To obtain the dispersion relation, let us make the plane wave approximation, that is, we assume that the coefficient at different unit cells differ only by a phase related to their spatial separation, \( c_{A_n} = e^{ik(n-1)a}c_{A_1} \) and \( c_{B_n} = e^{ik(n-1)a}c_{A_1} \), where \( k \) is the wave number and \( a \) is the lattice constant. Using these properties, we obtain a \( 2 \times 2 \) system

\[
\begin{bmatrix}
\epsilon_A + (e^{ika} + e^{-ika})t' & t'(1 + e^{-ika}) \\
\epsilon_B + (e^{ika} + e^{-ika})t'' & \epsilon_B + (e^{ika} + e^{-ika})t''
\end{bmatrix}
\begin{bmatrix}
c_A \\
c_B
\end{bmatrix}
= E
\begin{bmatrix}
c_A \\
c_B
\end{bmatrix}
\tag{A.4}
\]

where we have written \( c_A \equiv c_{A_1} \) and \( c_B \equiv c_{B_1} \). Using the Euler’s formula \( e^{i\alpha} = \cos \alpha + i \sin \alpha \) we may write the system as

\[
\begin{bmatrix}
\epsilon_A + 2\cos(ka)t' & t'(1 + e^{-ika}) \\
\epsilon_B + 2\cos(ka)t'' & \epsilon_B + 2\cos(ka)t''
\end{bmatrix}
\begin{bmatrix}
c_A \\
c_B
\end{bmatrix}
= E
\begin{bmatrix}
c_A \\
c_B
\end{bmatrix}
, \tag{A.5}
\]

The characteristic equation of this system gives

\[
(\epsilon_A - E + 2\cos(ka)t')(\epsilon_B - E + 2\cos(ka)t'') - (t')^2(1 + e^{-ika})(1 + e^{ika}) = 0 \tag{A.6}
\]

which can be written as

\[
(\epsilon_A - E)(\epsilon_B - E) + 2\cos(ka)(\epsilon_B - E)t + (\epsilon_A - E)t' + 4\cos^2(ka)t' - 2(t')^2(\cos(ka) + 1) = 0 . \tag{A.7}
\]

A more advanced way to achieve the same result is to work in the second quantization. The Hamiltonian is then

\[
\hat{H}_{\text{sawtooth}} = \sum_{i\sigma} \left[ \epsilon_A \hat{c}_{A,i\sigma}^\dagger \hat{c}_{A,i\sigma} + \epsilon_B \hat{c}_{B,i\sigma}^\dagger \hat{c}_{B,i\sigma} \\
+ t\hat{c}_{A,i+1\sigma}^\dagger \hat{c}_{A,i\sigma} + h.c. \\
+ t'\hat{c}_{B,i+1\sigma}^\dagger \hat{c}_{B,i\sigma} + h.c. \\
+ t''\hat{c}_{A,i-1\sigma}^\dagger \hat{c}_{A,i\sigma} + h.c. \\
+ t''\hat{c}_{B,i-1\sigma}^\dagger \hat{c}_{B,i\sigma} + h.c. \right] . \tag{A.8}
\]

The target is to find the independent degrees of freedom of the system, that is, to write the Hamiltonian as a sum of independent harmonic oscillators described by new operators \( \hat{a}_k \), where \( k \) is the label of the degrees of freedom. As the system is assumed to be large and invariant under discrete spatial transformation by a Bravais lattice vector, the crystal momentum is a good quantum number in the system. The various crystal momentum states span the Hilbert space of the solutions. We may write

\[
\hat{c}_{A,i\sigma} = \sum_k e^{-ikx}\hat{c}_{A,k\sigma}, \quad \hat{c}_{B,i\sigma} = \sum_k e^{-ikx}\hat{c}_{B,k\sigma} \tag{A.9}
\]
where $x$ labels spatial position of the unit cell $i$. We obtain as an auxiliary result:

$$
\hat{\mathcal{E}}_{A,i\sigma} \hat{\mathcal{E}}_{A,j\sigma} = \sum_{k,k'} e^{-i(k'x + k'x - kx)} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \hat{\mathcal{E}}_{A,k'\sigma}^{\dag}
= \sum_{k,k'} e^{-i(k'x + k'x - kx)} \hat{\mathcal{E}}_{A,k\sigma} \hat{\mathcal{E}}_{A,k'\sigma}
= \sum_{k,k'} e^{-ik(k' - x)} e^{-i(k' - k)x} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \hat{\mathcal{E}}_{A,k'\sigma}
= \sum_{k} e^{-ik(k' - x)} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x} \hat{\mathcal{E}}_{A,k'\sigma},
$$

(A.10)

and similarly for combinations of A and B. Inputting this to the Hamiltonian, we obtain

$$
\hat{\mathcal{H}}_{\text{sawtooth}} = \sum_{\sigma} \left[ e_{A} \sum_{k} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x_{i}} \hat{\mathcal{E}}_{A,k'\sigma}
+ e_{B} \sum_{k} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x_{i}} \hat{\mathcal{E}}_{B,k'\sigma}
+ t \sum_{k} e^{-ika} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{A,k'\sigma} + \text{h.c.}
+ t' \sum_{k} e^{-ika} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{B,k'\sigma} + \text{h.c.}
+ t' \sum_{k} e^{-ika} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{B,k'\sigma} + \text{h.c.}ight]
= \sum_{\sigma} \left[ e_{A} \sum_{k} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \sum_{k'} \sum_{i} e^{-i(k' - k)x_{i}} \hat{\mathcal{E}}_{A,k'\sigma}
+ e_{B} \sum_{k} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} \sum_{i} e^{-i(k' - k)x_{i}} \hat{\mathcal{E}}_{B,k'\sigma}
+ t \sum_{k} e^{-ika} \hat{\mathcal{E}}_{A,k\sigma}^{\dag} \sum_{k'} \sum_{i} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{B,k'\sigma} + \text{h.c.}
+ t' \sum_{k} e^{-ika} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} \sum_{i} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{B,k'\sigma} + \text{h.c.}
+ t' \sum_{k} e^{-ika} \hat{\mathcal{E}}_{B,k\sigma}^{\dag} \sum_{k'} \sum_{i} e^{-i(k' - k)x_{i+1}} \hat{\mathcal{E}}_{B,k'\sigma} + \text{h.c.}ight]
$$

(A.11)
By utilizing the fact $\sum_i e^{-i(k' - k)x_i} = \delta(k' - k)$ we obtain

$$
\hat{H}_{\text{sawtooth}} = \sum_{k,\sigma} \left[ \begin{array}{c}
\varepsilon_A \hat{c}_{A,k\sigma}^{\dagger} \hat{c}_{A,k\sigma} \\
+ \varepsilon_B \hat{c}_{B,k\sigma}^{\dagger} \hat{c}_{B,k\sigma} \\
+ te^{-ika} \hat{c}_{A,k\sigma}^{\dagger} \hat{c}_{A,k\sigma} + h.c. \\
+ t''e^{-ika} \hat{c}_{B,k\sigma}^{\dagger} \hat{c}_{B,k\sigma} + h.c. \\
+ t'\hat{c}_{B,k\sigma}^{\dagger} \hat{c}_{A,k\sigma} + h.c. \\
+ t'\hat{c}_{A,k\sigma}^{\dagger} \hat{c}_{B,k\sigma} + h.c. \end{array} \right]. \tag{A.12}
$$

The result can be written in a matrix form

$$
\hat{H}_{\text{sawtooth}} = \sum_{k,\sigma} \left[ \begin{array}{c}
\hat{c}_{A,k\sigma}^{\dagger} \\
\hat{c}_{B,k\sigma}^{\dagger} \\
\end{array} \right] \left[ \begin{array}{c}
\varepsilon_A + 2t \cos(ka) \\
+ \varepsilon_B + 2t'' \cos(ka) \\
\end{array} \right] \left[ \begin{array}{c}
\hat{c}_{A,k\sigma} \\
\hat{c}_{B,k\sigma} \\
\end{array} \right]. \tag{A.13}
$$

We find that the system is almost diagonalized but there are cross terms at the level of a single value of $k$. We may introduce new operators on the level of single unit cell by writing

$$
\hat{c}_{k}^{\dagger} \hat{H}_{k} \hat{c}_{k} = \hat{c}_{k}^{\dagger} S D S^{-1} \hat{c}_{k} = \hat{d}_{k}^{\dagger} D \hat{d}_{k} \tag{A.14}
$$

where $S$ contains the eigenvectors of $\hat{H}_{k}$, the single $k$ Hamiltonian matrix, and $D$ is a diagonal matrix of the related eigenvalues, and $\hat{d}_{k} = S^{-1} \hat{c}_{k}$ is a vector of new operators in terms of old operators. This choice diagonalizes the Hamiltonian. The eigenvalues of Hamiltonian matrix are given by the equation

$$
(e_A + 2t \cos(ka) - E)(e_B + 2t'' \cos(ka) - E) - (t')^2(e^{-ika} + 1)(e^{ika} + 1) = 0 \tag{A.15}
$$

which is solved by

$$
E = \frac{1}{2} \left[ e_A + e_B + 2t \cos(ka) + 2t'' \cos(ka) + \sqrt{(e_A + e_B + 2t \cos(ka) + 2t'' \cos(ka))^2 - 4(e_A + 2t \cos(ka))(e_B + 2t'' \cos(ka))} \right]^{1/2} \\
= \frac{1}{2} \left[ e_A + e_B + 2t \cos(ka) + 2t'' \cos(ka) \right] \\
\pm \sqrt{e_A + 2t \cos(ka) - e_B - 2t'' \cos(ka))^2 + 4(t')^2(2 + e^{ika} + e^{-ika})} \\
= \frac{1}{2} \left[ e_A + e_B + 2t \cos(ka) + 2t'' \cos(ka) \right] \\
\pm \sqrt{(e_A + 2t \cos(ka) - e_B - 2t'' \cos(ka))^2 + 8(t')^2(1 + \cos(ka))} \tag{A.16}
$$

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To find the conditions for a flat band let us implicitly differentiate the equation with respect to wavenumber $k$ and assume that the dispersion relation is flat, that is, $\frac{\partial E}{\partial k} = 0$. We obtain
\[
-2a \sin(ka)[(\epsilon_B - E) t + (\epsilon_A - E) t'''] - 8a \cos(ka) \sin(ka) tt'' + 2a(t')^2 \sin(ka) = 0, \quad (A.17)
\]
which can be written as
\[
-\sin(ka)[(\epsilon_B - E) t + (\epsilon_A - E) t'''] + 2 \sin(2ka) tt'' + (t')^2 \sin(ka) = 0 \quad (A.18)
\]
Since the relation must hold for all $k$ and we know that $\sin(\alpha)$ and $\sin(2\alpha)$ are independent, the two equations follow
\[
\begin{align*}
(\epsilon_B - E) t + (\epsilon_A - E) t''' - (t')^2 &= 0 \\
2t'' &= 0.
\end{align*} \quad (A.19)
\]
Thus, either tunneling from A to adjacent A or from B to adjacent B must be prohibited for the flat band solution. Let us assume that the latter is the case, that is, $t'' = 0$. From the first equation, we obtain that $\epsilon_B - E = (t')^2/t$ or
\[
E = \epsilon_B - (t')^2/t. \quad (A.20)
\]
With these conditions, the above equation turns to
\[
\left(\epsilon_A + 2t \cos(ka) - \epsilon_B + \frac{(t')^2}{t}\right) \left(\frac{(t')^2}{t} - (t')^2(e^{-ika} + 1)(e^{ika} + 1) = 0 \quad (A.21)
\]
where we obtain
\[
(\epsilon_A - \epsilon_B) \left(\frac{(t')^2}{t} + \frac{(t')^4}{t^2} - 2(t')^2 = 0 \quad (A.22)
\]
as $\cos(ka)$ terms cancel. From this we obtain
\[
\left(\frac{(t')^2}{t} \left(\epsilon_A - \epsilon_B + \frac{(t')^2}{t} - 2t\right) = 0 \quad (A.23)
\]
or
\[
t' = \sqrt{2t^2 + (\epsilon_B - \epsilon_A)t}. \quad (A.24)
\]
This is the flat band condition. When this is put to the solution, we obtain
\[
E = \frac{1}{2} \left[\epsilon_A + \epsilon_B + 2t \cos(ka) \pm \sqrt{(\epsilon_A - \epsilon_B + 2t \cos(ka))^2 + (16t^2 + 8(\epsilon_B - \epsilon_A)t)(1 + \cos(ka)))}\right] \\
= \left[\epsilon_A + \epsilon_B + 2t \cos(ka) \pm \sqrt{(2t \cos(ka) + \epsilon_B - \epsilon_A + 4t)^2}\right] \\
= \left\{\epsilon_B + 2t(\cos(ka) + 1) \right\} \left\{\epsilon_A - 2t \right\} \quad (A.25)
\]
The other band is seen to be flat as expected. Next, we demonstrate that the localized states
\[
|V_{i\sigma}\rangle = \left( \sqrt{2 + \frac{e_B - e_A}{t} \hat{c}^\dagger_{A,i\sigma} - \hat{c}^\dagger_{B,i\sigma}} \right) |0\rangle \quad (A.26)
\]
are eigenstates of the Hamiltonian \( \hat{N}_{\text{sawtooth}} \) at the flat band. We have at flat band with the given conditions that
\[
\hat{N}_{\text{sawtooth}} = \sum_{i\sigma} \left( e_A \hat{c}^\dagger_{A,i\sigma} \hat{c}_{A,i\sigma} + e_B \hat{c}^\dagger_{B,i\sigma} \hat{c}_{B,i\sigma} + t \hat{c}^\dagger_{A,i+1,\sigma} \hat{c}_{A,i\sigma} + \sqrt{2t^2 + (e_B - e_A)t\hat{c}^\dagger_{B,i\sigma} \hat{c}_{A,i\sigma}} + h.c. \right) \quad (A.27)
\]
By applying this to the localized state \( |V_{i\sigma}\rangle \) we obtain
\[
\begin{align*}
\hat{N}_{\text{sawtooth}} |V_{i\sigma}\rangle &= \sum_{i\sigma} \left( e_A \hat{c}^\dagger_{A,i\sigma} \hat{c}_{A,i\sigma} + e_B \hat{c}^\dagger_{B,i\sigma} \hat{c}_{B,i\sigma} + t \hat{c}^\dagger_{A,i+1,\sigma} \hat{c}_{A,i\sigma} + \sqrt{2t^2 + (e_B - e_A)t\hat{c}^\dagger_{B,i\sigma} \hat{c}_{A,i\sigma}} + h.c. \right) |V_{i\sigma}\rangle \\
&= \left( \sqrt{2 + \frac{e_B - e_A}{t} \hat{c}^\dagger_{A,i\sigma}} - \hat{c}^\dagger_{B,i\sigma} - \hat{c}^\dagger_{B,i-1}\sigma \right) |0\rangle \\
&= (e_A - 2t) \left( \sqrt{2 + \frac{e_B - e_A}{t} \hat{c}^\dagger_{A,i\sigma}} - \hat{c}^\dagger_{B,i\sigma} - \hat{c}^\dagger_{B,i-1}\sigma \right) |0\rangle \quad (A.28)
\end{align*}
\]
where the brackets are opened one term of the second bracket at a time.
Appendix B

From Fermi-Hubbard Model to BCS Hamiltonian

In this chapter, we derive the mean field form of the interaction term in the Fermi-Hubbard model. We consider the Hartree and pairing terms and neglect the Fock term. To make the mean-field approximation properly, we utilize the Wick’s theorem [61]. Wick’s theorem is about writing an operator in normal ordered form where the operators annihilating the vacuum are on the right of the respective creation operators. The \( \hat{O} \) denotes normal ordering of the operator \( \hat{O} \) when represented as sum of creation and annihilation operators. The contraction of two operators \( \hat{A}_i \hat{B}_j \) is defined as \( \hat{A}_i \hat{B}_j \equiv \hat{A}_i \hat{B}_j - \hat{A}_i \hat{B}_j \). We also denote \( \hat{A}_x \cdots \hat{Y}_p \equiv (-1)^p \hat{A}_x \hat{Y}_p \cdots \hat{Y}_p \) where \( p \) is the number of operators \( \hat{X} \cdots \hat{Y} \). With this notation, Wick’s theorem states

\[
\begin{align*}
\epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} = & \, \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \\
& \quad \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} \\
& \quad \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} + \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij}.
\end{align*}
\]  

(B.1)

By definition, the vacuum expectation value of \( \epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} \) is zero. The mean field approximation is that the operator itself is also zero, that is we approximate

\[
\epsilon_{ij}^\dagger \epsilon_{ij} \epsilon_{ij}^\dagger \epsilon_{ij} \approx 0.
\]  

(B.2)

Next, we evaluate the contractions. An important result states that if the anticommutator \( \{ \hat{A}, \hat{B} \} \) is a complex number it follows that \( \hat{A} \hat{B} \) is a complex number and so we have directly from definition \( \hat{A} \hat{B} = \langle \hat{A} \hat{B} \rangle \) as the mean value of a complex number is the complex number and the mean value of normal ordered product is zero [62]. Thus, after
the approximation and utilization of this result, we find the following
\[
\langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger e_{\downarrow} e_{\uparrow}\rangle \approx \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle + \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle + \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle + \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle
\]
\[
+ \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle.
\]
(B.3)

By utilizing the Wick's theorem on two operators we find
\[
\hat{A}\hat{B} = \hat{A}\hat{B} + \hat{A}\hat{B} = \hat{A}\hat{B} + \langle \hat{A}\hat{B} \rangle.
\]
(B.4)

We can reorder this to read
\[
\hat{A}\hat{B} = \hat{A}\hat{B} - \langle \hat{A}\hat{B} \rangle.
\]
(B.5)

Using this result, we arrive at
\[
\langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger e_{\downarrow} e_{\uparrow}\rangle \approx \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle + \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle + \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle + \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle
\]
\[
+ \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle
\]
\[
- \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle \langle e_{\downarrow} e_{\uparrow}\rangle - \langle e_{\downarrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\uparrow}^\dagger \rangle.
\]
(B.6)

Now, we may insert this into the definition of the interaction term of the Hamiltonian
\[
\hat{\Pi}_I \approx \hat{\Pi}_I^{MF} = \sum_i U_i \left( \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle + \langle e_{\uparrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle - \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle \right) \quad \text{Pairing terms}
\]
\[
+ \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle + \langle e_{\uparrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle - \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle \right) \quad \text{Hartree terms}
\]
\[
- \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle - \langle e_{\uparrow} e_{\uparrow}\rangle \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle + \langle e_{\uparrow}^\dagger e_{\downarrow} \rangle \langle e_{\uparrow} e_{\uparrow}\rangle \right) \quad \text{Fock terms}
\]
(B.7)

where we have identified the terms of Hartree-Fock approximation and the pairing terms.
Appendix C

Derivation of the current operator

The current operator from a site $j$ to a site $i$, $\hat{I}_{ij}$ of a lattice system may be evaluated in the Heisenberg picture using the Heisenberg equation of motion

$$\frac{d\hat{n}_i}{dt} = \frac{i}{\hbar} [\hat{H}_{\text{BCS}}, \hat{n}_i] + \frac{\partial \hat{n}_i}{\partial t},$$

(C.1)

where $\hat{n}_i$ is the number operator of particles at site $j$ and the continuity equation

$$\frac{d\hat{n}_i}{dt} = \sum_j \hat{I}_{ij} + \hat{R}_i,$$

(C.2)

where $\hat{R}_i$ is the operator related to the rate of creation of particles at the site $i$ by the pairing term of the BCS Hamiltonian. The number operator does not depend explicitly on time, so it is sufficient to evaluate the commutator $[\hat{H}_{\text{BCS}}, \hat{n}_i]$. Let us do this term by term.

First, the commutator is zero for the on-site terms because the particle number operators commute with each other. Secondly, from the hopping terms we obtain the following contribution

$$\left[ -\sum_{j,\sigma'} t_{ij} (\hat{c}_{j,\sigma'}^\dagger \hat{c}_{j,\sigma'} + \hat{c}_{j,\sigma'}^\dagger \hat{c}_{j,\sigma'}^\dagger), \sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} \right] = \sum_{j,\sigma} -t_{ij} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{i,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{i,\sigma}^\dagger),$$

(C.3)

where $j$ sum is over the sites that there can be hopping from the site $i$. Writing out the commutators, we find

$$\sum_{j,\sigma'} t_{ij} (\hat{c}_{j,\sigma'}^\dagger \hat{c}_{j,\sigma'} + \hat{c}_{j,\sigma'}^\dagger \hat{c}_{j,\sigma'}^\dagger), \sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$$

$$= \sum_{j,\sigma} t_{ij} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{i,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{i,\sigma}^\dagger - \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{c}_{j,\sigma}^\dagger - \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{c}_{j,\sigma}^\dagger - \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{c}_{j,\sigma}^\dagger - \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{c}_{j,\sigma}^\dagger)$$

(C.4)

$$= \sum_{j,\sigma} t_{ij} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} - \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma} - \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}^\dagger)$$

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where we used the anticommutation relations of the creation and annihilation operators.

Thirdly, there is a contribution from the BCS pairing terms. For those, we need the following commutation relations

\[
[\hat{c}_{i\downarrow} \hat{c}_{i\uparrow}^\dagger, \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger] = \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} - \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} = \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}^\dagger
\]

(C.5)

and

\[
[\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger, \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}] = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} - \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger = -\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger.
\]

(C.6)

By comparing the obtained sums of the commutator to the continuity equation, we obtain for the operators

\[
\hat{I}_{ij} = \frac{i}{\hbar} \sum_\sigma t_{j,i} (-\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma})
\]

(C.7)

\[
\hat{K}_i = \frac{i}{\hbar} \left( \Delta_i^* \hat{c}_{i\uparrow} \hat{c}_{i\uparrow}^\dagger - \Delta_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \right)
\]

The operators are Hermitian, so they are proper observables.
Appendix D

Derivations of Anderson mixing and Broyden’s method

In this section we derive the Anderson/Broyden mixing method and the Broyden’s method. In order to make this chapter independent, some of the details from the Methods section are repeated.

Various mixing methods are often used to ensure and to speed-up the self-consistent convergence. The mixing algorithms mix previous iterates with the newest iteration to obtain a balanced solution. The simplest mixing algorithm mixes the current and the previous values in the following manner:

\[ x_{n+1} = (1 - \alpha)x_n + \alpha f(x_n) \]  \hspace{1cm} (D.1)

where \( 0 < \alpha \leq 1 \) is the mixing parameter giving the proportion of new and previous iterates in the new value. For the following discussions, it is useful to define a function \( G(x) \equiv f(x) - x \) and write

\[ x_{n+1} = x_n + \alpha G(x_n) \]  \hspace{1cm} (D.2)

If the mixing converges, it is readily seen that the same fixed point equation is fulfilled. It has been shown that for a proper initial guess for the vector \( x \) and a small enough mixing parameter \( \alpha \), the iteration converges to a unique value which corresponds to a minimum in energy [54].

The problem with the simple mixing iteration is that, as the new solution is only partly given by the function \( f \), the convergence can still be slow even though it converges. Also, one has to choose the mixing parameter by hand via testing, which is time consuming for practical tasks. Here we consider two solutions to these problems by introducing the DIIS (direct inversion in the iterative subspace) method, which is also known as the Pulay mixing [55] or the Anderson method [56], and the Broyden method [57]. The methods have distinct advantages. In practice, it is an empirical task to find which method is the most suitable. In the following, we present these algorithms briefly.

The Anderson method is a generalization of the simple mixing introduced above. It utilizes the \( M \) previous iterations to form optimized density vectors and residual
vectors in the spanned subspace. These optimal vectors are then mixed as in the simple mixing. The method assumes that the residuals are linear, that is, one can consider the residual vectors in the same subspace as the density vectors. The method finds the density vectors in the space that correspond to residual vectors minimizing the Euclidean norm, as is the target in fixed-point iteration. In other words, if a new minimal residual vector is obtained in the subspace formed by the \( M + 1 \) subsequent residuals, then the corresponding optimal density vector is obtained by same weights in the space of previous \( M + 1 \) density vectors \( \mathbf{X} \). The Anderson mixing converges faster and is more robust against divergence problems than the simple linear mixing.

It has been shown that in certain cases combining simple mixing and the Anderson mixing, called the Periodic Pulay method [58], is more optimal. This method uses the Anderson method only once in \( k \) iterations and otherwise uses the simple mixing. Choosing the hyperparameters for the iterations is an empirical task.

Let us derive the Anderson method update equation. The derivation is similar as in Ref. [63]. In order to collect the history of \( M \) previous iterates and the current iterate, let us define the density difference matrix at iteration \( n \) as \( (\Delta \mathbf{X}_n)_{ij} \equiv X_{n-M+i,j} - X_{n-M+j-1,i} \) where \( X_{i,j} \) is the \( i \)th component of the vector \( \mathbf{X}_i \) of \( j \)th iterate, and the residual difference matrix \( (\Delta \mathbf{G}_n)_{ij} \equiv G(X_{n-M+i}) - G(X_{n-M+j-1}) \) where \( G(X_i) \) is the \( i \)th component of the residual vector \( G(X_n) \). As a note, it is more convenient to work with the residual vectors \( G(X) \) than the vectors \( F(X) \) as implied in the notation choice above, but in principle one could use either one. We define the \( n + 1 \)th iterate as

\[
\mathbf{X}_{n+1} = \bar{\mathbf{X}}_n + \alpha \bar{\mathbf{G}}_n
\]  

(D.3)

where \( 0 < \alpha \leq 1 \) is the mixing parameter and \( \bar{\mathbf{X}}_n \) and \( \bar{\mathbf{G}}_n \) are averaged density and residual vectors defined as

\[
\bar{\mathbf{X}}_n = \mathbf{X}_n - \Delta \mathbf{X}_n \Gamma_n
\]  

(D.4)

\[
\bar{\mathbf{G}}_n = G(\mathbf{X}_n) - \Delta \mathbf{G}_n \Gamma_n
\]  

(D.5)

where \( \Gamma_n \) is a vector of weights of past \( M \) and the current iterate. The weights \( \Gamma_n \) are chosen so that the Euclidean norm of the averaged residual is minimized:

\[
\Gamma_n = \arg \min_{\Gamma_n} ||\bar{\mathbf{G}}_n||.
\]  

(D.6)

We can solve \( \Gamma_n \) directly. The square of the norm of the averaged residual is

\[
||\bar{\mathbf{G}}_n||^2 = ||G(\mathbf{X}_n)||^2 + ||\Delta \mathbf{G}_n||^2 - G(\mathbf{X}_n)^T \Delta \mathbf{G}_n \Gamma_n - \Gamma_n^T \Delta \mathbf{G}_n^T G(\mathbf{X}_n).
\]  

(D.7)

Taking gradient with respect to \( \Gamma_n \) and demanding that it is zero, we obtain

\[
\Delta \mathbf{G}_n^T \Delta \mathbf{G}_n = \Delta \mathbf{G}_n^T G(\mathbf{X}_n).
\]  

(D.8)

Thus, we may write

\[
\mathbf{X}_{n+1} = \mathbf{X}_n + \alpha G(\mathbf{X}_n) - (\Delta \mathbf{X}_n + \alpha \Delta \mathbf{G}_n) (\Delta \mathbf{G}_n^T \Delta \mathbf{G}_n)^{-1} \Delta \mathbf{G}_n^T G(\mathbf{X}_n).
\]  

(D.9)

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which is the update equation of the Anderson mixing. The fact that the solution involves a solution for the optimal weights inspires the name direct inversion in the iterative subspace.

The Broyden method is essentially a quasi-Newton method, which updates both the density vector and the Jacobian. Thus, it is called a secant method. It makes the same assumption as the Anderson mixing that the residual vectors can be expanded in linear order of the density vectors. However, instead of minimizing the Euclidean norm of the residual, the method minimizes the norm of the difference of the Jacobian iterate.

Let us derive the Broyden method update formulas. The derivation follows Ref. [64]. From the linearity assumption of the residual it follows that

\[ G(X_{n+1}) \approx G(X_n) + J_n(X_{n+1} - X_n) , \]  

where \( J_n \) is the Jacobian matrix at the \( n \)th iterate, approximated by

\[ J_{n,ij} \approx \frac{G(X_{n+1})_i - G(X_n)_i}{X_{n+1} - X_n} . \]  

We find an update formula for \( X \) by assuming that \( G(X_{n+1}) \) vanishes in the approximation:

\[ X_{n+1} = X_n - J_n^{-1}G(X_n) . \]  

This is a multidimensional generalization of Newton’s algorithm. This algorithm has the disadvantage that far from the solution the assumption that the residual vector \( G(X_{n+1}) \) vanishes does not hold in general. To fix this problem, instead of using the secant formula, we define new Jacobian \( J_{n+1} \) so that the Eq. D.10 is exact. In other words, we have

\[ \Delta G_n = J_{n+1}\Delta X_n , \]  

where we have defined \( \Delta G_n \equiv G(X_{n+1}) - G(X_n) \) and \( \Delta X = X_{n+1} - X_n \). The equation for \( J_{n+1} \) gives the components of \( J_{n+1} \) only in the direction of \( \Delta X \), so we have freedom in its definition. We define it so that the Frobenius norm

\[ \| J_{n+1} - J_n \|_F^2 = \sum_{ij} |J_{n+1,ij} - J_{n,ij}|^2 \]  

is minimized under the constraint of Eq. D.13. Using the method of the Lagrangian multipliers we have the minimized Lagrangian

\[ L = \sum_{ij} |J_{n+1,ij} - J_{n,ij}|^2 + \sum_i \lambda_i \left( \Delta G_{n,i} - \sum_j \Delta X_{n,j} \right) \]  

where \( \lambda_i \) are the Lagrangian multipliers for different components of the constraint. Taking derivative with respect to \( J_{n+1,ij} \) and demanding that it is zero, we find

\[ 2J_{n+1,ij} - 2J_{n,ij} - \lambda_i \Delta X_{n,j} = 0 \]  

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which can be written in matrix form as

\[ J_{n+1} - J_n = \frac{1}{2} \lambda \Delta X_n^T \Delta X_n \]  

(D.17)

where \( \lambda \) is the vector of the constraints. Combining the result with the constraint equation Eq. D.13 we have

\[ \Delta G_n = J_n \Delta X_n + \frac{1}{2} \lambda \Delta X_n^T \Delta X_n \]  

(D.18)

and finally, by noticing that \( \Delta X_n^T \Delta X_n \) is a scalar, we can solve for the constraint vector and insert it to D.17 again, to obtain

\[ J_{n+1} = J_n + \frac{\Delta G_n \Delta X_n^T - J_n \Delta X_n \Delta X_n^T}{\Delta X_n^T \Delta X_n} \]  

(D.19)

which is the update equation for the Jacobian.

The Broyden method above has the disadvantage that, in order to update \( X \), the Jacobian must be inverted. To solve this problem, we can use the Sherman-Morrison formula

\[ (A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^TA^{-1}}{1 + v^TA^{-1}u} \]  

(D.20)

where \( A \) is an invertible matrix and \( v \) and \( u \) are vectors such that \( v^T u \neq 1 \), to write

\[ J_{n+1}^{-1} = J_n^{-1} + \frac{\Delta X_n - J_n^{-1} \Delta G_n}{\Delta X_n^T J_n^{-1} \Delta G_n} \Delta X_n^T J_n^{-1}, \]  

(D.21)

Using this formula has the advantage that it does not require evaluating the inverse.

As a note, one could derive another Broyden type method for the inverse Jacobian by demanding instead that \( \|J_{n+1}^{-1} - J_n^{-1}\|_F \) is minimized with the constraint \( J_n^{-1} \Delta G_n = \Delta X_n \). This leads to the update formula

\[ J_{n+1}^{-1} = J_n^{-1} + \frac{\Delta X_n \Delta G_n^T - J_n^{-1} \Delta G_n \Delta G_n^T}{\Delta G_n^T \Delta G_n}, \]  

(D.22)

which has the same form as Eq. D.19 but the roles of \( \Delta G_n \) and \( \Delta X_n \) have changed, which follows from the symmetry of the terms. The method would actually have the advantage to have less algebraic operators to evaluate. However, which method is the best is determined by the use case.