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Publication Date

2026-05-01

Peer reviewed|Thesis/dissertation

Ultracold Bosons and Fermions in Hexagonal Optical Superlattices

by

Shao-Wen Chang

A dissertation submitted in partial satisfaction of the

requirements for the degree of

Doctor of Philosophy

in

Physics

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Dan Stamper-Kurn, Chair

Professor Hartmut Häffner

Professor Boubacar Kanté

Spring 2026

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Abstract

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Professor Dan Stamper-Kurn, Chair

Quantum simulation using ultracold fermions in optical lattices provides valuable insights for strongly correlated many-body phenomena in regimes challenging for classical simulations. In this dissertation, we report the design and construction of an apparatus capable of producing quantum degenerate Bose and Fermi gases. The atoms are then loaded into hexagonal optical superlattices created using two commensurate wavelengths. The apparatus lays the foundation for studying interacting fermions in geometrically frustrated lattices.

We also report our experimental results on the characterization of the quantum geometry of Bloch band structures. Using rubidium Bose-Einstein condensates in the honeycomb lattice, we were able to measure the quantum distance around band touching points using parallel transport. Additionally, by simulating optical excitations using noninteracting fermions in a periodically modulated lattice, we observe quasimomentum-dependent optical selection rules, which stem from interband quantum geometry of the honeycomb lattice.

To my family

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Acknowledgments

First of all, I would like to thank my advisor, Prof. Dan Stamper-Kurn, for his support as I fumble my way towards becoming a physicist. I was often inspired by Dan's tireless pursuit of physics, especially the excitement that pierced through our discussions of new ideas. While very knowledgeable at both theory and experiment know-how, Dan is above all a great teacher who adapts conversations to the audience. It took me several years to come to appreciate how much I had benefited as a mentee, not only in terms of scientific knowledge, but also in developing physical intuitions, effective communication skills, and so much more. I would also like to thank Prof. Hartmut Häffner and Prof. Boubacar Kanté for reviewing my dissertation.

I was fortunate to be welcomed to the kagome lattice experiment (or E5, as we call it in the group) by Zephy (Tsz-Him) Leung, the senior graduate student back then, and Malte Schwarz, an exchange student at that time. Joined by the postdoc Charles Brown shortly after, we were a team with great dynamics, unparalleled sense of humor, and a strong motivation to make ambitious projects come true. Even with the episode of COVID in 2020, we still somehow managed to wrap up two projects in E5, and at the same time designed and constructed an almost new apparatus.

I owe much to Zephy and Charles, who patiently introduced to me all the basics required to work in an AMO lab. I wouldn't have been able to adapt so quickly to the monstrous complexity of E5 without Zephy's help, and he also made the first years of my PhD much more colorful with a few great trips and group dinners. Charles was (and is) a memorably good communicator between the group and collaborators, and also within the group. Being possibly the strongest physicist in the world, he was indispensable in building the ultrahigh vacuum system, which he also led the design of.

I am also truly amazed by the uncanny rapport that Malte and I have established. We could seamlessly switch from working on individual projects to taking on a marathon effort, whichever brought us closer to our goal. (Maybe sharing exactly the same birthday helped.) We also spent an unbelievable amount of time fighting the impossible fight against the ever growing entropy — lab cleanups —, and there are no better comrades than Malte for this. He is also the driving force for changes, from experiment upgrades, office organizations (although I never use the office) to lunch get-togethers. For sure, the experiment and the whole group will not be the same without him.

As the experiment grew, I also had the opportunity to work with several fellow graduate students. Rowan Duim joined us in late 2021, and contributed to several foundational parts of the experiment. I am especially grateful for her heroic endeavor to make ARTIQ work. Outside of the lab, she is a source for inspiration on her many pursuits related to and beyond the academia. She is also an accomplished lab DJ.

Later in my PhD, we were first joined by Erin Moloney, and later Ke Lin, around 2024 summer. Erin is marked by an urge to understand and lead the experiment, and she has been learning the experiment, both good and bad parts of it, at an impressive pace, and I am confident that she will make it better in the future. With a clear resolution of the physics

he wants to explore, Ke has already dived much deeper into the literatures than me. I am glad that E9 (the name of the new machine) is succeeded by two very talented minds, and also really enjoyed my last two years working in the lab with the new team.

I also had the pleasure of working with several undergraduate students. I had spent a remarkable three years working with John Ciavarra. John reminds me of a locomotive rushing with incredible momentum when it comes to physics. With an insatiable appetite to learn, he had laid his hand on an amazing number of projects, often outpacing how fast I can come up with new projects, and became an important source of motivation for me. Together with Ryan Everly, Nikhil Maserang and Nathaniel Grinkrug, they had not only contributed to the experiment, but also helped me grow as a physicist. I would like to say a special thank you to Nikhil and Nati for rating my playlist “sick.”

Working with the Dan Stamper-Kurn group had been an amazing experience. I fully enjoyed the broad scientific interest of the group, and I really appreciated how everyone is helpful and supportive of each other whenever anyone has a question. I am fortunate to be in a group where people are not just merely each other’s colleagues, but also friends.

And of course, no experiments can be built without a competent administrative team. Whenever I have any administrative tasks, I am confident that our administrative support (I hope I got the title right) Claire Legas got me. I would also like to thank our Storeroom Assistant Carlos Bustamante, and the Facilities Managers Anthony Vitan and Esperanza Munoz-Riddle for working closely with us throughout my PhD.

Finally, I would like to thank my family for their unconditional support. Seven years is a long commitment, and this journey wouldn’t have been possible without them.

Chapter 1

Introduction

When I joined the optical kagome lattice experiment in September 2019, we had an operational rubidium BEC machine. However, about half of this thesis will focus on the new ^{40}K Fermi gas setup, which is the culmination of efforts that span more than three years of my PhD. While there definitely are rich physics to study with bosons in kagome lattices [1, 2], we decided that the rich physics that will be enabled by loading fermions into kagome lattices is a rewarding pursuit to go after. In this chapter we provide an overview of the various research directions enabled by our endeavour.

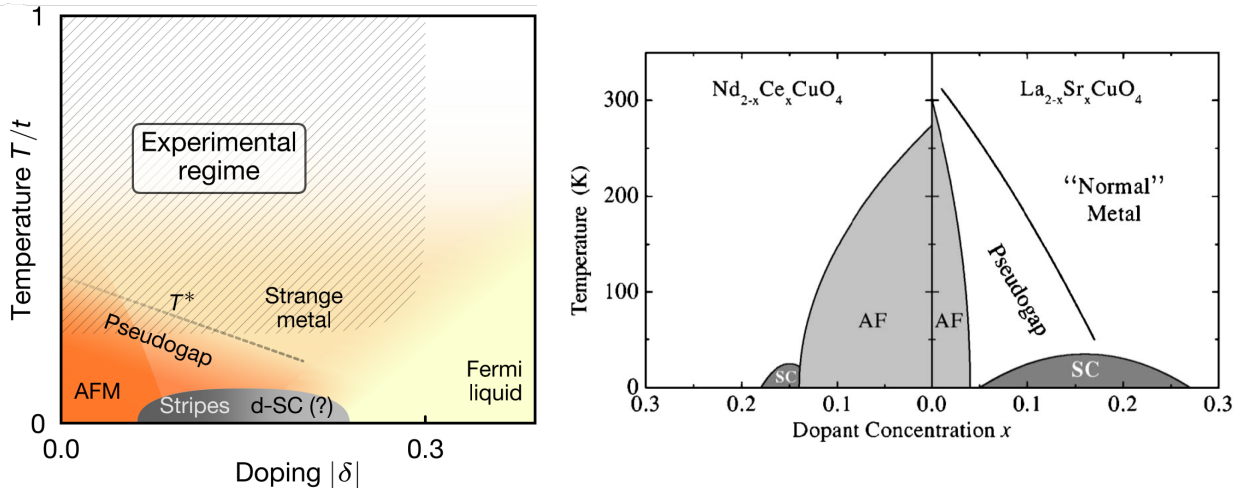


Figure 1.1: Left: one of the proposed phase diagram of the Fermi-Hubbard model on a square lattice at some intermediate ($U/t = 6.5$) repulsive interaction strength. Reproduced from Ref. [3]. Right: a similar proposed phase diagram for high- T_c superconductors. Reproduced from Ref. [4].

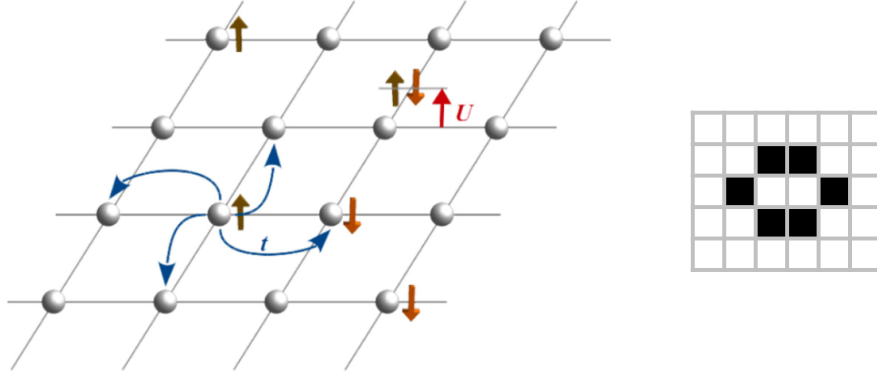


Figure 1.2: Left: an illustration of the Fermi-Hubbard model. Reproduced from Ref. [7]. Right: the *beehive*, a still life in *Conway's Game of Life*. Black (white) squares are live (dead) cells. Figure credit: wikipedia.

1.1 Quantum simulation using fermions

Quantum simulation, loosely speaking, is to use one physical system that behaves quantum mechanically to mimic another. The realization of degenerate Fermi gases in ultracold atom systems opens up the prospect to use them as a resource for quantum simulation of solid state systems, or more precisely, theoretical models that describe solid state systems [5, 6, 7]. In particular, fermions in optical lattices are well-described by the Fermi-Hubbard model (see Fig. 1.2), which is a deceptively simple model with only two ingredients: particles are allowed to hop to a neighboring site with a tunneling energy t if it is not already occupied by another particle of the same state, and there is an interaction energy U if a site is occupied by two particles.

Despite its simplicity, the Fermi-Hubbard model has received significant interest, as it is believed to give rise to strongly correlated phases, such as the high- T_c superconductivity [4]. Fig. 1.1 shows proposed phase diagrams of the doped square lattice with $U > 0$, which also show other correlated phases that emerge at low temperatures, such as the pseudogap phase and the antiferromagnetic phase. This is an example of emergent phenomena, where a system with a large number of constituents interacting under a simple set of rules exhibits complicated behaviors [8]. While the Fermi-Hubbard model of a square lattice at half-filling is relatively well understood (see e.g. [7] for a phase diagram in that case), there is still disagreement even on a qualitative level on the phase diagram as a function of doping [9], and still less is known about the phase diagram of frustrated lattices. As a result, there has been intense experimental [6, 7, 10] and theoretical [11, 12, 13] effort to understand the properties of the Fermi-Hubbard model.

Emergent phenomena are not unique to quantum systems. For example, the rules of *Conway's Game of Life* (see Fig. 1.2), which is a specific version of a two-dimensional cellular automaton, are very simple: the system evolves in discrete time steps. In each step,

a live cell stays live if two or three out of the eight neighbors are live, or otherwise turns into a dead cell. A dead cell turns into a live cell if three of the neighbors are live. These simple rules generate structures that are stationary (*still lives*), evolve with a finite periodicity (*oscillators*), or translate themselves indefinitely (*spaceships*). By arranging these structures in the right way, it can also be shown that the *Game of Life* is a universal Turing machine.

The quantum mechanical nature of our system of interest, however, poses a formidable challenge for classical computation. This can be seen by considering a system of, say, $N = 30$ particles, each of them can be in either the “0” state or “1” state. Let us consider the amount of resource required to record the state of the system. In a classical system, one only needs to keep track of the state of each particle individually, for example on a 5×6 grid similar to the *Conway’s Game of Life*. If N is doubled, the grid size required is also doubled. On the other hand, in the quantum mechanical case, since each of the particle can be in a superposition of the 0 and 1 state, there are in principle 2^{30} coefficients to keep track of, each of them a complex number. This grows exponentially to 2^{60} if N is doubled, and for a system of a few hundred particles, the state of the system already becomes intractable. (Things are worse if we consider density matrices.) As Feynman pointed out in his famous speech [14], if a system is described by quantum mechanics, attempts to mimic the behavior of this system should also be governed by quantum mechanics.

The classical simulation of fermionic systems faces additional challenges. The wave function of a multipartite fermionic state changes sign under the exchange of particles, which gives rise to the Pauli exclusion principle. To see how this is a problem, we look at an example of a state-of-the-art numerical simulation technique, the quantum Monte Carlo (QMC) algorithm. While the configuration space of quantum mechanical systems grow exponentially with the system size, as described above, QMC allows one to calculate thermodynamical quantities of interest with polynomially growing costs. QMC relies on mapping a quantum mechanical problem to a classical one, and averaging over results randomly sampled from the Boltzmann distribution [15]. The sign change from fermionic statistics proves to be troublesome, since it results in negative weights in the mapped system, and standard approaches adopted to work around the negative weights result in exponential growths of error. This is referred to as the “sign problem” [15, 16, 17], and is a strong motivation for the quantum simulation of fermionic systems.

On the other hand, fermions in the same internal state do not interact with each other under ultracold temperatures due to Pauli blockade (unless under special conditions, such as magnetically tuned p -wave Feshbach resonance [18]), and occupy all the available states up to the Fermi energy. Ultracold, noninteracting Fermi gas is therefore a useful tool for probing the single particle properties of the system [19, 20, 21, 22].

1.2 Geometry of the band structure

Before focusing on the specific lattice structure that our experiment is designed for, let us first discuss a fundamental concept for periodic systems, which is the band structure. As a

consequence of the Bloch's theorem, the energy spectrum of a periodic system is separated into different energy bands, and each band hosts a continuity of states parametrized by the quasimomentum. Given the Fermi energy and the band structure, solids are broadly categorized as band insulators and metal, with drastically different conductivity. They also determine the shape of the Fermi surface, which is the basis for many-body calculations. A material only absorbs (and emits) photons at frequencies corresponding to the band gap between a valence band and a conduction band. It can be said that the band structure provides the basis for understanding the electronic properties of a material.

In chapter 5 and 6 of this thesis, we will focus not on the energy of the bands, but the quantum geometry of Bloch states [23]. Geometry requires a concept of distance, which is defined by the metric of the space being studied. In a quantum mechanical system, this object is aptly called the quantum metric, defined as the real part of the quantum geometric tensor $\mathcal{B}$ [24]. The quantum metric measures the overlap of neighboring states, or the distance in *amplitude*. There is also an imaginary part to $\mathcal{B}$, which turns out to be the Berry curvature, and it can be understood as the distance in the *phase* of the wave functions [23]. It turned out that our works contribute to novel methods for measuring both components of the quantum geometry: the geometric probe experiment described in chapter 5 directly measures the quantum distance, the (intraband) *amplitude* overlap, while chapter 6 is concerned with the interband Berry connection, the (interband) *phase* distance.

In some sense, the topological properties of materials have attracted greater interests. The most prominent example is perhaps the Chern number, which underlies phenomena such as the quantum Hall effect [25, 26], topological insulators and the associated edge modes [27, 28], and quantized optical responses [29]. But in recent years, quantum geometrical measures, such as the quantum metric mentioned above, have found direct connection to physical observables, such as the bound for superfluid weight in flat band superconductivity [30, 31, 32, 33], and the emergence of anomalous Landau levels in singular flat bands [34]. We expect that the ability to characterize the quantum geometry of solid state systems will find increasing relevance in the future.

1.3 Kagome lattice

The expertise of our experiment is the capability to generate and stabilize a particular lattice geometry known as the kagome lattice, which is shown in Fig. 1.3. Immediately from the triangular motifs, one might already (correctly) guess that frustration plays an important role in the physics of kagome lattices. In this work, instead of following the typical narrative that introduces geometric frustration through stationary spins with antiferromagnetic interactions, we will focus on the kinetics of particles in the system.

Even without the interaction term in the Fermi-Hubbard model, the frustrated nature of the kagome lattice already makes it an interesting animal. One of the manifestation is the existence of compact localized states (CLS) (Sec. 3.4.3), which are eigenstates that only live on a finite number of sites. From Fig. 1.3, we see that the state cannot tunnel out,

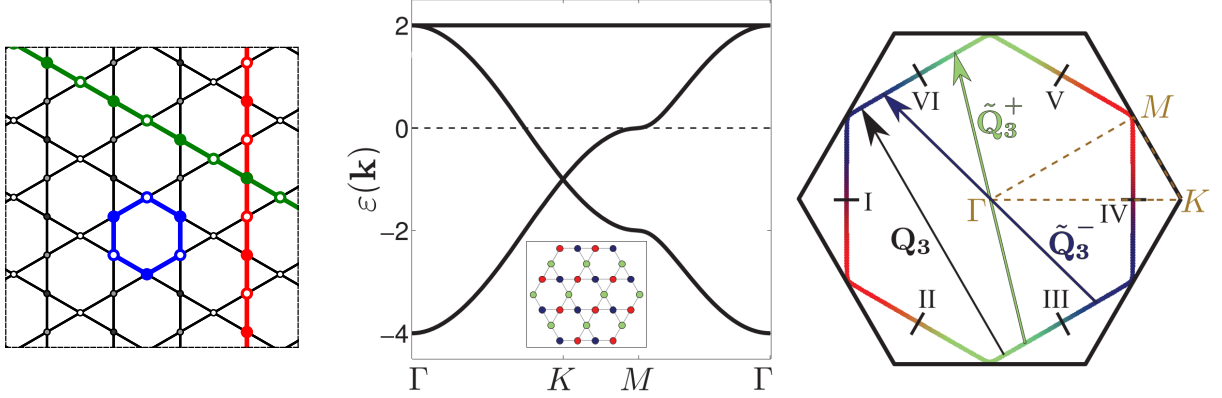


Figure 1.3: Left: a CLS (blue) and the two NLS (red and green) of the kagome lattice. The wave function of the state has opposite signs on the filled versus unfilled sites. Middle: the tight-binding band structure of the kagome lattice. The dashed line is at the van Hove point energy. Right: Fermi surface nesting at van Hove filling. The color of the same-energy contour reflects the wave function amplitude on each sublattice sites, following the color coding in the middle figure. $\mathbf{Q}_3$ is one of the three nesting vector that one would guess based on the constant energy contour. Due to the variation in the sublattice amplitudes, the on-site interaction is instead enhanced at $\tilde{\mathbf{Q}}_3^\pm$ in the momentum space. Middle and right figures are reproduced from Ref. [35].

since the tunneling amplitudes from two sites with opposite phases cancel each other. For a kagome lattice with $3N$ sites, there are N hexagons, each of them hosting a CLS. Together, they *almost* form a basis for the flat band of the kagome lattice. Since every hexagon looks the same in the kagome lattice, every CLS has the same energy. We said *almost*, because a CLS can actually be formed by the linear superposition of all the others, so we are one state short from forming a basis. This is complemented by two noncontractible loop states (NLS) that extend over the whole system. But now we have one state too many — this is why there must be a band touching point with a neighboring band [36]. Systems filled to flat bands have attracted considerable attention, since the kinetic energy no longer plays a role in determining the ground state of the system. This makes the kagome lattice a promising platform for studying strongly correlated phases, such as the flat band ferromagnetism [37, 38, 39], and flat band superconductivity that was formerly mentioned.

Beside from the (quadratic) touching point and the flat band, there are other features of interest in the band structure of the kagome lattice, shown in Fig. 1.3. Similar to the honeycomb lattice, the two dispersive bands host Dirac points at two nonequivalent quasi-momenta, and two van Hove points in each band, which are energy saddle points with a logarithmically divergent density of states. Looking more closely at the states themselves, we find that even though the dispersion relation of the lower two bands look exactly the same as the honeycomb lattice, the wave function amplitudes vary in a different way [35] — the two lattices have different quantum geometry. This difference leads to unconventional

instabilities and a rich phase diagram when the Fermi energy of a kagome lattice is at the van Hove filling [35, 40, 41, 42].

As we get excited at the strongly correlated physics that lies ahead, we would like to point out a substantial challenge for fermionic quantum simulators. From the phase diagram shown in Fig. 1.1, we see that correlated phases of interest happen at very low temperatures of $T/t \sim 0.1$. While the phase diagrams of the kagome lattice would look very different, we expect that the system needs to similarly be prepared at very low temperatures for strong correlations to emerge. To this end, we borrow intuition from recent breakthroughs in entropy redistribution techniques [43, 44], and ask if the flat band can be used as an entropy reservoir.

At first sight, this seems like a weird proposal, because one of our main goal is to study correlated physics when particles are loaded *into* the flat band, so we should be thinking about how to cool the flat band itself. But as we have pointed out for the case of van Hove filling, there are filling factors within the dispersive bands that are also highly nontrivial. It has also been predicted that systems filled to either the linear or quadratic band touchings demonstrate instabilities towards interesting correlated phases, such as topological insulating states [45, 46, 47] and the fractionalization of charges [48].

1.4 The optical kagome lattice experiment

The previous generation of the kagome lattice experiment only cooled Rb, which means that we only had access to bosons. Trapping and loading a fermionic isotope into the kagome lattice has been a long standing goal in our group, as motivated in previous sections. However, cooling neutral atoms to quantum degeneracy is typically more involved for fermions than for bosons, since the Pauli exclusion principle prevents efficient evaporative cooling in a gas of spin-polarized fermions. In the new apparatus described in this thesis, our fermion of choice is ^{40}K , and we cool and trap Rb atoms alongside with ^{40}K . The Rb atoms are mainly used as a coolant for ^{40}K atoms during evaporative cooling, an approach also known as sympathetic cooling. (Refer to the introduction of chapter 4 for more discussions.)

Fig. 1.4 provides an overview of the layout of the optical lattice experiment. Around every minute, a quantum degenerate cloud of atoms is produced in isolation to the external environment under ultrahigh vacuum. The atoms are trapped by two tightly focused laser beams, known as optical dipole traps, that propagate along the direction labeled B1 and B3 in Fig. 1.4. The dipole traps provide confinement in all directions, and support the atoms against the gravitational pull. The optically trapped atoms are then loaded into the optical lattice formed by three laser beams. Each of the lattice beams contains outputs from two lasers, with commensurate wavelengths at 532 nm and 1064 nm. By adjusting the intensity of each beam and the relative phase between each pair of beams, we have flexible and dynamical control over the geometry of the lattice.

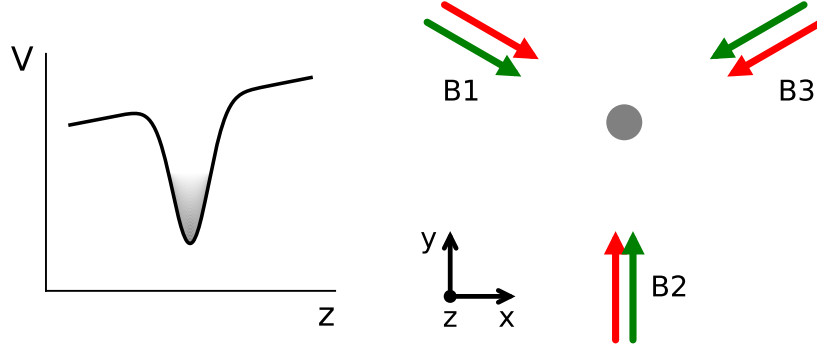


Figure 1.4: Left: trapping potential of the optical dipole trap along the direction of gravity. Right: the layout of the optical lattice beams. Green (red) arrows represent $\lambda = 532$ (1064) nm lattice beams.

1.5 Outline of this thesis

Chapter 2 describes the details of the optical kagome lattice machine. Since the design and construction of the new potassium machine is mainly a collective effort with Malte Schwarz, this thesis will document the parts of the experiment that I have personally contributed more effort to.

Chapter 3 briefly reviews the theoretical background necessary for understanding the results presented in the following chapters. As the basic diagnosis tool for the cold atoms, we summarize the relation between important thermodynamical quantities and experimentally measured density distribution for Bose and Fermi gases. We review two different approaches for calculating the band structure: solving the Schrödinger equation using plane wave expansion provides quantitatively accurate results, while the tight-binding model provides intuitive picture of the Bloch states.

Chapter 4 provides a description of a typical experiment sequence, and the typical parameters achieved in daily experiments at the time of writing. As every experiment apparatus is different, I include personal experience and understanding of the experiment where I believe is helpful.

Chapter 5 begins with a theoretical background for the experiment published in Ref. [49], which measures the quantum distance around singular touching points. This section provides details on the implementation of the experiment protocol that complements the published results. We highlight the importance of quasimomentum resolution for experiments that characterizes the quantum geometry of a system, which is an important feature in our measurement scheme that enabled the characterization of the quadratic band touching point.

Chapter 6 is a partial account of the most recent work from the experiment, and the first work done with fermions. I aim to establish the relation between optical excitation and interband quantum geometry, and show that optical lattices are versatile platforms

for the quantum simulation of optical excitations. I will describe our observations of the quasimomentum-dependent optical selection rules as a demonstration of the formalism presented in this chapter, and refer the reader to Ref. [50] for details on the measurement of the full interband Berry connection.

Chapter 7 is a theoretical work based on the idea of entropy redistribution. We ask: can the flat band be used as a resource for cooling? We show that, under the assumption that the system thermalizes isentropically, the answer is affirmative in the presence of weak interaction in a finite size system. We discuss possible implementations and challenges to realizing this cooling effect, and point out outstanding questions for further theory investigation.

Chapter 8 concludes this thesis and gives a list of planned experiment upgrades to be implemented by future generations. We briefly discuss the new possibilities enabled by the experiment upgrades, as well as extensions of the work described in this thesis.

Chapter 2

Experimental apparatus

We will first briefly review the working principle of the previous setup, which is helpful for understanding what changes were necessary in order for us to cool ^{40}K . For a complete description of the experiment sequence performed in the previous machine, see Ref. [51, 52, 53].

- Rb 3D magneto-optical traps (MOT) were loaded from a Zeeman slower for 14 s to 30 s;
- The Rb atoms in the MOT were then loaded into a magnetic trap, and transferred to an uncoated rectangular glass cell using magnetic transfer;
- A microwave sweep was applied to selectively evaporate the hottest atoms away from the magnetic trap;
- The atoms were then transferred into a crossed dipole trap, where we performed forced optical evaporation to get Rb Bose-Einstein condensates;
- The condensate is loaded into intensity- and phase-stabilized optical lattices.

As mentioned in the introduction, we decided to sympathetically cool ^{40}K using Rb during evaporative cooling. This means that the new machine should still be able to cool Rb to degeneracy, while at the same time also cool ^{40}K atoms. We decided to follow the same overall cooling scheme as before to reduce design overhead. Still, this required a major reconstruction. Most importantly, a new set of MOT infrastructure (an atom flux that loads the 3D MOT, a new atom source, and near-resonant lasers) are required for ^{40}K .

We chose to use a 2D MOT for ^{40}K instead of a Zeeman slower mainly because of the high cost of ^{40}K -enriched potassium sources. Zeeman slowers typically burn through a few grams of alkali metal every year, while 50 mg of 3.15% ^{40}K -enriched sample (in the form of KCl salt) is a few thousand dollars. It was in principle possible to valve off the Zeeman slower region using the gate valves in the old setup, and only replace the Zeeman slower, which can be a tricky process. Instead, we decided to take this opportunity to perform more

vacuum system upgrades. In particular, we replaced the uncoated rectangular glass cell with a compact hexagonal glass cell with nano-textured anti-reflection coating. Since Rb and K experience similar optical potentials for the optical trapping beams and the lattice beams that we had been using in the previous setup (see Sec. 3.1.2), we did not have to modify the lattice optics design.

To summarize, the main changes include:

- A new ultrahigh vacuum system
- A new set of coils that are compatible with the new vacuum system
- Redesigns for the Rb cooling lasers to create a Rb 2D MOT
- A new set of cooling lasers for potassium
- A new plug laser to prevent Majorana losses during sympathetic cooling
- A new experiment control system, ARTIQ

The design and construction of the apparatus are detailed in the following sections.

2.1 Lasers

In this section we provide an overview of the lasers used for cooling, trapping, and creating optical lattices. Some setups, such as the potassium cooling lasers and the plug laser, are new additions to the kagome experiment, and will be described in detail. The high power lasers used for optical potentials are largely the same as the previous rubidium machine, and we will only focus on modifications to the setup. More detailed descriptions of the 1064 nm and 532 nm setup can be found in Ref. [51, 52, 53].

2.1.1 Rb D2 lasers

Since we have replaced the Zeeman slower with a 2D MOT, the required detunings of the $F = 2 \rightarrow F' = 3$ (cooling) and $F = 1 \rightarrow F' = 2$ (repump) transition are different (closer to atomic resonance). The 2D MOT also requires much more power to operate. This is achieved by adding a tapered amplifier specifically for the 2D MOT. Otherwise, the rubidium setup is conceptually the same as the previous generation, with modifications made to make the setup more modular and easier to realign.

A simplified layout of the $F = 2 \rightarrow F'$ setup is given in Fig. 2.1. Compared to the previous setup, the main changes are

- Instead of first combining the cooling and repump light with orthogonal polarizations on a polarizing beam splitter (PBS) before sending light through a polarization-maintaining (PM) fiber, we couple all the frequencies individually into their own fibers and combine light on the science table (see Fig. 2.15).

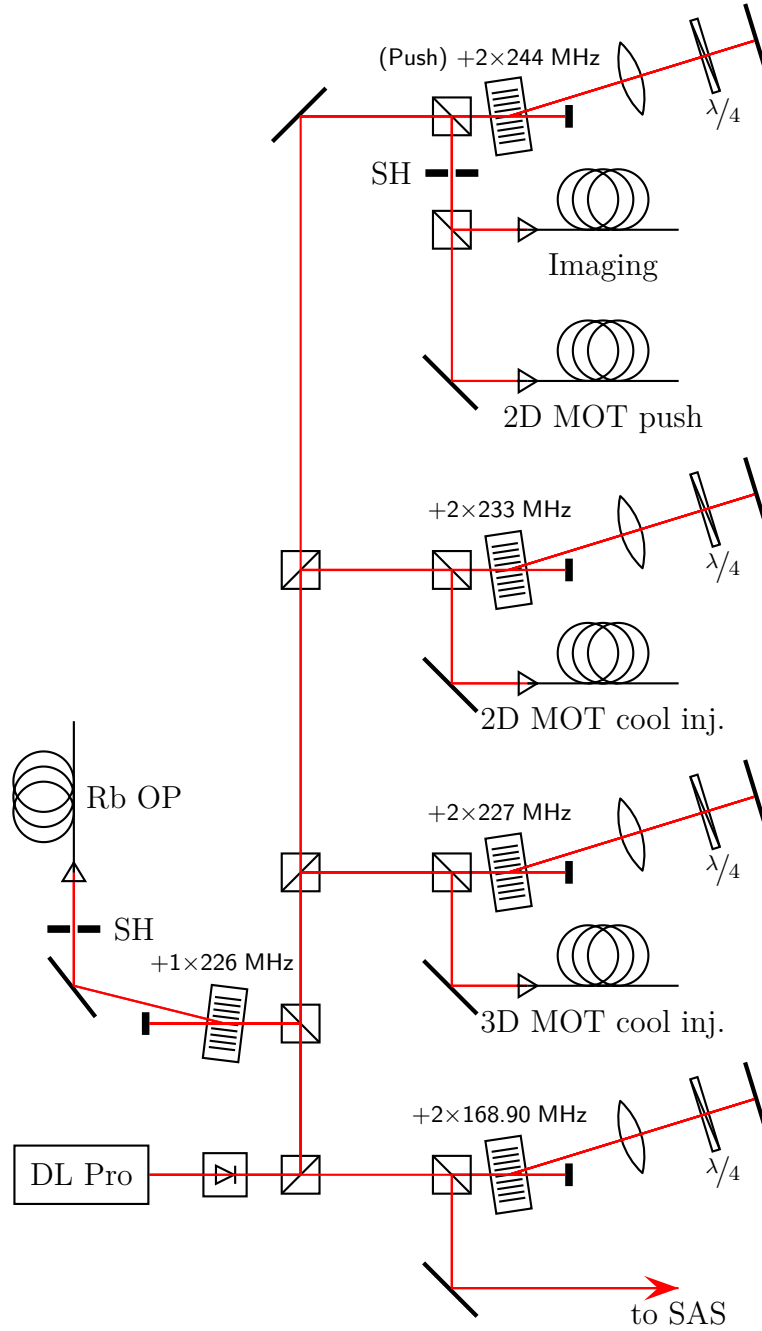


Figure 2.1: Simplified layout of Rb D2 optics. Half-wave plates used to change power distribution before each PBS are not plotted. SH: shutter.

- The imaging beam and the new 2D MOT push beam shares an AOM, since they are never used at the same time. It would be more ideal to have separate shutters for the two beams, but this is not currently implemented due to spatial constraints on the optical table.
- We added a new $F = 2 \rightarrow F' = 2$ optical pumping (OP) beam to pump Rb atoms to the $|2, 2\rangle$ state before turning on the magnetic trap (see Sec. 4.1.2). The previous experiment worked with a BEC in the $|1, -1\rangle$ state, and beside from turning off the repump beam to pump atoms into the $F = 1$ manifold, no additional effort was made to pump the m_F state of atoms.

The layout for the $F = 1 \rightarrow F' = 2$ (repump) setup is essentially the same as before, except that now a single AOM is shared between 2D MOT, 3D MOT, and imaging repump. I will hence omit the layout in this thesis.

Tapered amplifiers

Currently, both Rb 2D MOT and 3D MOT light are amplified with tapered amplifier (TA) chips mounted on home-built mounts. The 3D MOT mount has been in use since the beginning of the group, and while it is very efficient (providing more than 16 dB of gain at an injection current of only 1100 mA), it also drifts the most from day to day, likely due to its poor thermal management design. We have to redo the fiber coupling of the output of this mount every two to three days. The 2D MOT mount is designed by Malte Schwarz, and its alignment is much more stable, requiring realignment only roughly monthly.

We decided to first frequency shift the seed light for the TAs using acousto-optical modulators (AOMs) before amplifying the light with TAs. This is good for optical power, since a double pass AOM setup typically has an efficiency of 60~70%. The downside is that we no longer have the ability to change the intensity after the TA. The speed with which we can turn off the MOT beams is also limited by the mechanical shutters, which is around 2 ms. So far these limitations have not caused serious trouble, although one might benefit from changing 3D MOT cooling power during compressed MOT.

Injection lock module

In our lab, we have historically used injection locks to get the optical power required to seed TAs. They also have the benefit that when the injection light is accidentally turned off, the seed light is not lost, thereby preventing possible thermal damage to the TA chips. When properly set up, the seed frequency can be scanned by several GHz while maintaining the lock.

When we rebuilt part of the rubidium setup to install the 2D MOT TA, we have decided to isolate the injection lock setup into a fully fiber-coupled module, see Fig. 2.2. The benefit for doing so include the following:

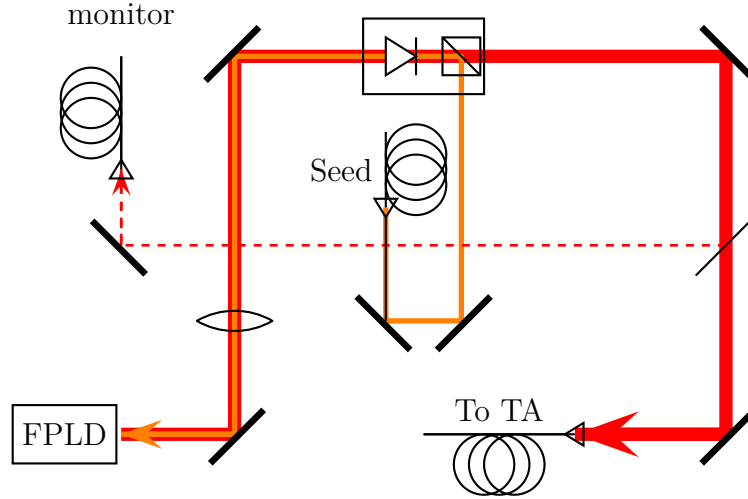


Figure 2.2: The complete layout of the Rb injection lock module. The seed light is injected through the front PBS housed in the isolator. The monitor pickoff is sent to a Fabry-Perot cavity (Toptica, FPI100). FPLD: Fabry-Perot laser diode.

- No need to recouple the seed light for free space TAs after replacement, since the input mode is completely defined by the fiber coupler.
- Easier to switch between different setups if we ever build new ones. One can imagine having a second backup setup handy if the laser diode currently in use fails. To provide a perspective, the lifetime of a laser diode is on the order of 20,000 hours, or roughly 28 months. With N laser diodes in the lab, one laser diode is expected to fail every $28/N$ months. In our case $N = 7$ (not counting the TAs).
- Option to spatially separate different modules. This allows one to keep the most important and sensitive setup on optical tables, which is vibrationally damped, while moving less important modules to racks. This is particularly important for our lab, which is rather limited in space.

Obvious drawbacks include the loss of optical power at fiber coupling, sensitivity to polarization drifts, and susceptibility to back reflections, which tends to provide optical feedback to the light source and destabilize the output. We have found that the isolator that we typically use for the laser diodes (such as IO-3-780-HP¹ from Thorlabs with around 35 dB isolation) is enough to prevent noticeable negative effects in our experiments, while the temperature

¹A low power variant of isolator with the rejected port accessible for injection locking is no longer available from Thorlabs.

stability in the lab is good enough so that we are not strongly affected by the polarization drifts.

We have found that QLD-780-80S from QPhotonics work pretty well for our setup, requiring only occasionally adjusting the injection current by around 1 mA to stay in lock. However, since the rubidium lasers are still in general less stable than the potassium lasers due to the injection locks occasionally failing, we plan to replace most of the setup described here with a fiber coupled DL Pro and BoosTA in the future.

2.1.2 K D2 lasers

The relevant transitions are labeled in Fig. 2.3. Similar to Rb, the D2 transition is used to trap and image K atoms. We also use the D1 transition for optical pumping, see Sec. 2.1.3. The SAS spectroscopy locks the lasers to the crossover features labeled as “xover” in the plot. As usual, one uses the transitions between the stretched states in the maximal F manifold to get cycling transitions for cooling, while the optical pumping transitions are chosen such that the desired states are dark states.

Design considerations

The potassium laser setup is designed so that we can easily switch between ^{39}K and ^{40}K . This requires changing the frequencies of both the cooling and repump beams by around 800 MHz [54]. While it is possible to achieve this detuning using different diffraction orders of an AOM (which is used in the Cambridge kagome lattice experiment [55]), we decided to look for an electronics solution to simplify the optics setup. This is the guiding principle for the design of the K D2 seed laser system (Fig. 2.5), which closely follows the initial plan of our previous graduate student, Tsz-Him Leung. Fig. 2.4 summarizes the detunings required in our design to bridge the gap between the crossover feature that we lock to and the resonant frequencies of the relevant transitions.

Offset locking requires that the lasers being locked emit in a single spectral mode. Since the linewidth of the cooling laser is not too important for us, we decided to use distributed Bragg reflector (DBR) laser diodes from Photodigm, instead of the more expensive and bulky ECDLs such as DL Pro. They are easy to operate and output up to 80 mW of optical power, which is more than enough for seeding a TA. However, they are very sensitive to back reflections, and we need to use at least one tandem isolator to prevent optical feedback. In one case we even had to add another isolator after the tandem isolator. They also require sub-mK temperature stability. In our experience, each 767 nm laser diode survives for 1.5~2 years, although the 780 nm laser diode for Rb repump has been running for more than seven years.

Also, during the compressed MOT stage, one needs to decrease the power in the repump beam within 1 ms, which requires the 3D MOT repump beam to be controlled by an AOM.

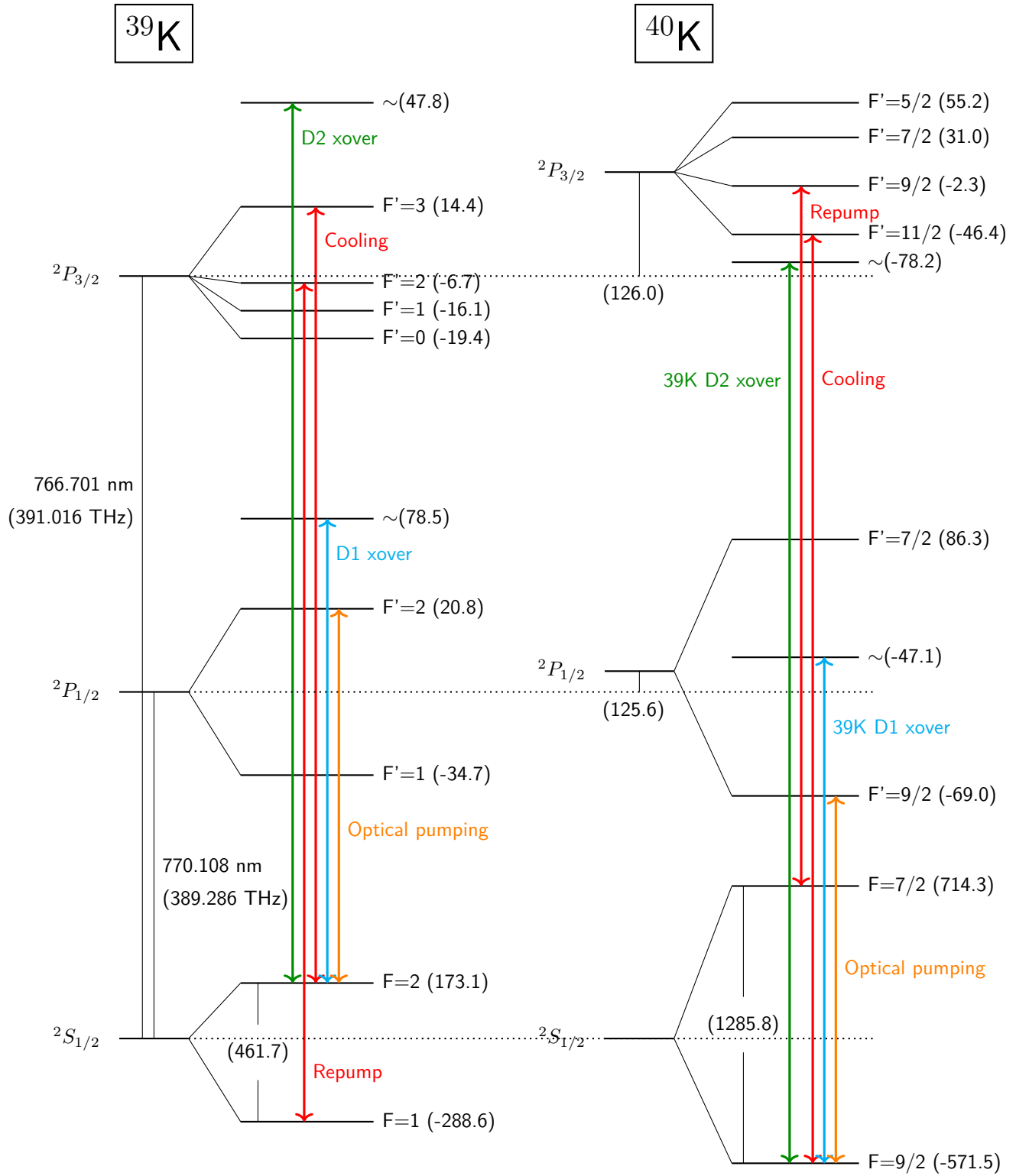


Figure 2.3: The atomic level structures of ^{39}K and ^{40}K and relevant transitions for laser cooling. All numbers without units are in MHz. Level spacings are not to scale.

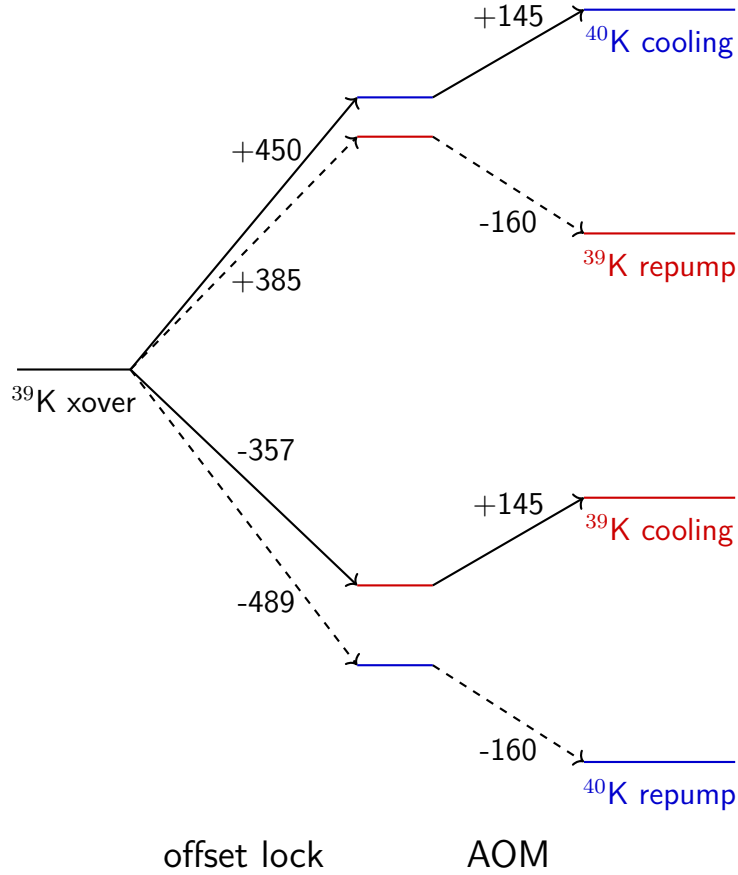


Figure 2.4: Required detunings at each step from the crossover feature for relevant transitions in MHz. Actual values might differ slightly depending on MOT optimization. Solid (dashed) arrows represent detunings on the cooling (repump) side. Refer to Fig. 2.3 for the actual transitions used.

Saturation absorption spectroscopy (SAS)

Due to the low natural abundance of ^{40}K , the signal we see is dominated by the absorption of ^{39}K . Similar to the rubidium setup, the error signal is obtained with a frequency modulation spectroscopy setup, in which the light that enters the K reference cell is modulated by an EOM and then back-reflected.

Offset locks

The offset lock design is based on Ref. [56]. A simplified optics setup is shown in Fig. 2.5, where two beams with the same polarization are combined on a non-polarizing beam splitter (NPBS). Consider a reference beam at frequency f_r overlapped with a control beam detuned from the reference by δ . In our case, f_r is stabilized by SAS described in the last section. The

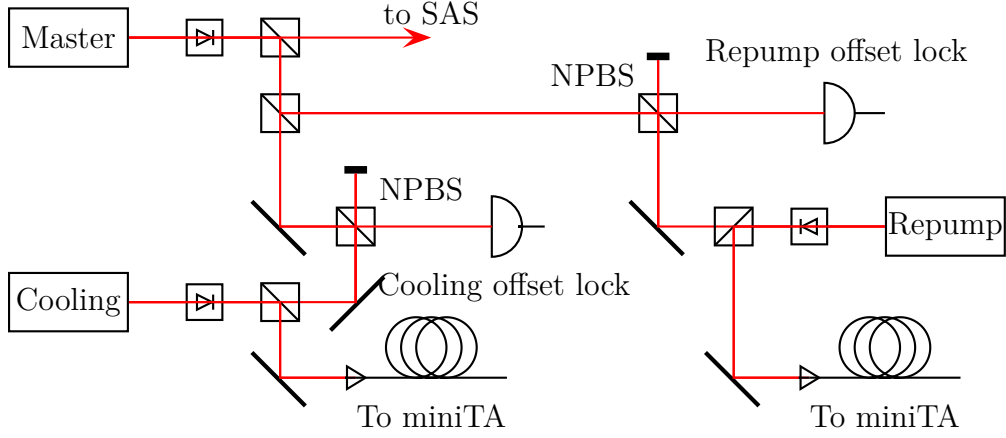


Figure 2.5: Simplified layout for the K D2 seed lasers optics. NPBS: non-polarizing beam splitter. Unlabeled cubes are PBS's.

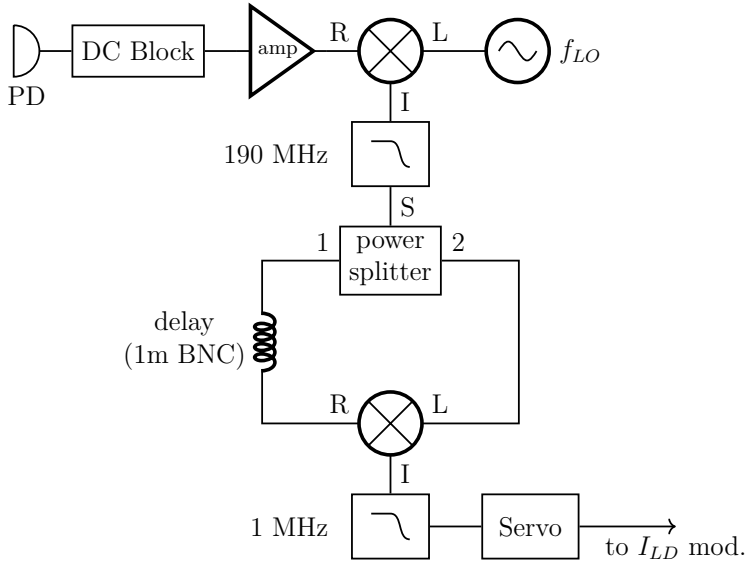


Figure 2.6: Left: simplified electronics setup for the offset locks. Right: (Blue) error signal for the repump laser. (Yellow) sweep signal for current modulation, which generates a linear frequency scan. Right hand side corresponds to larger frequency. The green and red circles are lock points for ^{40}K and ^{39}K , respectively. The yellow arrows label where the detuning between the reference and control beams is the same as f_{LO} . For all the lasers in our lab, the sign of the servo gain is set such that we always lock to upward slopes as shown on oscilloscopes.

beat note between the two beams oscillates at frequency $|\delta|$, which we detect on a photodiode (PD).

We stabilize $|\delta|$ using the circuit shown in Fig. 2.6. The beat note is detected on a photodiode and mixed with a local oscillator (LO) at frequency f_{LO} . The lower frequency part of the signal at frequency $|f_{LO} - |\delta||$ is split in two ways, with a $L = 1$ m delay line in one of the path. The delay line converts the frequency of the beat note to a phase, which can be detected using a phase detector. The resulting signal for the repump laser is shown in Fig. 2.6. Since the signal is proportional to $\cos(2\pi |f_{LO} - |\delta|| L/c_L)$, where $c_L = 2 \cdot 10^8$ m/s is the propagation velocity in a RG-58 cable, the zero crossings are actually at $|\delta| = f_{LO} \pm (2m - 1)c_L/4L$ ($m \in \mathbb{N}$) with alternating slopes. In our setup, this gives

$$\delta = \begin{cases} \text{(left)} & -f_{LO} \pm (2m - 1) \cdot 50 \text{ MHz}, \\ \text{(right)} & f_{LO} \pm (2m - 1) \cdot 50 \text{ MHz}, \end{cases}$$

where left and right refers to the position of the two “lobes” of the error signal as they are displayed in Fig. 2.6. The sign of $\pm$ is determined by the sign of the servo gain (+ for cooling, $-$ for repump). The envelope of the lobes are limited by the bandwidth of the phase detector.

Small changes in frequency can be done by changing f_{LO} , which is occasionally useful for optimizing MOT cooling or repump frequencies. Locking to the opposite lobe jumps the frequency by around $2f_{LO}$, and by choosing a voltage-controlled oscillator (VCO) or direct digital synthesis (DDS) frequency generator that operates in the range 350 to 450 MHz, we can easily switch between ^{39}K and ^{40}K by locking to different lobes. Note that all the beams derived from the control beam are shifted at the same time when one changes f_{LO} , so for individual frequency scans we prefer to use AOMs.

Power distribution

More repump optical power is required to make a MOT of ^{39}K compared to that of Rb, which is the main design consideration of the power distribution scheme. This is due to the narrow hyperfine structure in the $^2\text{P}_{3/2}$ states. Since the polarization in an actual 3D MOT is never completely circularly polarized, the $F = 2 \rightarrow F' = 2$ transition is also strongly driven by the cooling beam, and atoms quickly falls into the $F = 1$ manifold. This means that what is conventionally considered the repump beam, which drives the $F = 1 \rightarrow F' = 2$ transition, now contributes significantly to the trapping forces. Empirically, the experiment at JILA has operated with as much repump power as cooling in their 3D MOT [57]. Therefore, we decided to also use TAs to amplify the repump laser.

We note that while ^{40}K is famous for the inverted hyperfine structure, and the hyperfine structure is also not very broad, the inversion is actually good for avoiding driving the unwanted transition, since a red detuned cooling beam is farther detuned from the unwanted $F = 9/2 \rightarrow F' = 9/2$ transition. ^{40}K is therefore similar to Rb in terms of making a MOT, and the repump beam does not participate appreciably in trapping. We do however seem to observe a small dependence on the loading speed as we vary the 2D MOT repump detuning.

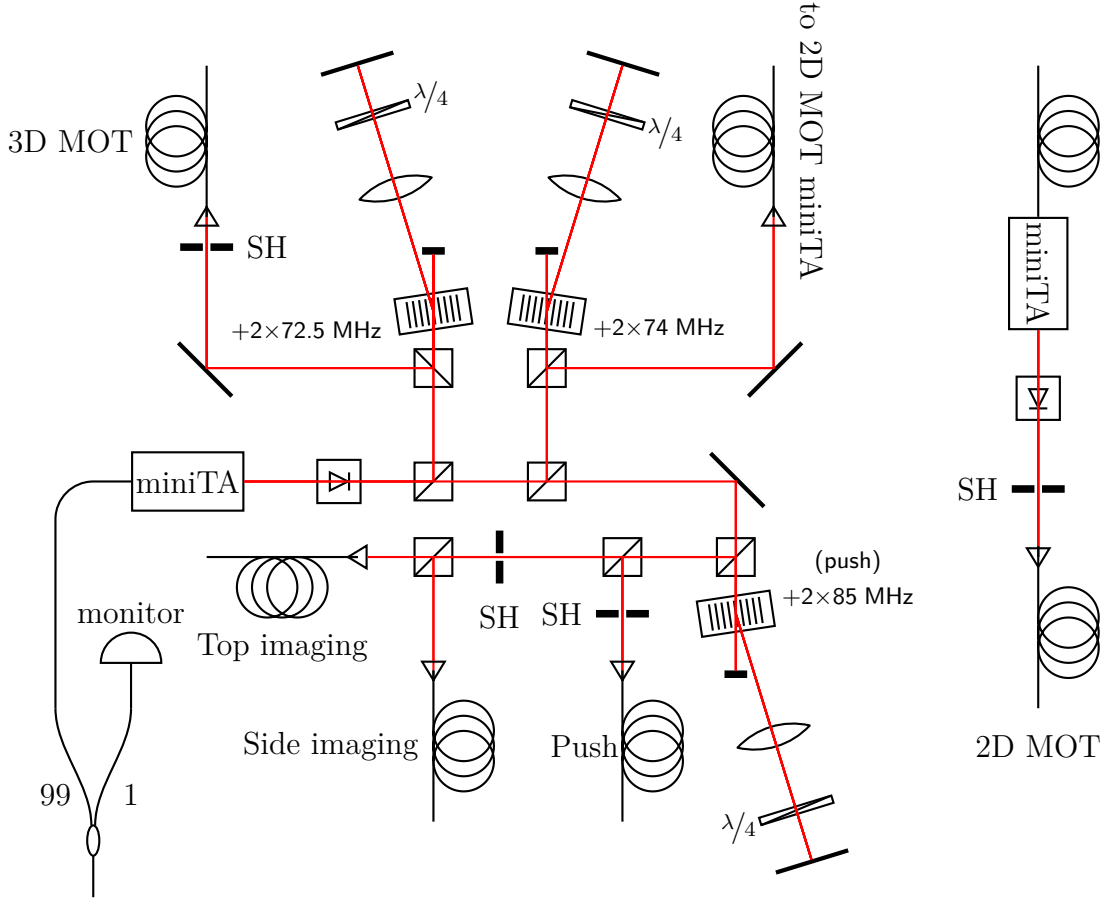


Figure 2.7: Simplified layout for K D2 cooling light power distribution. The repump light setup is similar.

As opposed to the Rb setup, in our K laser system, the seed light from the DBR is first amplified by a miniTA before frequency shifting with AOMs. This decision is mainly a historical one, when we initially thought that we didn't need separate TAs for the 2D MOT, and the free space TAs we were using required at least 20 mW to saturate. The 2D MOT miniTAs are then added in a way that minimally disturbed the original setup, and when we decided to replace the free space TAs with miniTAs we did not modify the power distribution scheme. Experimentally, we have found that the ^{40}K 3D MOT is optimized at an intermediate power (in contrast to Rb, which only loads more and more atoms as the 3D MOT power is increased), which is possibly due to light-assisted inelastic collisional losses [58]. So far this design has been working well for us, but it is possible that we might need more 3D MOT cooling power when we implement a dark spot MOT for ^{40}K or when we decide to work with ^{39}K .

We have been very satisfied by the performance of miniTAs (Eagleyard, EYP-TPA-0765-01500-3006-BTU02-0000). They are installed in Eagleyard evaluation boards (model number

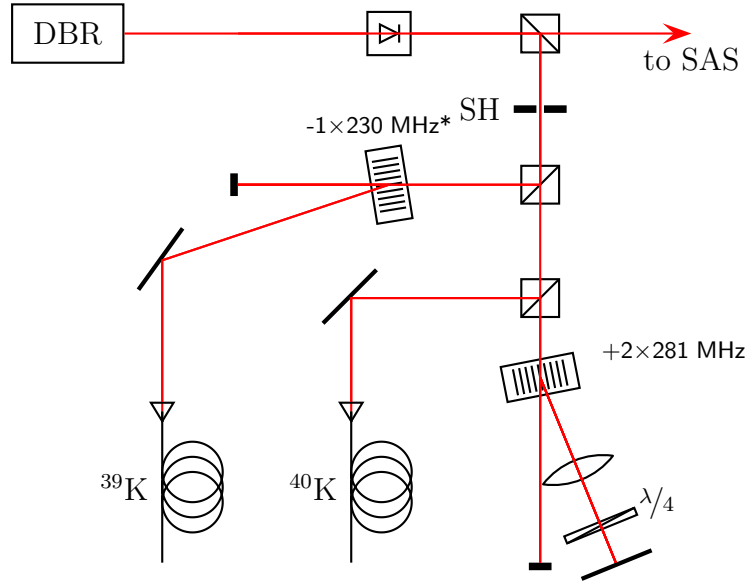


Figure 2.8: Simplified K D1 optics layout. *: expected frequency (we have not attempted to transfer ^{39}K into magnetic traps).

9001), and mounted on water cooling plates. Temperature of the chip is usually stabilized within a few seconds after turning on the injection current, so misalignment due to slow thermal drifts is not longer a problem. The output from miniTA is more Gaussian compared to free space TAs, which allows us to reach 50~60% fiber coupling efficiency. The input is saturated at less than 10 mW of power. Currently we have five miniTAs in the lab, the two oldest ones having been operating for about 18 months, and have shown no signs of degradation. But in case we need to replace them, the fiber coupled input and beam path defined by evaluation boards mean that the replacement can be done very quickly.

2.1.3 K D1 laser

Currently we only use the 770 nm laser for optical pumping before transferring atoms into the magnetic trap in the MOT chamber. Since each atom only needs to scatter at most a few photons before being pumped to the dark state, we don't need a lot of power in this beam. The setup is similar to the master laser of the other setups, where a small fraction of the output power is used for spectroscopy, and the rest of the power is frequency shifted and then fiber coupled to the science table. The modulation required for the SAS is directly applied to the injection current of the DBR diode, similar to our Rb repump setup.

We have considered adding gray molasses cooling on the D1 transition before transferring into the magnetic trap, and this is the original reason why we bought the 770 nm laser. We

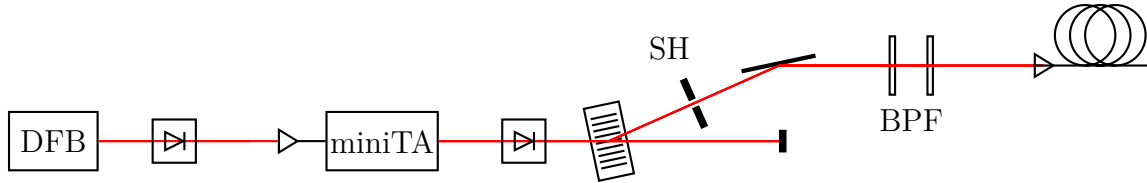


Figure 2.9: Simplified 760 nm plug optics layout. BPF: bandpass filters.

have never actually tried this, since the current sequence without a sub-Doppler cooling stage works reasonably well, and we don't yet have a good way to combine the 770 nm light with the MOT beams. Besides from the difficulty of combining one more beam in the switch yard, one also must remember that the dual-wavelength wave plates used to distribute power between different MOT beams are by design multi-order, and is not at a conventional phase retardance for 770 nm². The power balance of the gray molasses setup is therefore expected to be very imbalanced.

2.1.4 Plug laser

This is perhaps the simplest laser setup in our lab, since it doesn't need frequency stabilization. The seed light from a distributed feedback (DFB) laser (Eagleyard, EYP-DFB-0760-00040-1500-BFW01-0005) is amplified by a 765 nm miniTA and then sent to the science table. The AOM is used solely as a switch, so that we can slowly ramp off the plug potential when loading into the crossed dipole trap.

The 760 nm light is several THz detuned from the D1 and D2 transitions of both Rb and K, and frequency fluctuations on the order of tens of GHz is negligible. We however do want a single mode emitter to ensure that the output spectrum contains no near-resonance component. Since a single absorption is enough to pump an atom into an anti-trapped state, we cannot tolerate any resonant light. It was found that two 760 nm bandpass filters (Thorlabs, FBH760-10) are required to suppress the near-resonant light from the spontaneous emission of the miniTA to a tolerable level (i.e. similar lifetime with and without the plug beam at initial stages of evaporation cooling). We have attempted to use the 532 nm lattice laser as the plug beam, but the plug is not strong enough at the maximum power we tried (2 W) due to the much larger detuning.

We note that 760 nm is somewhat close to the D2 line of potassium, so the plug potential is around three times stronger for K than for Rb, meaning that K atoms are pushed farther

²To elaborate, these wave plates are based on a birefringent material with different birefringence at the two specified wavelengths, in our case 767 nm and 780 nm. Since the difference in the birefringence at the two wavelengths is small, the wave plate must be thick enough to accumulate enough difference in the phase retardance at the two wavelengths to reach the desired specification. For other wavelengths, the birefringence is different still from that of 767 nm and 780 nm, and the resulting phase retardance can be very different. For example, our 767 nm half wave plate / 780 nm full wave plate provides a phase retardance of 28.38 waves at 770 nm.

away by the plug beam. This is good for protecting K atoms from Majorana losses, but bad for thermalization. The position of the minima of the combined trap potential differ by around $10\text{ }\mu\text{m}$ between the two species, which proved to not be a problem for us.

2.1.5 1064 nm fiber amplifier

This is the only part of the lattice laser setup that is modified. In the past we used to use a Nufern fiber amplifier, which has a track record of failing regularly [51], is noisy [59], and the company that manufactures them is out of business. Our last Nufern served us for roughly five years of operation (with around two years of inactivity), a surprisingly long period, but in its last months the output started to randomly turn off intermittently for a few seconds every minute, before it completely failed.

The fiber amplifier is now replaced by a fiber amplifier from Azurlight (ALS-IR-1064-50-A-SF). We followed the same beam path as Nufern to minimize interruption to the experiment. The Azurlight is now continuously running (as opposed to Nufern, which we turned off everyday in hope to extend its lifespan) and requires no additional care.

2.2 Vacuum chamber

In this section, I will only include a brief overview of the final hardware of the vacuum chamber. Since I am mostly involved in the construction of the vacuum chamber, I will focus on the major incidents that resulted in long delays, and what could have been done to avoid these delays in future designs. An account of the vacuum system design considerations can be found in Malte Schwarz’s thesis [50].

I recommend starting with *Building Scientific Apparatus* [60] to learn about the basics of vacuum systems. Good tutorials are also available from major vacuum component companies, such as Pfeiffer or Lesker.

2.2.1 Overview

The construction begins with meticulously cleaning the vacuum parts. We follow the empirically tested procedure by Ryan Olf. Each of the part is first cleaned with dish soap if it is oily to the touch. Then, using an ultrasonic bath, the parts are cleaned in the following order, with 30 minutes each cycle:alconox $\rightarrow$ tap water (heavy rinsing) $\rightarrow$ deionized water $\rightarrow$ (deionized water again, until there is no bubble at all) $\rightarrow$ methanol $\rightarrow$ acetone. We found that copper gaskets cleaned using this procedure don’t form a air-tight seal, so all the gaskets are only wiped with methanol right before use.

The parts that can withstand high temperatures (namely, the stainless steel parts, except for the all-metal valves) are baked at $500\text{ }^{\circ}\text{C}$ for 38 hours after vacuum cleaning and before assembling the vacuum chamber. This is commonly referred to as hydrogen bake or prebake, as the goal of this bake is to remove the hydrogen that is dissolved in stainless steel. Following



Figure 2.10: Left: parts after a successful hydrogen bake at the chemistry glassblowing shop. Right: parts destroyed in another hydrogen bake attempt.

the observation in [61], we bake the parts in atmospheric condition. The bake is done at the glassblowing shop in the chemistry department over weekend, see Fig. 2.10. A few observations from the hydrogen bake:

- Rotatable flanges can stick to the parts after the bake, presumably due to oxidation layers formed at the contact. In some cases but not always, they can be separated again by gently hitting with a rubber mallet at a certain angle. To prevent this from happening in subsequent bakes, we made sure that the rotatable flange is not in contact with the main body of the part using UHV foil before baking.
- We have tried to use a smaller oven at the physics machine shop, which ended up burning the UHV foil and destroying our parts, see Fig. 2.10. This is possibly because the heating element in the smaller oven is too close to the parts, or that the temperature of the oven is not calibrated correctly.

The vacuum chamber was built on a empty region of the science table, away from the lattice beam optics, which we did not modify when disassembling the old Rb machine. After the water bake, we summoned half of the group members to slide the vacuum chamber in place. Peripherals, such as magnetic transport coils and MOT optics, are installed after the slide.

While I will not discuss the considerations behind the vacuum system design, here I include a brief description of the vacuum setup for better understanding the next sections. See Fig. 2.11 for a CAD rendering of the UHV chamber design. The atom sources (K: 50 mg of 3.15% ^{40}K -enriched KCl salt from Oak Ridge National Laboratory, distilled into two glass ampoules by Precision Glass; Rb: 5 g of 99%+ purity Rb in a prescored ampoule, Strem 93-3735) are attached to the 2D MOT cell through a custom-made 2.75" conflat flange with a 1.33" nipple welded on an opening on the side. We also refer to them as ovens, since they are designed to be heated up to increase the vapor pressure of alkali metals in the 2D MOT

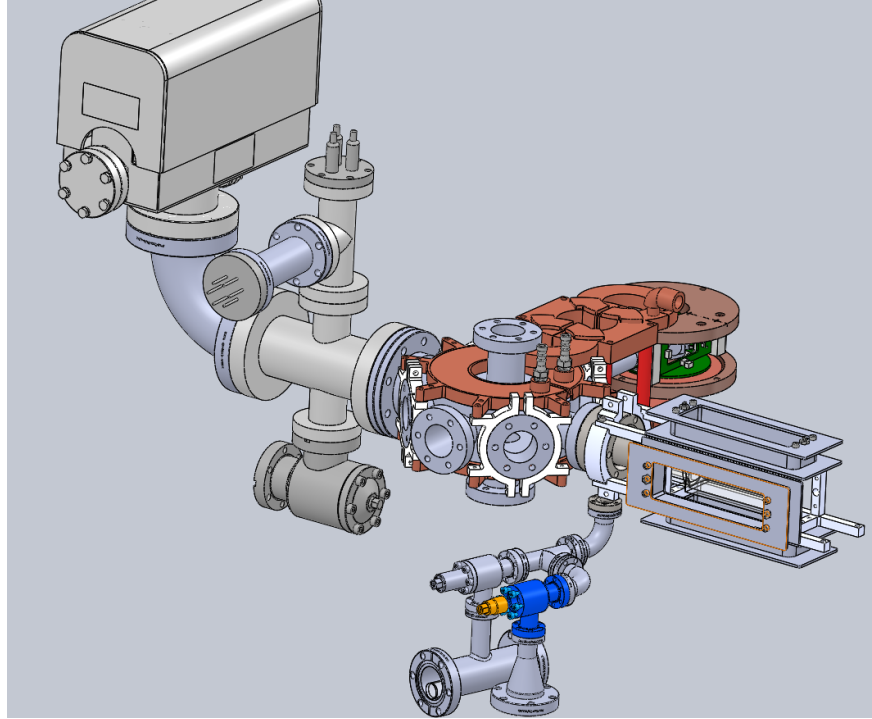


Figure 2.11: CAD rendering of the vacuum chamber design. The 2.75” angled valve is attached to the reducing cross on the other flange in the experiment (as it should).

cell. The 2D MOT cell is connected to the 3D MOT chamber through a differential pumping tube to maintain the pressure difference on the two sides. The opposite end of the 3D MOT chamber is connected to the pumping arm, which consists of a titanium sublimation pump (Ti-sub), an ion gauge and an ion pump. The science cell is connected to the 3D MOT chamber through two additional flanges for length adjustment. In our current setup, there is an additional valve after the angled valve, and the potassium oven is replaced by a new design, due to reasons stated below.

2.2.2 Incident I: a K ampoule under high vacuum

Alkali metals are pyrophoric, and they rapidly form oxide when in contact with the atmosphere. In our case, Rb reacts violently with bursts of flame, and ^{40}K -enriched potassium is so small in quantity that in metallic form, it completely reacts in a matter of seconds. Therefore, it is necessary to release the metal under vacuum. There are two common ways to introduce alkali atoms into the vacuum system, either using getters or by breaking ampoules containing the alkali metal under vacuum. In our experiment, we decided to work with alkali metals in ampoules, which is only broken after the water bake. A magnetic ball made of 440C stainless steel is placed next to the ampoule, and we use a strong magnet from outside of the vacuum chamber to smash the ampoule open.

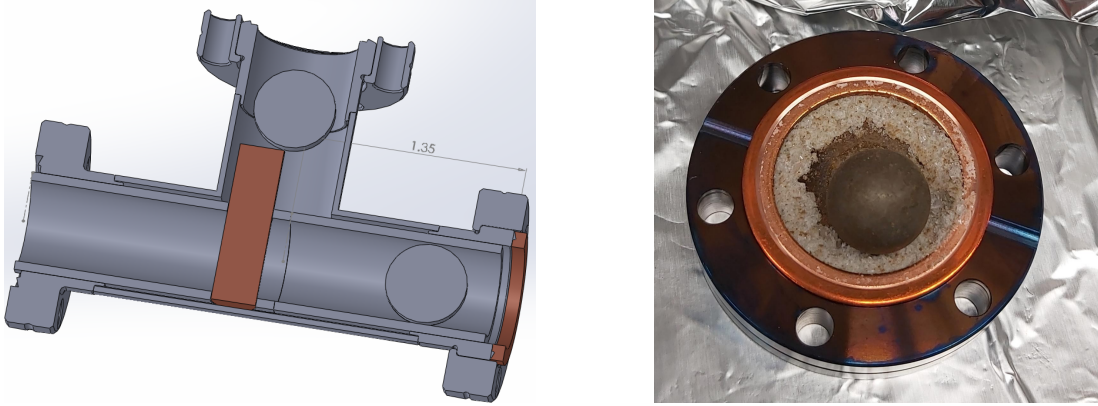


Figure 2.12: Left: a cross-sectional view of the new K ampoule holder design. Right: the remains of the first K ampoule. The brown color of the glass shards comes from potassium oxide.

The rubidium ampoule was sealed with argon and was prescored, so it was easily broken, and we see a sharp increase in pressure when it was broken. However, the potassium ampoule was small, not prescored, and sealed under high vacuum at around 10^{-8} Torr. This means that we did not have a reliable way to tell if the ampoule is broken. We note that simply smashing the steel ball against the stainless steel vacuum chamber would slightly increase the pressure, possibly by releasing hydrogen from the stainless steel part. This adds further confusion when trying to tell if the ampoule was broken.

After smashing the potassium ampoule for half an hour, we decided to try to propagate the two alkali metals to the 2D MOT cell by gently heating up the ovens, during which the interior of the vacuum chamber is coated by a thin layer of alkali. This process empirically takes a few days for rubidium, but perhaps should take longer for potassium due to the lower vapor pressure. We then checked the existence of alkali vapor using a resonant probe beam three days after breaking the ampoule. We were immediately able to see the Doppler-broadened absorption feature of rubidium, but we didn't see any signal from potassium.

After a month of monitoring with intermittent episodes of K oven heating, we concluded that we didn't actually smash open the ampoule, and I designed a new K oven so that we know for sure the ampoule is smashed open when the magnetic ball is dragged to the other side of the tee, see Fig. 2.12. The magnetic ball on the right arm of the tee can only be dragged to the left arm if the ampoule (shown as a brown cylinder) is broken. The ball sitting on the ampoule prevents large shards from going up towards the 1.33" angled valve. We removed the original K holder on September 16th, 2022, and to our dismay, it turned out that we have broken the ampoule very well (Fig. 2.12), and there simply weren't enough potassium atoms in the vacuum system yet. The enriched potassium source oxidized in the atmosphere in a matter of seconds.

In any case, given the new holder design, we installed a new source, this time with confidence that the ampoule is broken, and after heating all the parts between the holder

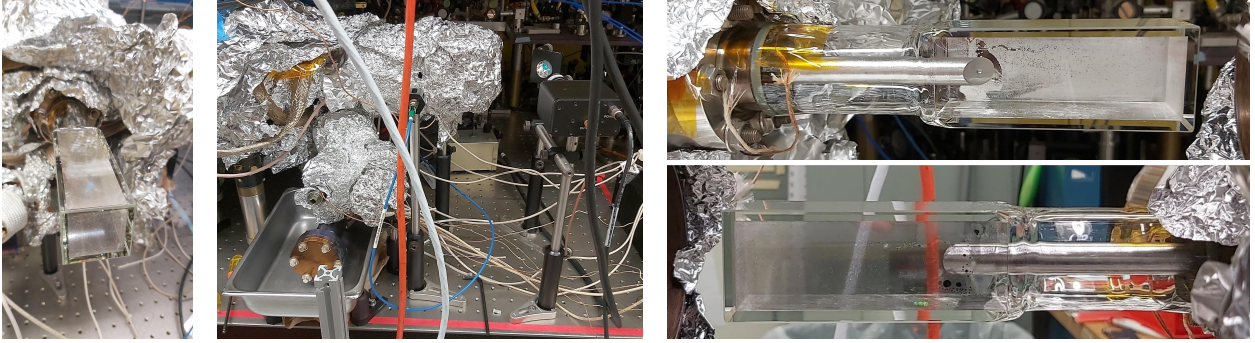


Figure 2.13: Left: 2D MOT cell coated with Rb. Middle: the setup for reversing Rb atoms into the Rb oven. Right: images after the first reversal attempt, which was neither hot nor long enough to remove all the Rb atoms.

and the cell to 100°C for ten days (this time with the valve to Rb oven fully closed), we were finally able to see signs of absorption at the K D2 line.

2.2.3 Incident II: a 2D MOT cell coated with Rb

Even before we put in the new potassium source, we had already unfortunately coated the 2D MOT cell with a layer of Rb atoms when trying to transfer K to the 2D MOT cell, see Fig. 2.13. This happened because we didn't fully close the valve for the Rb oven, and because the vapor pressure of Rb is much higher than K (see Fig. 2.14). I recommend anyone who works with VAT valves to practice with the actuating part so that similar events don't happen again in the future.

The layer of Rb atoms rendered the cell reflective, so the Rb layer had to be removed. We did this with a setup similar to our water bakeout, but only on the 2D MOT side. All parts except for the Rb oven are heated up to around 160 to 200°C , whereas the Rb oven is immersed in an ice bath, so that the Rb atoms solidify at this single cold spot. This is carried out in four separate sessions before the original K oven was replaced. The valve to the K oven was closed to prevent Rb atoms from entering this region. This is a tiring process, as the ice bath has to be replenished every 20 minutes with new ice, which means that at least one person has to be on duty throughout the reversal process, the longest one being 30 hours. For the last two attempts, we had a probe beam scanned around the Rb D2 transition that is reflected off the angled differential pumping tube surface, and we monitored the absorption signal to determine whether Rb atoms were removed successfully.

We were able to remove almost all the Rb atoms such that there is no noticeable absorption signal at 110°C and below. Since we don't have a gate valve separating the 2D MOT section from the ultrahigh vacuum (UHV) section, we were worried that we might put too much Rb into the main chamber, thereby degrading the vacuum or even damaging the ion pump. Fortunately, so far we haven't noticed any detrimental effect on our vacuum quality. I would however still suggest future designs to add a gate valve for ease of trouble-shooting.

2.2.4 Incident III: a viton valve

Ever since we first established UHV in the main chamber, we have been plagued by a recurring problem: after firing the Ti-sub, the pressure reading at the ion gauge initially drops to around $2 \cdot 10^{-10}$ Torr (subpar for a quantum gas experiment). The pressure then slowly increases to above 10^{-9} Torr over a course of a few months. We have fired the Ti-sub a few times, only to see the pressure creep up again.

The culprit turned out to be the valve in the pumping arm, which is the only valve between the whole vacuum chamber (before the K oven replacement) and the atmosphere. During vacuum system construction, we found that the all-metal VAT valve removed from the previous vacuum system that we were planning to reuse for our chamber was leaky. In a hurry to finish the vacuum system construction, and also complicated by the logistics drag due to COVID, we decided to use what was available at hand, and found an angled valve with viton seal (MDC, AV-IV-150) that was specified to work down to $1 \cdot 10^{-11}$ Torr. This specification might have been for setups in which it is installed in a section of a UHV system, with both sides of the valve under vacuum. There are many reasons why one should avoid using anything other than all-metal valves in a UHV system:

- Viton, or other elastomers that are often used to forming seals for non-all-metal valves, have larger outgassing rates. For example, depending on whether the viton part is baked at around 150°C , the outgassing rate varies from 10^{-7} to 10^{-10} Torr $\text{L s}^{-1} \text{cm}^{-2}$ [62], whereas we expect the outgassing rate of hydrogen-baked stainless steel parts to be on the order of 10^{-15} Torr $\text{L s}^{-1} \text{cm}^{-2}$ [61].
- Viton is a fluorocarbon, and upon excess baking it releases fluorocarbon monomers, which is difficult to remove once introduced into a vacuum system [62].
- Most relevant for us, viton is permeable to water. The equilibrium permeation flow of atmospheric water through a viton O-ring, 5 mm cross section diameter, 6 cm torus diameter, similar to what we have in the MDC valve, is about 10^{-7} Torr L s^{-1} , and is established after around two months (assuming normal atmospheric condition, for example 20 mbar of water vapor pressure) [63]. This means that we effectively have a leak for water vapor.

This issue was finally resolved in March 2024, after we installed another all-metal VAT angled valve after the MDC viton valve. The pressure reading on the ion gauge immediately after installation was around $6 \cdot 10^{-10}$ Torr. We had tremendous difficulty trying to fire the Ti-sub this time, and while in the end we were able to successfully fire the Ti-sub and lower the pressure reading to $6 \cdot 10^{-11}$ Torr, the last titanium filament in our Ti-sub also broke in this attempt. The pressure has since been stable, but in case the pressure in the main chamber worsens again, for example due to a newly developed leak, one might need to replace the Ti-sub, which would be a daunting task. (We note that this gauge reading is achieved when we water-cool the nipple that houses the ion gauge.)

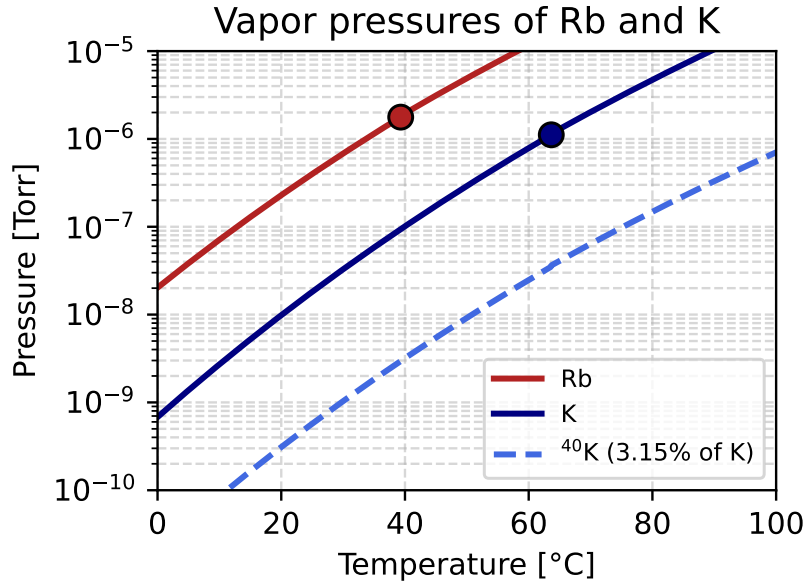


Figure 2.14: Vapor pressures of Rb and K as a function of temperature. An additional curve accounted for the 3.15% enrichment factor of our ^{40}K sample is also plotted.

2.2.5 Oven temperature and vapor pressure

The decision to use a dual-species design for 2D MOT greatly simplifies the vacuum chamber design and reduces space overhead, but comes at the cost of a slightly more complicated 2D MOT optics setup, trade-off between Rb and K optimizations, and most importantly, uncertainty in vapor pressure.

The 2D MOT coils are glued to four copper blocks connected to cooling water tubings, which were intended to cool the 2D MOT coils. It became clear as we run the experiment that we actually want to heat the cell up, since we are not limited by the pressure in the 2D MOT chamber yet, and we still benefit greatly by having a larger vapor pressure in the 2D MOT cell. As a result these remain unused (or one can even imagine running hot water through them to further heat up the cell). We have additionally stuck several resistive wires (braided to avoid generation of unwanted magnetic fields) to the inner surfaces of the 2D MOT coil holders, and added rectangular window panels on the openings of the holder, to heat up the 2D MOT cell indirectly through air.

After the work in Sec. 2.2.2, we believed that there was a small amount of visible potassium deposit in the corner of the 2D MOT cell, while the amount of rubidium is not high enough to be seen by eye. Based on the ion gauge reading and lifetime in the science cell magnetic trap, the pressure in the science cell does not increase as we heat the 2D MOT section from room temperature to 60°C, while the loading rate increases significantly for both species. This has been a stable working condition for us for around one year. However,

the amount of alkali atoms in the cell region seem to have changed gradually, and eventually the vapor pressure in the 2D MOT dropped. We have observed that occasionally turning off the heating around the cell for around two days increases the vapor pressure in the cell for around two weeks, which is reflected by a faster loading rate and separately confirmed with an optical depth measurement. After trial and error, we are now working with the valve to the Rb oven open, and the Rb holder heated to 33 °C. The potassium loading rate is at least twice slower than the fastest loading that we have achieved, which suggests that we can significantly reduce our experiment cycle time if we can increase potassium vapor pressure in some way. We have tried to use a 405 nm LED from Thorlabs (L405-66-60-550) in hope to increase the vapor pressure through light-induced atomic desorption [64] without heating up the cell further, but we saw no change in the MOT loading rate.

In a future design, one might want to implement mixing nozzles between the two alkali sources to allow independent control over the vapor pressure of each species [65]. This can be implemented in our current system when we again have to replace the potassium source (, which we might not ever need to do, considering the small atomic flux out of the 2D MOT chamber).

2.3 Science table optics

To accommodate the cooling of an additional atomic species, the MOT optics from the previous apparatus had to be entirely rebuilt. The optical trapping beams and optical lattice beams, on the other hand, are the same as before, since Rb and K have similar D1 and D2 line transition wavelengths, and the lattice setup built for Rb also works for K. I will therefore only describe the changes made for these optics. More detailed description can be found in previous theses [51, 52, 53]. A description of the magnetic coils, in particular the magnetic transport coil designs, will be discussed in Malte Schwarz’s thesis [50].

2.3.1 Magneto-optical traps

The cooling and repump beams for both species are combined on what we call “switch yards,” mainly built by a former undergraduate student Ryan Everly, see Fig. 2.15. We opted to not use a fiber power splitter to split MOT beam power. While this significantly increases the space required for power distribution, we have benefitted a lot from fine-tuning the power balancing between different beams from time to time. There is additionally a $\sim 8.5\times$ magnification telescope on the 3D MOT switch yard after all the beams are combined to enlarge the MOT beams to the desired sizes. 2D MOT beams are expanded with four individual telescopes following the design in our group’s optical cavity experiment [66].

Our power distribution scheme results in different splitting ratios of cooling and repump power among the different 3D MOT beam pairs. They have opposite polarizations when combined on a PBS, so at PBS1 in Fig. 2.15, they are split into different ratios unless the splitting is equal in the two exit ports. This is roughly the case for our 2D MOT, but not the

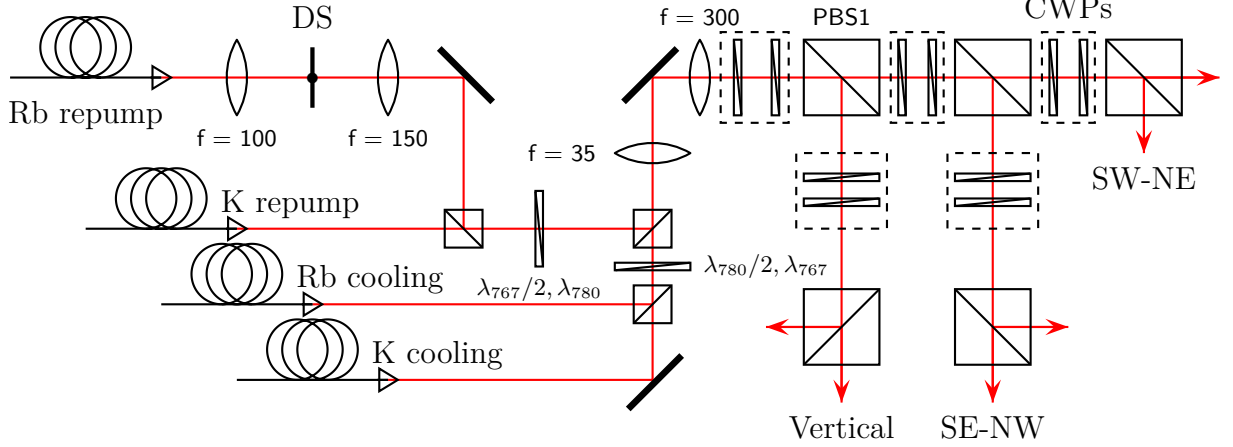


Figure 2.15: Simplified optics layout for the 3D MOT switch yard. The design of the 2D MOT switch yard is similar, except that the beams are only split into two pairs. DS: dark spot (currently removed from the setup). CWPs: pair of customized wave plates, see text.

3D MOT. Since the cooling and repump transitions we use are at the same wavelength, there don't seem to be simple alternatives to combine the two beams with the same polarization.

After the switch yards, the MOT beams are separated into four (2D MOT) or six (3D MOT) beams. We are able to change the power splitting ratio for the 767 nm and 780 nm lights separately using a combination of customized wave plates from Tower Optics (part numbers 4505-0323 $\sim$ 4505-0331) and broadband PBS cubes. These wave plates are half-wave plates for one wavelength, and full-wave plates for the other.

When designing the beam path of individual MOT beams, additional care was taken to make sure that the path length of the MOT beams are as close as possible. This allows one to implement a dark spot MOT by adding an opaque mask in the K repump beam path before it is combined with other beams. Additional lenses are added in the K repump beam path so that the dark spot is imaged at the position of the MOT, while making sure that the beam size of the repump beam is roughly unchanged. We have not implemented the dark spot in the experiment yet, but this can potentially give us a several-fold increase in ^{40}K atom number [58]. For this purpose, it might have been better to start with a larger beam from collimators, instead of using a small beam followed by an aggressive telescope, which makes it harder to avoid diffraction fringes when imaging the dark spot to the MOT position.

The push beam is mounted on a four-axis optics mount, providing all the relevant degrees of freedom for fine tuning. The beam waist of the push beam is comparable to the differential pumping tube, whose hole diameter is 0.0595". The input of the push beam collimator is connected to a fused fiber polarization combiner (Thorlabs, PFC780A) that combines the 767 nm and 780 nm push beams. The output first goes to a 767 nm- λ , 780 nm- $\lambda/2$ wave plate to match the polarization of the two wavelengths, and then to a quarter wave plate. The rough alignment was done by eye using a green light fiber checker.

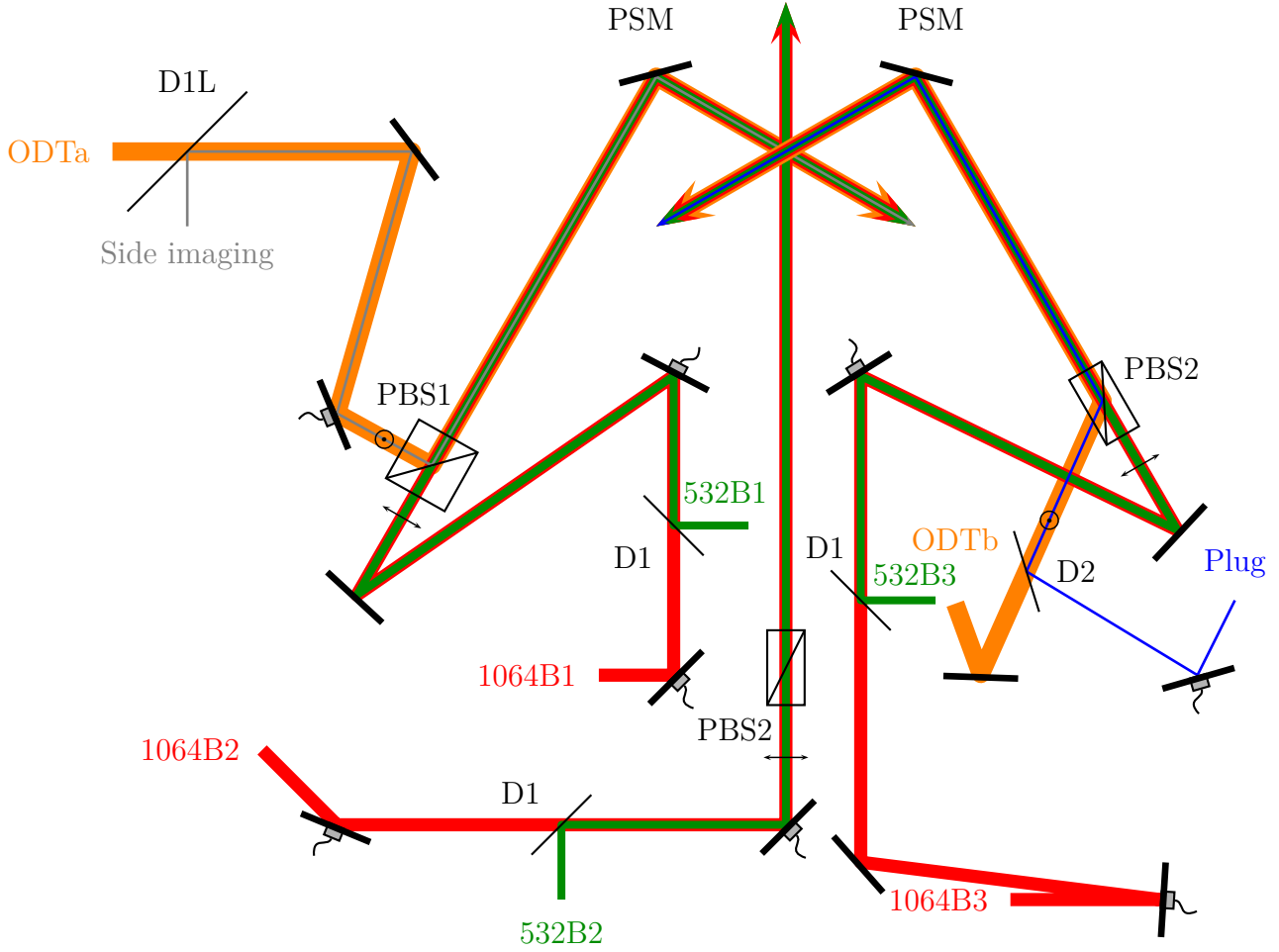


Figure 2.16: Simplified optics layout around the science cell. The thickness and color of each beam is only used to differentiate different beams. D1(L): Thorlabs, DMLP950(L); D2: Thorlabs, DMLP900; PBS1: EK SMA Optics, 435-1224D; PBS2: Advanced Thin Film, PBS1005-SBB. PSM: Thorlabs, PF1011-P01. Unlabeled mirrors are 1" dielectric mirrors with appropriate coatings.

2.3.2 Science cell optics

We did not remove the science cell optics, which included the lattice beams and the dipole trap beams, while disassembling the E5 vacuum system. We were able to realign the trapping beams and the lattice beams to the atoms without too much difficulty. A simplified but geometrically informed layout of the lattice beam optics is given in Fig. 2.16. The main changes are listed below.

- The beam waist of ODTa is changed to $w_h = 105\text{ }\mu\text{m}$ in the lattice plane and $w_v = 26.3\text{ }\mu\text{m}$ in the direction of gravity. A tighter confinement is beneficial for sympathetic cooling K with Rb during forced optical evaporation, since otherwise the trap center would be lower for Rb due to its larger mass, and the overlap between the two species would be worse. (See Ref. [50] for an in-depth discussion on optical evaporation with two species.) The beam waist of ODTb is roughly the same as before (measured to be $w_h = 51\text{ }\mu\text{m}$ and $w_v = 71\text{ }\mu\text{m}$), and as a result the final optical trap depth is mostly controlled by the strength of ODTa, while ODTb mainly provides confinement along the direction of ODTa propagation.
- The fine alignment of lattice beams can now be controlled by piezo-controlled mirror mounts. For each beam, one of the mount affects both beams, and the other only affects the 1064 nm beam. This design is due to historical reasons, because the 1064 nm piezo mounts were installed later. We use AG-M100N from Newport for all of them. For long-term stability, however, I learned from Newport technicians that it is better to use picomotor mounts, such as model 8807 from Newport, because they are held in place with the restoring force of springs similar to normal mirror mounts. So far, our beam alignment stability seems to be better than the previous machine due to the enclosure around science table, and better lab temperature stability due to the Birge chiller upgrade in March 2024.
- The new 760 nm plug beam is first combined with ODTb using a long-pass dichroic filter (Thorlabs, DMLP900), and then combined on the original PBS cube with the lattice beams.

Arbitrary phase lock

Hardware wise, the setup is almost exactly the same as described in Tsz-Him Leung's thesis [53]. Notable changes include

- One interferometer compensation plate (BCP4210, Thorlabs) is installed for the lattice beam pair B23. We haven't installed one for B12.
- The photodiodes for 532 nm lattice beams are replaced with PDA8A2, Thorlabs (used to be PDA10A, Thorlabs). This increased the gain by more than 10 dB.
- The low pass filters after the mixer for demodulation are removed, and the modulation frequency of the 532 EOM is changed from 0.7 MHz to 10 MHz. These filters (even for 1 MHz cutoff frequency) are found to introduce a frequency dependent phase shift to the error signal between DC to 10 kHz. The high frequency component at 20 MHz is much faster than the bandwidth of the servo, and is not expected to affect the performance of the servo even if left unfiltered.

2.4 Experiment control

Due to the complexity of a dual species experiment, we realized in the experiment design stage that we need to add more digital and analog output channels to the control system setup. Instead of upgrading the original control program, Cicero, we decided to use ARTIQ instead for our control system.

Cicero is a home-brewed control program developed in MIT designed to work mainly with National Instruments PCI cards, and peripherals that communicates through RS232 or GPIB. While it has a very intuitive GUI, the PCI cards compatible with the program are no longer in production and are pretty outdated. Cicero also runs the best on Windows XP, and we were worried that it will eventually become incompatible with newer operating systems.

ARTIQ is a control system solution provided by M-Labs. Spun off from the Ion Storage Group at NIST, ARTIQ is a combination of python-like programming language and FPGA-based hardware devices (called “sinara core devices”). Benefits that lead to the decision to switch to ARTIQ include

- It is maintained by a company, and has a large user base in the AMO community.
- The Sinara devices cover most of the common devices we use in the experiment, including digital and analog I/O, DDS frequency generators, and phase lock loops (PLL), making it easier to centralize the control system and control them under the same high level programming language.
- It is cheap compared to other options, such as Quantum Machines.

We have had many issues with ARTIQ hardware, which will be detailed in Malte Schwarz’s thesis [50]. In this thesis I will focus on the programming aspect of our implementation of ARTIQ.

2.4.1 Design considerations

Optical lattice experiments are slow in the sense that the timescale is on the order of ms set by the hopping strength. Even if we consider the smoothness of a variable output, our experiment only requires at most μs level precision and sampling rate. We can often tolerate solving a time sequence error by adding a few μs of delay at appropriate times. We are also not too worried about overhead in e.g. generating output (if any), since our experiment cycle time is on the order of one minute. Doing these computationally expensive sequence generation during time-consuming steps, such as MOT loading or magnetic transport, provides another workaround.

Therefore, instead of maximizing performance, we try to focus on ease of programming, and optimizing everyday workflow. We are very much inspired by the GUI of Cicero, where one can run the experiment up to different sections in the sequence, and easily switch between diagnosis, calibration and data taking in just a few clicks.

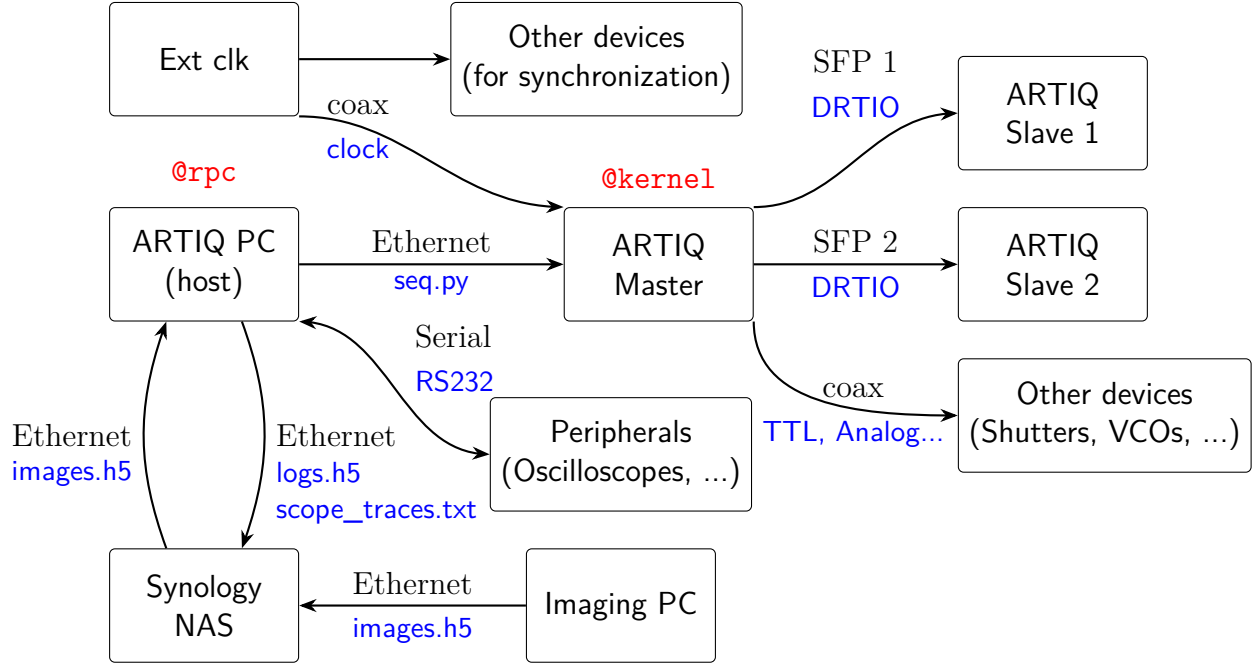


Figure 2.17: Connection between devices in the control system. See the official overview for a more complete diagram. The device at which a given piece of python code is compiled is determined by the decorator attached to the code, indicated in red text here. Each connection shows the physical connection type in black texts, and signal transmitted (either the protocol used, or the data transmitted) in blue texts.

2.4.2 Overview

A sketch of connections between relevant devices is given in Fig. 2.17. Conceptually, there are three kinds of devices controlled by an experiment sequence:

- DRTIO devices (basically, things in the ARTIQ crates). These include TTL, DAC, DDS, PLL, etc. Most of the time, the outputs of these devices are the control signals for other devices. In the code, they can only be accessed by code blocks with the `@kernel` decorator. The DRTIO system ensures that the output timings of events from different crates are synchronized.
- Devices controlled directly by the PC. For example, ARTIQ PC communicates with Tektronix oscilloscopes and Thorlabs K-cubes through serial ports. In the code, they are accessed by code blocks with the `@rpc` decorator (or no decorator, since this is the default). No timing precision can be guaranteed. For example, one can imagine a situation where the PC freezes after submitting an experiment. DRTIO devices will run normally (and so do the devices controlled by them), but PC-controlled devices will not output.

- Devices that are not a part of DRTIO nor connected to PC, but triggered by some signal, usually from DRTIO devices. Keep in mind that even though the DRTIO signals are precise to nanosecond resolution, there might be additional delays before the receiving device actually changes its state. For example:
 - All the shutters in our lab are controlled by shutter controllers that changes the state of shutters upon receiving TTL signals. The delays are a few milliseconds, with fluctuations on the order of tens of microseconds.
 - Home-built VCOs are controlled by a TTL (on/off) and two analog inputs (amplitude and frequency), with negligible delays. The three channels combined provide the same degrees of control as a single urukul DDS.

When an experiment is submitted through the ARTIQ dashboard, code blocks without `@kernel` are compiled on the ARTIQ computer, while those with `@kernel` are compiled on the FPGA of ARTIQ (in our case, a Kasli-SoC). Since they use different compilers, the `@kernel` codes have less or modified functionalities compared to the python installation being run in the host PC. This is often a point of confusion in the lab.

Each experiment is associated with a unique identifier called RID. An `.h5` log file is generated for each RID, which contains all the variables and datasets used in the experiment. We store the log file and any experiment data in the same folder, which is a slightly nontrivial task, given that the camera is connected to a different PC. Currently we rely on the file creation time to associate an image with its RID, but in the future this can be trivialized if we switch to a camera that is supported by the grabber module.

2.4.3 General remarks on working with ARTIQ

My goal is to (i) provide a very high level understanding that is sufficient for everyday lab works, and (ii) highlight some errors that we have encountered, along with our solutions / workarounds. The official ARTIQ documentation includes a good tutorial on the basics of RTIO concepts and an acceptable explanation of ARTIQ classes, which I will not reproduce here. The documentation is also constantly evolving, so it is worth going back to the same section from time to time. The author discovered a lot of previously unavailable documentation when writing this thesis.

2.4.4 Coding ARTIQ sequences in E9

In this section I give a brief description of the building blocks of our experiment sequence. While at first sight we seem to take an object-oriented approach, in reality the classes merely provides different namespaces for functions, and are defined mainly for readability. (Think of them as folders for python functions to avoid confusion between e.g. `Rb.MOT_on()` and `K40.MOT_on().`)

E9Word

This is similar to a “word” in Cicero, and we refer them as “words” in the lab. Each word should be a subclass of **E9Word**. It is a subclass of the **E9EnvExp** class, which is just the **EnvExperiment** class with a few convenience functions. For a word that doesn’t make use of the convenience functions defined in **E9EnvExp**, there is no meaningful difference between **E9Word** and **E9EnvExp** other than a few attributes accessed by **E9Seq**.

Each word should be a logically meaningful part of an experiment sequence, such as MOT loading, optical pumping, magnetic transport, etc. This rule is not enforced in the code but should be followed for mental clarity.

Variable vaults

We have several `xxx_vault.csv` files that store experiment parameters, such as

- Constants (values that we don’t expect to scan in experiments);
- Variables, and their default scan range, minimal / maximal allowed values, etc.;
- For each kind of DRTIO devices, the alias(es) for each channel, and output parameters when in idle mode (not actively running any sequence).

Currently we only have one vault for each kind of parameters, but one can imagine having multiple vaults, and quickly switch between different experiment configurations by simply loading a different vault.

Each vault is simply a `.csv` file. This file format is chosen because `.csv` files are very intuitive to work with when used with the Edit CSV extension in Microsoft VS Code. A potentially more ARTIQ-style solution is to work with `datasets` or `.h5` files, but we were not convinced that the extra work is worth the effort.

E9Seq

This is similar to a “sequence” in Cicero, and we refer them as “sequences” in the lab. Each sequence should be a subclass of **E9Seq**. It is also a subclass of the **E9EnvExp** class. This is the class that creates the parallel between our ARTIQ implementation and Cicero. Below I list the basic features and points for improvement.

The `build()` method for each **E9Word** in `E9Seq.all_words_and_cfg` is run during the build stage of an experiment. Additionally, a boolean value can be created for each word. These boolean values don’t do anything by themselves — one needs to program the conditional statements in `E9Seq.run_seq()`. Besides from controlling whether a word runs or not, we also use these booleans to e.g. automatically select the right imaging sequence.

The vaults to be loaded are currently coded as class attributes of **E9Seq**. Since they are already accessed in `build()`, switching between different vaults as suggested before would require editing the sequence code itself, if this implementation is not changed.

Scanning variables are made possible with the `MultiScanManager` (MSM). The MSM is an iterable that only uses outer products, which is undesirable, since it does not allow e.g. scanning two variables as pairs. This should be addressed by a python-savvy student in the future. Additionally, since `prepare()` is only run once, and the values scanned by the MSM are updated in `run()`, outputs that are generated in `prepare()` are not updated, even if the variable that derives them are scanned. In our case, this is an issue if one wants to scan the magnetic transport variables, since the current ramp shapes are generated in `prepare()`³. One workaround is to generate the ramp in `run()` instead, which adds a short computation overhead to each run. This not a big issue for us since our actual experiment sequence is much longer than the time that this computation takes.

At the end of `run()` of each sequence, or if any exceptions are raised during the execution of a sequence, the output automatically goes back to the idle value. This is implemented by `E9Seq.safe_exit()`.

In our lab, we mainly work with the ARTIQ dashboard, which provides a GUI for submitting sequences and other useful widgets. Some common pitfalls when using the dashboard under our framework:

- After editing and saving a constant or variable in a vault, they are NOT reflected in the actual sequence until one hits the “recompute” button for that value.
- If a scheduled experiment doesn’t run, check if “Due date” is set to some value. This often happens when one accidentally scrolled when the mouse is on the “Due date” scroll box.
- Override can be changed during an experiment, and is not saved in the run log.

³It is nontrivial to generate the output on the fly, as we do for all other outputs, since the ramp shape is not given by a simple function, but is numerically calculated.

Chapter 3

Quantum gases in optical potentials

In this chapter, we review the theory background required to understand the results from our experiment. This chapter also serves to define the notations used throughout this thesis. I will often use “a cloud of atoms,” “a gas of atoms,” and “atoms” interchangeably.

3.1 Properties of rubidium and potassium

The classic reference for atom trappers on the physical properties of rubidium is *Rubidium 87 D Line Data* by Daniel Steck [67]. Tobias Tiecke compiled a similar document for potassium, *Properties of Potassium* [54].

3.1.1 Atoms in external magnetic fields

The Zeeman shift due to a weak external magnetic field B is given by

$$V_Z = B\mu_B g_F m_F, \quad (3.1)$$

where μ_B is the Bohr magneton, and g_F is the Landé g -factor. Eqn. (3.1) is a good approximation as long as F is a good quantum number. This is no longer the case when V_Z is comparable to the hyperfine splitting of the atom under consideration. For the ground state manifold of alkali atoms, $L = 0$ and $S = 1/2$, and the Breit-Rabi formula applies [67, 54]:

$$E_{\text{Breit}}(B) = -\frac{\Delta E_{\text{hfs}}}{2(2I + 1)} + g_I \mu_B m_B \pm \frac{\Delta E_{\text{hfs}}}{2} \left(1 + \frac{4mx}{2I + 1} + x^2 \right)^{1/2}, \quad (3.2)$$

where ΔE_{hfs} is the hyperfine splitting, $m = m_I \pm m_J$, and $x = (g_J - g_I)\mu_B B / \Delta E_{\text{hfs}}$.

Eqn. (3.2) can be used to find the difference of energy gaps between neighboring m_F levels, $E_{m \rightarrow m-1} = E_m - E_{m-1}$. This is relevant when transferring atoms to a different m_F state using an applied RF field, which works by driving a series of rapid adiabatic passages. The values of $E_{m \rightarrow m-1}$ for different m -states as a function of magnetic field are shown in Fig. 3.1.

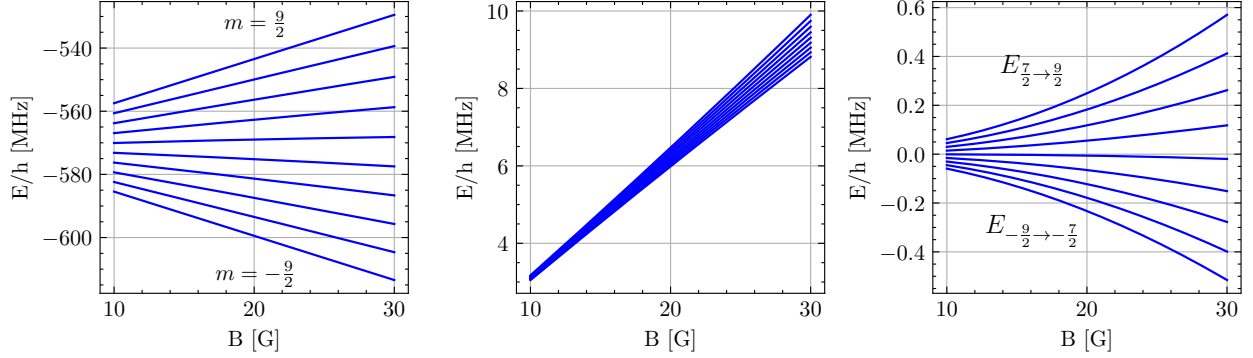


Figure 3.1: Left: Zeeman shifts in ^{40}K calculated using the Breit-Rabi formula. Middle: $E_{m \rightarrow m-1}$ between the neighboring m_F states as a function of magnetic fields. Right: $E_{m \rightarrow m-1}$ with the average set to zero to better visualize the differences in $E_{m \rightarrow m-1}$.

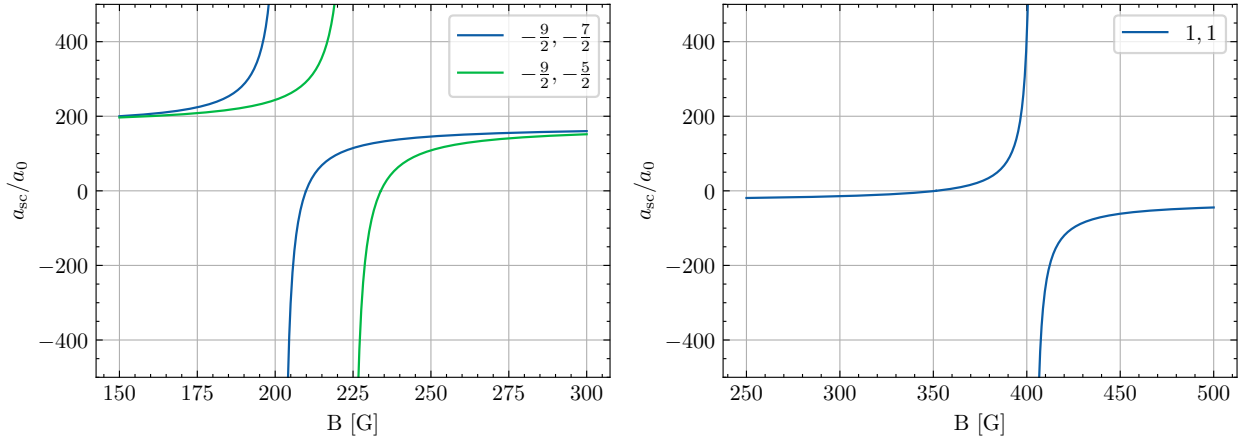


Figure 3.2: $a_{\text{sc}}(B)$ for selected internal state combinations, normalized by the Bohr radius a_0 . Left: ^{40}K ; Right: ^{39}K .

For example, starting with a cloud of ^{40}K atoms in the $|F = 9/2, m_F = 9/2\rangle$ state, one can apply a fixed magnetic field of, say, 20 G, where the differences in ΔE_{m_F} for different m_F states are sufficiently resolved. One can then apply a RF pulse scanning from, say, 6.7 MHz to 5.8 MHz, to transfer atoms to the $|F = 9/2, m_F = -9/2\rangle$, driving one adiabatic passage at a time.

Feshbach resonance

While none of the works described in this thesis make use of the magnetic Feshbach resonance, we include some basic facts of the experimentally relevant resonances in this section, since the apparatus is designed to make use of these resonances. For two atoms in an internal state combination with Feshbach resonances, the s -wave scattering length between them at

a magnetic field B is given by [68]

$$a_{\text{sc}}(B) = a_{\text{bg}} \left(1 - \frac{\Delta B}{B - B_0} \right), \quad (3.3)$$

where a_{bg} is the background scattering length, ΔB is the resonance width, and B_0 is the resonance position. By tuning the strength of the external magnetic field, one can change the interaction strength between atoms. Fig. 3.2 shows the resonances that this experiment is designed to utilize [54, 69]. While there are interspecies resonances between Rb and ^{40}K at around 500 G [58, 70, 71], we currently don't have plans to make use of these resonances. The resonances between Rb and ^{39}K are relevant during optical evaporation (See Sec. 3.2.2).

3.1.2 Atoms in far-detuned optical fields

The main transitions between the internal levels of alkali atoms are the D1 and D2 lines. The levels structures of ^{39}K and ^{40}K , including relevant transitions used in cooling, are shown in Fig. 2.3. We will refer the reader to [72, 67] for the Rb level structure. Since the oscillator strengths of other transitions are around two orders of magnitude or more weaker than the D lines [73], it is usually a very good approximation to ignore all other transitions when calculating the effective optical potential.

For detunings much larger than the hyper fine structure splitting of the $^2\text{P}_{J'}$ states, $\Delta \gg \Delta'_{\text{HFS}}$, the effective potential of $|F = F, m_F = m_F\rangle$ atoms in the $^2\text{S}_{1/2}$ manifold is given by [74]

$$U_{\text{dip}}(\mathbf{r}) = \frac{\pi c^2 \Gamma}{2\omega_0^3} \left(\frac{2 + \mathcal{P} g_F m_F}{\Delta_{2,F}} + \frac{1 - \mathcal{P} g_F m_F}{\Delta_{1,F}} \right) I(\mathbf{r}), \quad (3.4)$$

where $\mathcal{P} = 0 (\pm 1)$ for π - ($\sigma^\pm$ -) polarized light. Eqn. (3.4) is a good approximation for all our trapping beams. If, additionally, the detuning is so large that even the fine structure splitting is small compared to the detuning, $\Delta \gg \Delta'_{\text{FS}}$, then Eqn. (3.4) further simplifies to

$$U_{\text{dip}}(\mathbf{r}) = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} \left(1 + \frac{1}{3} \mathcal{P} g_F m_F \frac{\Delta'_{\text{FS}}}{\Delta} \right) I(\mathbf{r}). \quad (3.5)$$

Eqn. (3.5) holds for all the trapping beams except for the 760 nm plug beam. The polarization dependence introduces a small correction for us (up to $\pm 2.4\%$ for Rb in $|F = 2, m_F = 2\rangle$ state or $\pm 1.1\%$ for ^{40}K in $|F = 9/2, m_F = 9/2\rangle$ state), and can usually be safely ignored. (But see e.g. [51] for how this effect is amplified in Raman-Nath diffractions.) In terms of polarizability, this amounts to keeping only the scalar polarizability α^s , giving

$$U_s(\mathbf{r}) = -\frac{\alpha^s}{2\epsilon_0 c} I(\mathbf{r}). \quad (3.6)$$

So far, our discussions have been limited to the effective conservative potential experienced by atoms in a single long-lived state. We note that it is important to consider the

energy shifts of the excited states for *in situ* fluorescence imaging. In this situation, an atom scatters thousands of photons in the optical field, and with each optical excitation, the atom spends $2\pi/\Gamma$ in the excited state on average, where Γ is the decay rate of the excited state. If the optical potential experienced by an atom in the ground and excited states are mismatched due to differences in their polarizabilities, excitations create sudden changes in the confinement, which can undesirably heat up the atom. A commonly adopted solution, which sees extensive use in optical tweezer experiments, is to use a wavelength and/or polarization combination that results in the same trapping potential for the relevant states. These wavelengths and polarizations are referred to as being “magic.” The calculations of the polarizability mismatch typically consider the multilevel nature of the atoms, such as using the state summing method detailed in [75].

Let us consider what this implies for our experiment if we were to implement *in situ* fluorescence imaging after a future imaging system upgrade (see Sec. 8.2). We would likely use the $\lambda = 532$ nm optical lattice to “pin down” the position of atoms in the horizontal plane, and use a one-dimensional $\lambda = 1064$ nm lattice for confinement in the vertical direction. It turns out that there are magic wavelengths around 532 nm, which can be used to suppress heating in the lattice plane [76]. However, at $\lambda = 1064$ nm, ^{40}K atoms in the $^2\text{P}_{1/2}$ states experience an anti-trapping potential that is about 5.4 times stronger than the trapping potential of the ground state due to a strong $4p_{1/2} - 3d_{3/2}$ transition. This resulted in heating during fluorescence imaging, for example, in the first realization of the first ^{40}K quantum gas microscope [77].

3.2 Atomic gases in harmonic potentials

In this section, we review well-known results for atomic gases in a trapping potential. The main observable we have access to in our system is the density distribution of atoms, which is obtained through absorption imaging. Therefore, it is important to understand the relation between the thermodynamical variables and the density and momentum distribution of the atoms. This section covers enough background knowledge for us to diagnose the quantum gases in everyday experiments. For more extensive discussions, see Ref. [78, 79].

We will focus on harmonic trapping potentials, which are good approximations for optical dipole traps formed by Gaussian beams, or optically plugged magnetic quadrupole traps (if the temperature of atoms is low compared to the plug potential). For a three dimensional harmonic trap with potential given by

$$V(\mathbf{r}) = \frac{1}{2}m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (3.7)$$

the density of states (DoS) is given by

$$\rho_{\text{trap}}(E) = \frac{1}{2\hbar^3 \bar{\omega}^3} E^2 \equiv C_{\text{trap}} E^2, \quad (3.8)$$

where $\bar{\omega}^3 = \omega_x \omega_y \omega_z$ is the geometrical mean of the trap frequencies. Integrating the DoS from 0 to E then gives us the number of states whose energy is below E , $G_{\text{trap}}(E) = C_{\text{trap}} E^3/3$.

The main difference between bosons and fermions is that fermions cannot occupy the same state. We consider a grand canonical ensemble in thermal equilibrium, so the system is describe by the temperature T and the chemical potential μ . The occupation number of a state with energy E is then given by

$$f_{\mp}(E; \mu) = \frac{1}{e^{(E-\mu)/k_B T} \mp 1}, \quad (3.9)$$

where bosons (fermions) takes the upper (lower) sign. I will sometimes use the thermodynamical beta $\beta \equiv 1/k_B T$ instead of T . These are the famous Bose-Einstein distribution and Fermi-Dirac distribution, respectively. At high temperatures, the occupation number in each energy state is small, namely $e^{(E-\mu)/k_B T} \gg 1$, so Eqn. (3.9) simplifies to the Boltzmann distribution, $f(E; \mu) = e^{-(E-\mu)/k_B T}$, for both bosons and fermions. In this case, we will refer to the atomic gas as being “thermal,” and the quantum statistics is irrelevant. The difference between bosons and fermions is only important at ultracold temperatures.

The measure of the “quantumness” of a bulk gas is given by the phase space density, defined as (ϖ is `varpi`)

$$\varpi \equiv n \lambda_{\text{dB}}^3 = n \left(\frac{2\pi \hbar^2}{m k_B T} \right)^{3/2}, \quad (3.10)$$

where n is the density of the cloud, and $\lambda_{\text{dB}} \equiv h/\sqrt{2\pi m k_B T}$ is the thermal de Broglie wavelength. Intuitively, ϖ can be understood as the number of particle in a volume of λ_{dB}^3 , and when this number is on the order of unity, the matter waves of particles start to overlap each other.

3.2.1 Thermal gases

Under the semi-classical approximation, we will write the occupation number as [79]

$$f_{\mp}(\mathbf{r}, \mathbf{p}) = \frac{1}{\exp[(|\mathbf{p}|^2/2m + V(\mathbf{r}) - \mu)/k_B T] \mp 1}, \quad (3.11)$$

which holds for cases where $V(\mathbf{r})$ does not vary significantly over λ_{dB} . Integrating over the momentum space then gives us the density distribution,

$$n(\mathbf{r}) = \int \frac{d^3 \mathbf{p}}{(2\pi \hbar)^3} f_{\mp}(\mathbf{r}, \mathbf{p}) = \pm \frac{1}{\lambda_{\text{dB}}^3} \text{Li}_{3/2}(\pm \exp[(\mu - V(\mathbf{r}))/k_B T]), \quad (3.12)$$

where $\text{Li}_s(x) = \sum_{k=1}^{\infty} x^k/k^s$ is the polylogarithm function of order s . We can confirm that the quantum statistics becomes irrelevant for thermal clouds using the identity,

$$\lim_{|x| \rightarrow 0} \text{Li}_s(x) = x. \quad (3.13)$$

Eqn. (3.12) then reduces to

$$n(\mathbf{r}) = \frac{1}{\lambda_{\text{dB}}^3} \exp[(\mu - V(\mathbf{r}))/k_B T] \xrightarrow{\text{har.}} \frac{N}{\pi^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left[- \sum_i \frac{x_i^2}{\sigma_i^2} \right], \quad (3.14)$$

where for the harmonic potential, $\sigma_i = \sqrt{2k_B T / m \omega_i^2}$. The *in situ* density simply becomes a Gaussian function for thermal clouds in harmonic traps.

In experiments, we often perform time-of-flight (ToF) measurements, in which the gas is released from the confining potential and expands in free space. The spatial distribution after a ToF can again be found using Eqn. (3.11) (ignoring interaction effects). An atom of mass m initially at the spatial position $\mathbf{r}_0$ with momentum $\mathbf{p}$ will be at $\mathbf{r} = \mathbf{r}_0 + \mathbf{p}t/m$ after an expansion time t . Representing this condition with a delta function, we have [78]

$$n_{\text{ToF}}(\mathbf{r}, t) = \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} f_{\mp}(\mathbf{r}, \mathbf{p}) \delta^{(3)}(\mathbf{r} - \mathbf{r}_0 - \frac{\mathbf{p}t}{m}) \quad (3.15)$$

$$= \frac{1}{\lambda_{\text{dB}}^3} \prod_{i=1}^3 \left(\frac{1}{1 + \omega_i^2 t^2} \right)^{1/2} \text{Li}_{3/2} \left\{ \exp \left[\frac{1}{k_B T} \left(\mu - \frac{m}{2} \sum_{i=1}^3 \frac{\omega_i^2 r_i^2}{1 + \omega_i^2 t^2} \right) \right] \right\}. \quad (3.16)$$

For long ToF, this is approximately given by

$$n_{\text{ToF}}(\mathbf{r}, t) = \frac{1}{\lambda_{\text{dB}}^3} \frac{1}{\bar{\omega}^3 t^3} \text{Li}_{3/2} \left(\exp \left[\frac{1}{k_B T} \left(\mu - \frac{mr^2}{2t^2} \right) \right] \right) \quad (t \gg 1/\omega_{x,y,z}). \quad (3.17)$$

This again simplifies to a Gaussian function for thermal clouds using Eqn. (3.13). By identifying $p = mr/t$, we see that for t long enough such that the final cloud size is much larger than the original size, ToF measurements map momentum distributions to spatial distributions.

3.2.2 Bose gases

We first consider a gas of noninteracting bosons. In this case, the chemical potential of a Bose gas is capped at the ground state energy E_0 (for $T > 0$), since otherwise Eqn. (3.9) would predict a negative occupation number for the ground state, which is unphysical. This means that the occupation number of an excited state with energy E is capped at $1/(\exp[\beta(E - E_0)] - 1)$. As the temperature approaches zero ($\beta \rightarrow \infty$), the occupation number in excited states goes down. Eventually, the number of atoms in the excited states $N_{\text{ex}} = \int dE \rho(E) f_{-}(E)$ drops below the number of particles in the system N , and the remaining particles must all reside in the ground state, at which point the Bose gas undergoes a phase transition to form Bose-Einstein condensates (BEC).

The critical temperature is found by setting $N = N_{\text{ex}}$, which gives [80]

$$k_B T_c = \left(\frac{N}{2C_{\text{trap}} \zeta(3)} \right)^{1/3} = \hbar \bar{\omega} \left(\frac{N}{\zeta(3)} \right)^{1/3}, \quad (3.18)$$

where $\zeta(3) \approx 1.202$ is the value of Riemann zeta function. For $T < T_c$, $N_{\text{ex}} < N$, and all the remaining atoms must be in the ground state, giving

$$N_0 = N \left[1 - \left(\frac{T}{T_c} \right)^3 \right]. \quad (3.19)$$

Inverting Eqn. (3.19) gives us an expression of the temperature as a function of the condensate fraction

$$T = \left(1 - \frac{N_0}{N} \right)^{1/3} T_c. \quad (3.20)$$

At any finite $T < T_c$, the Bose gas consists of a condensate fraction and a thermal fraction. Experimentally, the ToF images reveal the onset of condensation through the famous bimodal distribution, namely, the momentum distribution is the sum of the two fractions. To find the spatial distribution of the condensate, we will base our calculation on the Gross-Pitaevskii equation, which accounts for the interaction between bosons at a mean field level:

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + U_0 |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}), \quad (3.21)$$

where $U_0 = 4\pi\hbar^2 a_{\text{sc}}/m$. We then make the Thomas-Fermi approximation, which neglects the kinetic energy term in Eqn. (3.21). Noting that $n(\mathbf{r}) = |\psi(\mathbf{r})|^2$, we obtain

$$n(\mathbf{r}) = \max([\mu - V(\mathbf{r})] / U_0, 0). \quad (3.22)$$

For harmonic traps, Eqn. (3.22) predicts that the distribution of atoms follows an inverse parabola, with sharp cutoffs¹ in density at the Thomas-Fermi Radii,

$$R_i^{\text{TF}} = \sqrt{\frac{2\mu_{\text{TF}}}{m\omega_i^2}}, \quad (3.23)$$

and the density at the trap center is given by

$$n_{\text{TF}} = \frac{\mu_{\text{TF}}}{U_0} = \frac{15^{2/5}}{2} \left(\frac{N_0 a}{\bar{a}} \right)^{2/5} \frac{\hbar\bar{\omega}}{U_0}, \quad (3.24)$$

Here, N_0 is the number of atoms in the condensate fraction, and $\bar{a} = \sqrt{\hbar/m\bar{\omega}^2}$ is the associated oscillator length. both expressed in terms of the chemical potential under Thomas-Fermi approximation, μ_{TF} , which is obtained by setting $\int d^3\mathbf{r} n(\mathbf{r}) = N_0$.

While Eqn. (3.22) gives the real space density, it has been shown that the inverse parabolic shape is maintained during ToF [78, 81], a fact useful when doing fits.

¹In reality, the change in density must be smooth, otherwise the kinetic energy diverges at the density glitches. The density is smoothed out over a length scale called the healing length, $\xi \equiv \sqrt{\hbar^2/2mnU_0} = \sqrt{1/8\pi na_{\text{sc}}}$.

The Thomas-Fermi approximation is justified by the fact that the interaction energy of a Bose gas scales faster than the kinetic energy as a function of atom number [80]. For species with negative background scattering length, this means that the cloud collapses above a critical number of atoms, which was first observed in ^7Li [82]. In the future, if we ever decide to work with ^{39}K BECs, care must be taken during the final evaporation step to make sure that the ^{39}K - ^{39}K scattering length is tuned to a positive value before condensation takes place. (Depending on the internal state of atoms during evaporation, the Rb- ^{39}K scattering length is tuned at the same time [83].)

3.2.3 Fermi gases

We consider fermions in a single internal state, which is often referred to as a “spinless” Fermi gas. In contrast to bosons, $f_+(E; \mu)$ approaches a step function as $T \rightarrow 0$,

$$\lim_{T \rightarrow 0} f_+(E; \mu) = \Theta(E_F - E) = \begin{cases} 1 & E < E_F \\ 0 & E > E_F \end{cases}. \quad (3.25)$$

The fact that each state is only occupied by one particle is exactly the Pauli exclusion principle. Here, we have defined the Fermi energy as the chemical potential at zero temperature, $E_F \equiv \mu(T = 0)$. The Fermi temperature is then defined as $T_F \equiv E_F/k_B$. Unlike bosons, there is no phase transition as a Fermi gas is cooled towards $T = 0$, but the Fermi energy defines a natural energy scale, and we call it a degenerate Fermi gas (DFG) when $T/T_F < 1$. E_F also defines the Fermi surface, which are constant energy surface(s) in the phase space.

Since there is one particle per state, we can find E_F by equating the particle number N to the number of states below the Fermi energy $G(E_F)$, giving

$$E_F = \left(\frac{3N}{C_{\text{trap}}} \right)^{1/3} = (6N)^{1/3} \hbar \bar{\omega}. \quad (3.26)$$

The density of a Fermi gas at zero temperature is given by

$$n_F(\mathbf{r})|_{T=0} = \int_{|\mathbf{p}| < \sqrt{2m(\mu - V(\mathbf{r}))}} \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} = \frac{1}{6\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (\mu - V(\mathbf{r}))^{3/2}. \quad (3.27)$$

The Thomas-Fermi radius given in Eqn. (3.23) is thus also the radius of the Fermi gas. For $0 < T \lesssim T_F$, the density is still given by the polylogarithm Eqn. (3.12), but the limiting identity Eqn. (3.13) that gave us Gaussian density distributions for thermal clouds no longer applies.

By inspecting regions at different values of local chemical potential $\mu(\mathbf{r}) \equiv \mu - V(\mathbf{r})$, we can understand how the density distribution of a fermionic cloud at finite temperatures approaches the form given by Eqn. (3.27). For regions where $\mu(\mathbf{r}) \gg k_B T$, Eqn. (3.12) approaches Eqn. (3.27):

$$n(\mathbf{r}) = \pm \frac{1}{\lambda_{\text{dB}}^3} \text{Li}_{3/2}(\pm \exp[(\mu - V(\mathbf{r}))/k_B T]) \approx \frac{1}{6\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (\mu - V(\mathbf{r}))^{3/2},$$

where we have made use of the following identity:

$$\lim_{\text{Re}[u] \rightarrow \infty} \text{Li}_s(\pm e^u) = -\frac{u^s}{\Gamma(s+1)} \quad (-s \notin \mathbb{N}). \quad (3.28)$$

This holds up to the “wings” of the cloud, where $\mu(\mathbf{r})$ is no longer large compared to $k_B T$. In the opposite limit $k_B T \gg \mu(\mathbf{r})$, the density distribution becomes

$$n(\mathbf{r}) \approx \frac{2\sqrt{\pi}}{\lambda_{\text{dB}}^3} e^{\beta(\mu - V(\mathbf{r}))/2}, \quad (3.29)$$

where we have used a different identity,

$$\lim_{|u| \rightarrow 0} \text{Li}_s(e^u) = \Gamma(1-s)(-u)^{s-1} \quad (\text{Re}[s] < 1). \quad (3.30)$$

This is the difficulty of measuring the onset of Fermi degeneracy (from real space distribution), since lower temperature only affects the wings. The density distribution of a cloud after a long ToF can again be shown to be related to its original shape with rescaling factors given by $b_i(t) = \sqrt{1 + \omega_i^2 t^2}$ [79], so this difficulty carries over to the momentum space measurements.

The fact that we have Rb atoms in the same optical dipole trap with ^{40}K during forced evaporation provides us an alternative and simpler way to measure the temperature of cold Fermi gases. Assuming that the Rb and ^{40}K atoms are in thermal equilibrium, we can use Rb atoms as a thermometer for the mixture, since it is much easier to measure the temperature of bosons from the bimodal distribution once the trap parameters are known [84].

From Eqn. (3.18) and (3.26), we see that both T_c and T_F are proportional to the trap frequency (of the corresponding isotope). The critical temperature of the BEC transition and the Fermi temperature in the same harmonic trap potential is simply related through

$$\frac{T_c}{T_F} = \tau \left(\frac{1}{6\zeta(3)} \right)^{1/3} \left(\frac{N_B}{N_F} \right)^{1/3} \approx 0.375 \left(\frac{N_B}{N_F} \right)^{1/3} \quad (3.31)$$

where τ is the ratio of trap frequencies in an optical dipole trap due to differences in polarizabilities and masses. To find τ , let us consider an optical trap formed by an optical field with intensity $I(\mathbf{r})$. Assuming that we only need to account for the scalar polarizability, the optical potential experienced by the bosonic isotope is given by Eqn. (3.6),

$$V_B(\mathbf{r}) = \frac{1}{2} m_B \omega_B^2 x^2 = -\frac{\alpha_B^s}{2\epsilon_0 c} I(\mathbf{r}), \quad (3.32)$$

and $B \leftrightarrow F$ for the fermionic isotope. We then find τ by eliminating $I(\mathbf{r})$ that appears in the two equations, and find

$$\tau \equiv \frac{\bar{\omega}_B}{\bar{\omega}_F} = \sqrt{\frac{\alpha_B^s m_F}{\alpha_F^s m_B}} \approx 0.725. \quad (3.33)$$

We have substituted the values for Rb and ^{40}K in the end, and the polarizabilities are calculated at 1064 nm. Assuming that the two species are at equilibrium, we can then use Eqn. (3.20) and (3.31) to find T/T_F :

$$\frac{T}{T_F} = 0.375 \left(1 - \frac{N_{B,0}}{N_B} \right)^{1/3} \left(\frac{N_B}{N_F} \right)^{1/3}. \quad (3.34)$$

The applicability of this thermometry scheme should be considered more carefully towards the end of optical evaporation. Due to the difference in the mass between Rb and ^{40}K atoms, the gravitational potential displaces Rb atoms more than ^{40}K in a weak optical dipole trap. Eqn. (3.34) assumes that the system is in thermal equilibrium, which requires that there is enough (elastic) collisions between the two species. This will not be true if there is no spatial overlap between the two species. The displacement between Rb and ^{40}K due to gravity should be compared to the Thomas-Fermi radius (, which is a pessimistic approximation, since the spatial extent of the thermal component of Rb atoms is larger). For now we will note that we can usually assume good thermalization between Rb and ^{40}K , and refer readers to Ref. [50].

3.2.4 Fitting functions for time-of-flight images

In our experiments, we almost exclusively make use of absorption imaging for measurements, which connects the measured the optical densities to column densities, $n_c(x, y) = \int dz n(x, y, z)$. The fitting functions should therefore account for the integral in the z direction.

For thermal gases or non-interacting Fermi gases (including DFG), the in-trap density distribution is given by Eqn. (3.12), and ToF density distribution by Eqn. (3.17), both containing $\text{Li}_{3/2}$. We make use of the polylogarithm identity (which only requires that the confinement is harmonic in the z -direction)

$$\int_{-\infty}^{\infty} dz \text{Li}_s(xe^{-z^2}) = \sqrt{\pi} \text{Li}_{s+\frac{1}{2}}(x), \quad (3.35)$$

which motivates using a dilogarithm function for fits,

$$n_c(x, y) = n_0 \text{Li}_2 \left[-\exp \left(q - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2} \right) \right] / \text{Li}_2(-e^q). \quad (3.36)$$

$q = \beta\mu$ is the logarithm of the fugacity, which is related to the temperature through [79]

$$\frac{T}{T_F} = [-6 \text{Li}_3(-e^q)]^{-1/3} \quad (3.37)$$

In our experience, using the fugacity itself in the fit function provides similar results.

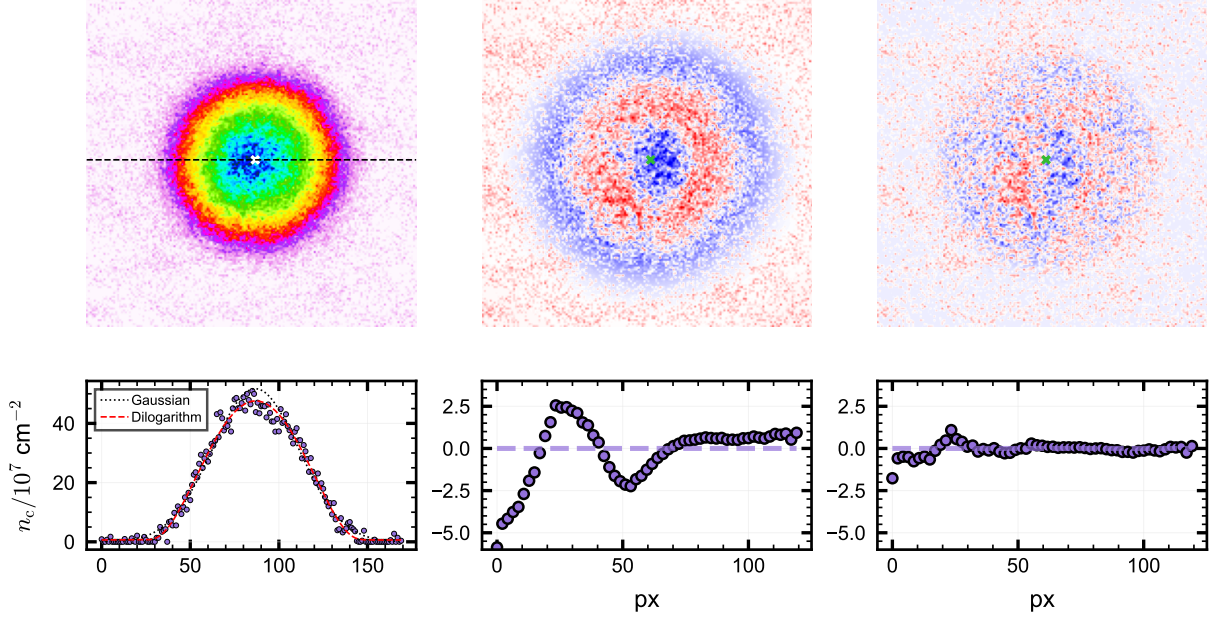


Figure 3.3: Extracting thermodynamical parameters from numerical fits of ToF images. Upper left: a DFG of $2 \cdot 10^5$ ^{40}K atoms after 14ms of ToF. The cross labels the center of the cloud used for the radial integral in the next two plots. Lower left: a cross section of the cloud at the black dashed line in the upper left plot. Middle: fit residue, $\varepsilon(r) = \int d\theta n_c(r, \theta) - n_{\text{fit}}(r, \theta)$, from fitting to a two dimensional Gaussian. The lower plot is a radial integral. Right: $\varepsilon(r)$ from fitting to a dilogarithm function. For this particular run, we find $T/T_F = 0.06$ using Eqn. (3.37).

Experimentally, we often fit to Gaussian functions for simplicity, and the limiting behavior Eqn. (3.13) means that Gaussian fits usually works pretty well. For degenerate gases, the deviation from Gaussian functions and Thomas-Fermi profiles (both bosons and fermions) is clearly visible from the fit residuals, see Fig. 3.3. The density profile of DFGs given in Eqn. (3.27) has a flatter distribution, and a more abrupt decrease in density near the edge of the cloud, so Gaussian fits usually overestimate the density near the center and the wings. The dilogarithm fitting function given in Eqn. (3.36) provides much better fits.

For BECs, the integral of the Thomas-Fermi profile (Eqn. (3.22)) along one dimension is straightforward. For harmonic potentials, the fitting function is

$$n_c(x, y) = n_0 \max \left(1 - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2}, 0 \right)^{3/2}. \quad (3.38)$$

The discussion here is suitable for characterizing bulk gases. For a brief discussion on thermometry of fermions in lattices, see Sec. 7.3.2.

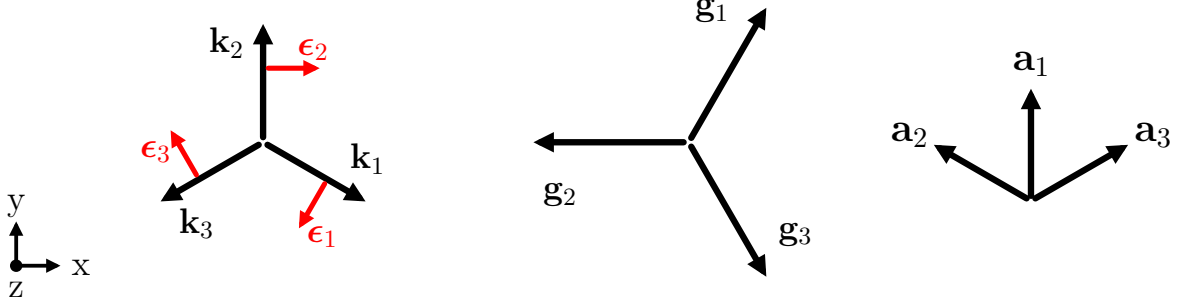


Figure 3.4: Directions of the lattice vectors defined in this section. y points south.

3.3 Lattice potential

3.3.1 Conventions

The conventions I use for lattice vectors in our lab are the same as in [52]. I made an effort to stick pedantically to the terminologies of Bravais lattice (see e.g. [85], chapter 4). The wave vectors of the three lattice beams lie in the x - y plane, and are given by

$$\mathbf{k}_1 = k \begin{pmatrix} \frac{\sqrt{3}}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix}, \quad \mathbf{k}_2 = k \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{k}_3 = k \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix}, \quad (3.39)$$

where $k = 2\pi/\lambda$. I will use lower case letters $\mathbf{k}$ for vectors defined with $\lambda = \lambda_{532} = 532$ nm, and upper case letters $\mathbf{K}$ for $\lambda = \lambda_{1064} = 1064$ nm, and similarly for other vectors defined below. ($\mathbf{k}_i = 2\mathbf{K}_i$.) I will often refer to the lattice beams propagating in the direction of $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$ as B1, B2 and B3, respectively.

The in-plane polarization vectors are perpendicular to the wave vectors, and are given by:

$$\boldsymbol{\epsilon}_1 = \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad \boldsymbol{\epsilon}_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \boldsymbol{\epsilon}_3 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}. \quad (3.40)$$

Lattices with out-of-plane polarizations are not used in the works described in this thesis, and interested readers are referred to [52].

The primitive vectors are defined as $\mathbf{G}_i = \mathbf{K}_j - \mathbf{K}_k$ for even permutations of $\{i, j, k\}$, giving

$$\mathbf{G}_1 = G \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad \mathbf{G}_2 = G \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad \mathbf{G}_3 = G \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad (3.41)$$

where $G = \sqrt{3}K$. This definition has a very nice physical picture: an atom in a far-detuned optical lattice undergoes a two-photon scattering process, where it virtually absorbs a photon from one of the beam, and emits into another beam. We will take $\mathbf{G}_1$ and $\mathbf{G}_2$ as our basis

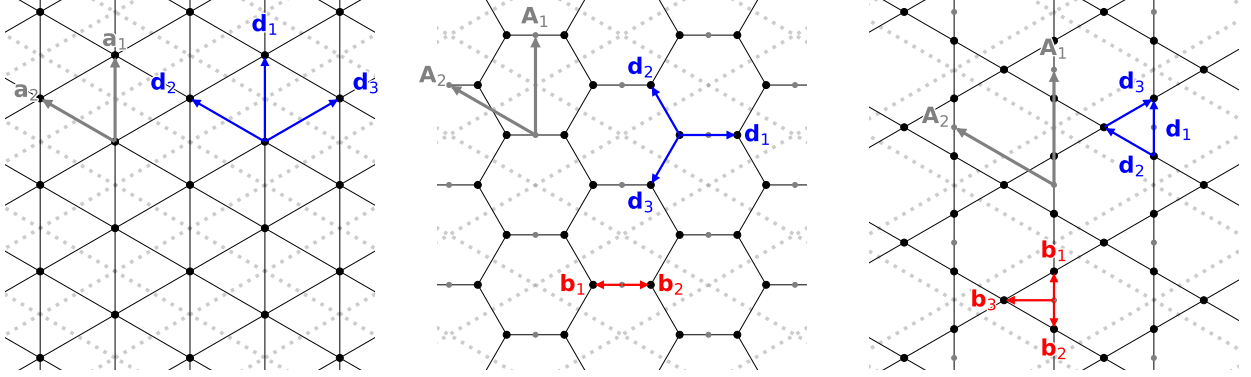


Figure 3.5: Visualization of the structures of the triangular, honeycomb, and kagome lattices. Unit cells are delineated by gray dotted lines. Black solid lines connect neighboring lattice sites.

vectors of the reciprocal space², and $\mathbf{G}_3$ is defined for convenience. ($\mathbf{G}_3 = -\mathbf{G}_1 - \mathbf{G}_2$) Any reciprocal lattice vector can then be written as a sum of integer multiples of the primitive vectors, $\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2 + n_3\mathbf{G}_3$.

The lattice vectors satisfy $\mathbf{A}_i \cdot \mathbf{G}_j = 2\pi\delta_{ij}$ ($i, j = 1, 2$), which give

$$\mathbf{A}_1 = A \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbf{A}_2 = A \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{A}_3 = A \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad (3.42)$$

where $A = 2\lambda_{1064}/3$ is the lattice constant. $\mathbf{A}_3$ is defined for convenience. Importantly, A is not the spacing between neighboring sites, but rather the spacing between unit cells.

Lattices with more than one sublattice sites is called a “lattice with a basis” in [85]. Basis vectors specify the positions of sublattice sites in a unit cell. The basis of the triangular lattice can be trivially chosen to be a single point, the zero vector. The lattice spacing is then given by $a_{\text{tri}} = 2\lambda_{532}/3 = 355 \text{ nm}$. This is also the lattice spacing of the kagome lattice, a_{kag} .

We will take the basis of the honeycomb lattice³ to be

$$\mathbf{b}_1^{\text{hc}} = a_{\text{hc}} \begin{pmatrix} -\frac{1}{2} \\ 0 \end{pmatrix}, \quad \mathbf{b}_2^{\text{hc}} = a_{\text{hc}} \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \quad (3.43)$$

where $a_{\text{hc}} = 2\lambda_{1064}/\sqrt{27} = 410 \text{ nm}$ is the lattice spacing of honeycomb lattices.

²“Basis vectors” in the language of linear algebra, i.e. they span the whole 2D momentum space. Not to be confused with the “basis” of Bravais lattices, which specifies the positions of sublattice sites in each unit cell.

³I will specifically use “hexagonal” lattice to refer to the Bravais lattice spanned by $\mathbf{G}_1$ and $\mathbf{G}_2$. All the lattices that can be realized in our experiment are hexagonal lattices, but with different bases. For example, “triangular” lattices are hexagonal lattices with a one-point basis. In literatures, honeycomb lattices are often referred to as hexagonal lattices, and hexagonal lattices are also called triangular lattices. Exactly...

Finally, the basis of the kagome lattice is taken to be

$$\mathbf{b}_1^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{b}_2^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} 0 \\ -\frac{1}{2} \end{pmatrix}, \quad \mathbf{b}_3^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}. \quad (3.44)$$

The vectors connecting neighboring lattice sites, which I will denote as $\mathbf{d}$, are given by (also see Sec. 3.4.2 on how they can be defined from the lattice and basis vectors)

$$\mathbf{d}_1^{\text{tri}} = a_{\text{tri}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbf{d}_2^{\text{tri}} = a_{\text{tri}} \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{d}_3^{\text{tri}} = a_{\text{tri}} \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad (3.45)$$

$$\mathbf{d}_1^{\text{hc}} = a_{\text{hc}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{d}_2^{\text{hc}} = a_{\text{hc}} \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad \mathbf{d}_3^{\text{hc}} = a_{\text{hc}} \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad (3.46)$$

$$\mathbf{d}_1^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbf{d}_2^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{d}_3^{\text{kag}} = a_{\text{kag}} \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad (3.47)$$

for triangular, honeycomb, and kagome lattices, respectively. See Fig. 3.5 for a visualization of the real space vectors.

The recoil energy defines the natural energy scale in the system. In our experiment, there are four of them, given by

$$\begin{aligned} E_{r,532}^{\text{K}} &= \frac{\hbar^2 k^2}{2m_{\text{K}}} = h \cdot 17.639 \text{ kHz} \\ E_{r,1064}^{\text{K}} &= \frac{\hbar^2 K^2}{2m_{\text{K}}} = h \cdot 4.410 \text{ kHz} \\ E_{r,532}^{\text{Rb}} &= \frac{\hbar^2 k^2}{2m_{\text{Rb}}} = h \cdot 8.111 \text{ kHz} \\ E_{r,532}^{\text{Rb}} &= \frac{\hbar^2 K^2}{2m_{\text{Rb}}} = h \cdot 2.028 \text{ kHz} \end{aligned} \quad (3.48)$$

m_{K} here is the mass of ^{40}K , since we have not yet cooled ^{39}K to degeneracy. I will often drop the species label when it is clear by context which species we are working with. I will typically use the recoil energy of the 532 nm (1064 nm) light as a unit for the 532 nm (1064 nm) lattice.

3.3.2 Optical lattice potential

We will assume that the lattice beam intensity is roughly uniform across the whole atom cloud, so that the lattice beams can be approximated as plane waves⁴. The intensity pattern is then given by

$$I(\mathbf{r}) = I_0 |r_1 e^{i(\mathbf{k}_1 \cdot \mathbf{r} + \phi_1)} \boldsymbol{\epsilon}_1 + e^{i\mathbf{k}_2 \cdot \mathbf{r}} \boldsymbol{\epsilon}_2 + r_3 e^{i(\mathbf{k}_3 \cdot \mathbf{r} + \phi_3)} \boldsymbol{\epsilon}_3|^2, \quad (3.49)$$

⁴This is a very good approximation for Rb BECs, where the Thomas-Fermi radius is around 8 μm . For a DFG with $8 \cdot 10^4$ atoms, the Thomas-Fermi radius is around 20 μm , which is still small compared to the beam waist of lattice beams, which is around 80 μm .

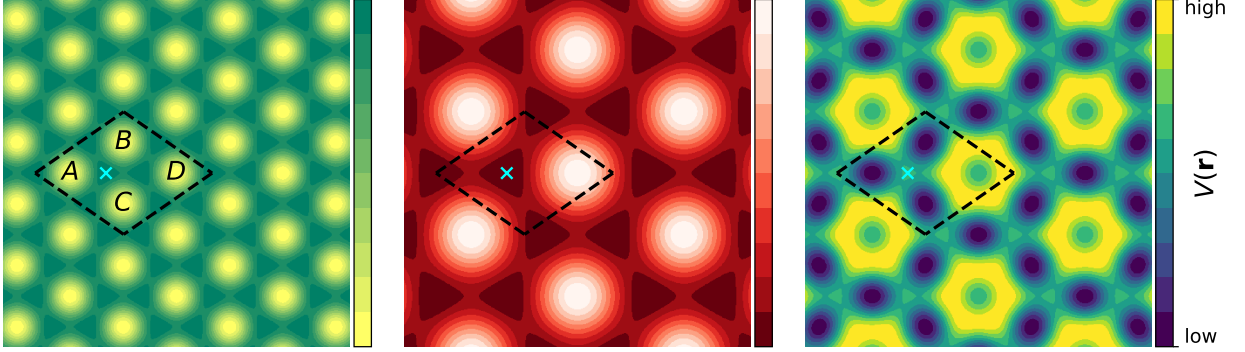


Figure 3.6: Real space potentials of the triangular (left), honeycomb (middle), and kagome (right) lattices. Cyan crosses are visual guides. Black dashed lines enclose one unit cell of the kagome lattice. (For the ; for the honeycomb lattice, this is displaced from the unit cell choice in Fig. 3.5)

where $\phi_{1(3)}$ and $r_{1(3)}$ are the detuning and relative field strengths between B1 (B3) and B2, respectively. $I_0 = 2\epsilon_0 c E_2^2$ is the intensity of B2 with electric field amplitude E_2 . Note that the relative intensities between B1 (B3) and B2 are given by $r_{1(3)}^2$.

Following appendix A, we find that Eqn. 3.49 simplifies to

$$I(\mathbf{r}) = I_0 [c_0 - r_1 \cos(\mathbf{g}_3 \cdot \mathbf{r} + \phi_1) - r_3 \cos(\mathbf{g}_1 \cdot \mathbf{r} - \phi_3) - r_1 r_3 \cos(\mathbf{g}_2 \cdot \mathbf{r} + \phi_3 - \phi_1)], \quad (3.50)$$

where $c_0 = r_1^2 + 1 + r_3^2$. Multiplying Eqn. 3.50 by $-\alpha^s/2\epsilon_0 c$ (see Eqn. (3.6)) then gives the optical potential experienced by the atoms.

The lattice depth is defined as the peak-to-peak value of $V(\mathbf{r})$. Therefore, we rewrite Eqn. (3.50) for the case $r_1 = r_3 = 1$ as

$$V(\mathbf{r}) = \frac{2}{9} V_{\text{lat}} [3 - \cos(\mathbf{g}_3 \cdot \mathbf{r} + \phi_1) - \cos(\mathbf{g}_1 \cdot \mathbf{r} - \phi_3) - \cos(\mathbf{g}_2 \cdot \mathbf{r} + \phi_3 - \phi_1)], \quad (3.51)$$

where $V_{\text{lat}} = -(9/4\epsilon_0 c)\alpha^s I_0$ is the lattice depth. This holds for both the 532 nm and the 1064 nm lattice, but they results in different lattice geometries since $\alpha^s < 0$ for 532 nm, and $\alpha^s > 0$ for 1064 nm. I will write $V_{532} > 0$ and $V_{1064} < 0$ for the two lattices.

To create an optical kagome lattice, we choose $\phi_1 = \phi_3 = 0$ in Eqn. (3.51) for both 532 nm and 1064 nm lattices. Fig. 3.6 shows the resulting lattice potentials, with lattice depths chosen to be $V_{532} = 2E_{r,532} = 8E_{r,1064} = -V_{1064}$. The unit cell of the superlattice is determined by the long wavelength 1064 nm lattice, which contains four 532 nm lattice sites that we label as A, B, C and D. When the chemical potential of atoms is lower than the D-site offsets, the other three sites form the kagome geometry shown in Fig. 3.5.

Imbalanced lattices break the rotational symmetry and can be interesting. Note, however, that the inversion symmetry cannot be broken by imbalancing the lattice beams alone, since cosine is an even function. The easiest way to break inversion symmetry in our system is then (i) by using diagonal polarization for a monochromatic lattice, or (ii) by forming a

superlattice with displacement without any particular symmetry. In both cases, different on-site offsets are introduced to each sublattice sites. For the case of two-band systems, the offsets correspond to diagonal “mass” terms, in analogy to quantum electrodynamics [86].

3.4 Band structure calculation

Since the lattice potential in our system is very simple, it is straightforward for us to numerically calculate the band structure and Bloch states to high precision (Sec. 3.4.1). It is nonetheless very instructive to model our system using tight-binding approximation, since it is conceptually simple, and is the basis of theoretical models of interest, such as the Hubbard model.

3.4.1 Plane wave expansion

The calculation presented in this section is already in previous theses [51, 52, 53], but is included again to (i) define notations used in later chapters, and (ii) to include relative detunings and intensity imbalances explicitly in the expression. The basic idea is to express the Bloch states with a Fourier series expansion, and then solve the Schrödinger equation.

The Bloch theorem states that the eigenstates, or Bloch states, can be written as

$$\psi_{\mathbf{q}}^{(n)}(\mathbf{r}) = \langle \mathbf{r} | \psi_{\mathbf{q}}^{(n)} \rangle = e^{i\mathbf{q} \cdot \mathbf{r}} u_{\mathbf{q}}^{(n)}(\mathbf{r}), \quad (3.52)$$

where $\mathbf{q}$ is called the quasimomentum, n labels the band number, and $u_{\mathbf{q}}^{(n)}(\mathbf{r}) = \langle \mathbf{r} | u_{\mathbf{q}}^{(n)} \rangle$ is a periodic function with the same periodicity of the lattice. Using (3.52), we can write the Schrödinger equation as

$$\left(\frac{(\hat{\mathbf{p}} + \hbar \mathbf{q})^2}{2m} + V_{\text{lat}}(\mathbf{r}) \right) u_{\mathbf{q}}^{(n)}(\mathbf{r}) = E_{\mathbf{q}}^{(n)} u_{\mathbf{q}}^{(n)}(\mathbf{r}), \quad (3.53)$$

where $E_{\mathbf{q}}^{(n)}$ is the eigenenergy of the n^{th} -band state with quasimomentum $\mathbf{q}$. This can be solved by expanding both $V_{\text{lat}}(\mathbf{r})$ and $u_{\mathbf{q}}^{(n)}(\mathbf{r})$ in Fourier series.

For the lattice potential term, we define three “J-subsets” to account for beam imbalances, one for each beam pair: (as a reminder, lower (upper) case letters are for the 532 nm (1064 nm) lattice, respectively)

$$\begin{aligned} \mathcal{J}_{12} &= \{(1, 1), (-1, -1)\} \\ \mathcal{J}_{23} &= \{(1, 0), (-1, 0)\} \\ \mathcal{J}_{13} &= \{(0, 1), (0, -1)\} \\ \mathcal{J} &= \mathcal{J}_{12} \cup \mathcal{J}_{23} \cup \mathcal{J}_{13} \end{aligned} \quad (3.54)$$

(for 532 nm lattice, multiply all the J-set components by 2), and the in-plane lattice potential, including relative intensities R 's and phases Φ 's, can now be rewritten as

$$V(\mathbf{r}) = V_{\text{lat}} \left(\frac{2}{3} - \frac{1}{9} \sum_{(a,b) \in \mathcal{J}} R_{(a,b)} e^{i(\mathbf{G}_{(a,b)} \cdot \mathbf{r} + \Phi_{(a,b)})} \right), \quad (3.55)$$

where $\mathbf{G}_{(a,b)} = a\mathbf{G}_1 + b\mathbf{G}_2$, and (similar for $r_{(a,b)}$ and $\phi_{(a,b)}$)

$$R_{(a,b)} = \begin{cases} R_1 & , (a,b) \in \mathcal{J}_{12} \\ R_3 & , (a,b) \in \mathcal{J}_{23} \\ R_1 R_3 & , (a,b) \in \mathcal{J}_{13} \end{cases} \quad \Phi_{(a,b)} = \text{sgn}(a+b) \times \begin{cases} -\Phi_1 & , (a,b) \in \mathcal{J}_{12} \\ -\Phi_3 & , (a,b) \in \mathcal{J}_{23} \\ \Phi_3 - \Phi_1 & , (a,b) \in \mathcal{J}_{13} \end{cases}$$

For the periodic function, we have

$$u_{\mathbf{q}}^{(n)}(\mathbf{r}) = \langle \mathbf{r} | u_{\mathbf{q}}^{(n)} \rangle = \langle \mathbf{r} | \left(\sum_{j,k} c_{(j,k)} |\mathbf{G}_{(j,k)}\rangle \right) = \sum_{j,k \in [-N,N]} c_{(j,k)} e^{i\mathbf{G}_{(j,k)} \cdot \mathbf{r}}, \quad (3.56)$$

where in the last line we restricted $|j|$ and $|k|$ to N , the largest plane wave component that we consider in the expansion. N is chosen such that the observables of interest (such as eigenenergies) does not change with larger N . For the lattice depths and quasimomenta used in our works, $N = 5 \sim 6$ is usually large enough.

We can now rewrite Eqn. (3.53) as

$$\begin{aligned} \sum_{j,k} \sum_{(a,b) \in \mathcal{J}} \sum_{(c,d) \in \mathcal{J}'} \left[\frac{\hbar^2(\mathbf{G}_{(j,k)} + \mathbf{q})^2}{2m} + V_{1064} \left(\frac{2}{3} - \frac{1}{9} R_{(a,b)} e^{i(\mathbf{G}_{(a,b)} \cdot \mathbf{r} + \Phi_{(a,b)})} \right) \right. \\ \left. + V_{532} \left(\frac{2}{3} - \frac{1}{9} r_{(c,d)} e^{i(\mathbf{G}_{(c,d)} \cdot \mathbf{r} + \phi_{(c,d)})} \right) \right] c_{(j,k)} e^{i\mathbf{G}_{(j,k)} \cdot \mathbf{r}} = \sum_{j,k} E_{\mathbf{q}}^{(n)} c_{(j,k)} e^{i\mathbf{G}_{(j,k)} \cdot \mathbf{r}}. \end{aligned} \quad (3.57)$$

Remember that $V_{532} > 0$ and $V_{1064} < 0$. By matching the coefficients of the terms with the same plane wave components in Eqn. (3.57), we then get the following linear equation for the coefficient $c_{(j,k)}$:

$$\begin{aligned} E_{\mathbf{q}}^{(n)} c_{(j,k)} = \left(\frac{\hbar^2(\mathbf{G}_{(j,k)} + \mathbf{q})^2}{2m} + \frac{2}{3}(V_{1064} + V_{532}) \right) c_{(j,k)} - \frac{1}{9} V_{1064} \sum_{(a,b) \in \mathcal{J}} R_{(a,b)} e^{i\Phi_{(a,b)}} c_{(j-a,k-b)} \\ - \frac{1}{9} V_{532} \sum_{(c,d) \in \mathcal{J}'} r_{(c,d)} e^{i\phi_{(c,d)}} c_{(j-c,k-d)}. \end{aligned} \quad (3.58)$$

This can be written as a matrix equation $\mathbf{H}(\mathbf{q}) |u_{\mathbf{q}}^{(n)}\rangle = E_{\mathbf{q}}^{(n)} |u_{\mathbf{q}}^{(n)}\rangle$, where (writing $s = (j, k)$ for simplicity)

$$\mathbf{H}(\mathbf{q})_{s,s'} = \begin{cases} \hbar^2(\mathbf{G}_s + \mathbf{q})^2/2m + (2/3)(V_{1064} + V_{532}) & s = s' \\ (R_l e^{i\Phi_l}/9)V_{1064} & l = s - s' \in \mathcal{J} \\ (r_l e^{i\phi_l}/9)V_{532} & l = s - s' \in \mathcal{I} \\ 0 & \text{otherwise.} \end{cases} \quad (3.59)$$

This is an eigenvalue problem that can be easily solved numerically for each $\mathbf{q}$. We note that while m is dependent on the species used in the experiment, the calculation can be made to adapt easily to different species if the lattice depths are measured in units of the 1064 nm recoil energy. For example, by writing $\tilde{V}_{1064} = V_{1064}/E_{r,1064}$ and $\tilde{V}_{532} = V_{532}/E_{r,1064}$, the diagonal terms in Eqn. (3.59) becomes

$$\mathbf{H}(\mathbf{q})_{s,s} = (\tilde{\mathbf{G}}_s + \tilde{\mathbf{q}})^2 + (2/3)(\tilde{V}_{1064} + \tilde{V}_{532}), \quad (3.60)$$

where $\tilde{\mathbf{G}} = \mathbf{G}/K$ and $\tilde{\mathbf{q}} = \mathbf{q}/K$. One then recovers energy in SI units by multiplying the resulting eigenvalues by $E_{r,1064}$.

Since $\mathbf{H}(\mathbf{q})$ is Hermitian, the eigenstates can be chosen to be real (i.e. $c_{i,j} \in \mathbb{R}$). There is still a gauge degree of freedom, since $c_{i,j} \rightarrow -c_{i,j}$ gives the same state. This will be relevant for chapter 6, where the choice of gauge affects the position of Dirac strings.

Given a state $|u_{\mathbf{q}}^{(n)}\rangle$, we can now calculate the population in peak (j, k) , given by

$$P_s = |c_s|^2. \quad (3.61)$$

For $\mathbf{q} = \mathbf{0}$, we note that $[\mathbf{H}, \mathcal{P}] = 0$, where $\mathcal{P}$ is the parity operator. This implies that $\mathcal{P} |u_{\mathbf{q}}^{(n)}\rangle \propto |u_{\mathbf{q}}^{(n)}\rangle$, and in particular, the time-of-flight images of the ground state ($\mathbf{q} = \mathbf{0}$, $n = 1$) of any lattice should be inversion symmetric.

3.4.2 Tight-binding model

The tight-binding model only considers one or a few orbitals on each site, called the Wannier states. Wannier states are most straightforwardly defined as the Fourier transform of Bloch states [85], but more sophisticated constructions that iteratively finds the maximally localized Wannier states exists [87]. As a first approximation, we can approximate each lattice site as a two-dimensional harmonic oscillator. There is exactly one ground state with Gaussian-like wave function, and the Bloch bands formed by only considering these states in the model are called s -bands. Similarly, there are two states with one unit of excitation, p_x and p_y , and the bands formed by considering these states are called p -bands.

This model is very convenient for studying few-band systems, and it is a good approximation of the numerical solution from Sec. 3.4.1 when the couplings between s -orbitals and

higher orbitals are small, and if the s -orbitals are sufficiently localized such that higher order hoppings can be ignored. Most generally, the tight-binding Hamiltonian is given by

$$\hat{H}_{\text{TB}} = \sum_{(t,i,j) \in \mathbb{T}} t \hat{c}_i^\dagger \hat{c}_j + \text{h.c.}, \quad (3.62)$$

where $\mathbb{T}$ specifies the connectivity of the lattice structure. Here we only consider models with translational invariance, so that they can be diagonalized after Fourier transform. For example, in a honeycomb lattice, one way to specify the lattice is to take the sublattice site operators to be a and b , and let $\mathbb{T} = \{(-t, i, j) | (i, j) \text{ are n.n.}\}$ (n.n. stands for nearest neighbors). In this case, the Hamiltonian becomes

$$\hat{H}_{\text{TB}}^{\text{hc}} = - \sum_{\langle i, j \rangle} t \hat{a}_i^\dagger \hat{b}_j + \text{h.c.}, \quad (3.63)$$

where it is understood that the lattice geometry is that of a honeycomb lattice. This is the most common but somewhat inconvenient way to write the Hamiltonian, since it looks the same for any lattice geometry, and when one perform Fourier transform to get the momentum space Hamiltonian, one must have the lattice structure in mind.

A different way to write down the same Hamiltonian that avoids this issue is to sum over *unit cells* instead of lattice sites. I will continue to use $\mathbf{A}_1$ and $\mathbf{A}_2$ as the lattice vectors. Now I will be more specific and write out both the unit cell spatial location $\mathbf{R}_m$ and the sublattice operator in $\mathbb{T}$. Now the same honeycomb lattice can be coded as

$$\mathbb{T} = \left\{ \left[-t, \hat{a}_{\mathbf{R}_m}, \hat{b}_{\mathbf{R}_m} \right], \left[-t, \hat{a}_{\mathbf{R}_m + \mathbf{A}_1}, \hat{b}_{\mathbf{R}_m} \right], \left[-t, \hat{a}_{\mathbf{R}_m + \mathbf{A}_2}, \hat{b}_{\mathbf{R}_m} \right] \right\}_{\forall m} \quad (3.64)$$

(there are many other ways to code this), and the tight-binding Hamiltonian is now written as a sum over unit cells,

$$\hat{H}_{\text{TB}}^{\text{hc}} = -t \sum_m \hat{a}_{\mathbf{R}_m}^\dagger \hat{b}_{\mathbf{R}_m} + \hat{a}_{\mathbf{R}_m + \mathbf{A}_1}^\dagger \hat{b}_{\mathbf{R}_m} + \hat{a}_{\mathbf{R}_m + \mathbf{A}_2}^\dagger \hat{b}_{\mathbf{R}_m} + \text{h.c.} \quad (3.65)$$

Since each of the terms take the form

$$\hat{h} = \sum_m -t \hat{a}_{\mathbf{R}_m + \mathbf{A}}^\dagger \hat{b}_{\mathbf{R}_m}, \quad (3.66)$$

we only need to know how to transcribe this particular expression in the momentum space. We can then just do this for each term mechanically.

Care must be taken on the basis used when doing Fourier transform. Throughout this thesis, I will use

$$\begin{aligned} \hat{a}_{\mathbf{k}} &= \frac{1}{\sqrt{V}} \sum_m e^{i\mathbf{k} \cdot (\mathbf{R}_m + \mathbf{r}_a)} \hat{a}_{\mathbf{R}_m} \\ \hat{a}_{\mathbf{R}_m} &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot (\mathbf{R}_m + \mathbf{r}_a)} \hat{a}_{\mathbf{k}} \end{aligned} \quad (3.67)$$

(and $a \leftrightarrow b$ for $\hat{b}$) for our transformation to the momentum space. V is the size of the system. Note the appearance of the basis vectors $\mathbf{r}_a$. The general term in Eqn. (3.66) now becomes

$$\tilde{h} = \sum_{\mathbf{k}} -te^{-i\mathbf{k} \cdot \mathbf{d}_{ab}(\mathbf{A})} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \quad (3.68)$$

where $\mathbf{d}_{ab}(\mathbf{A}) = \mathbf{A} + \mathbf{r}_a - \mathbf{r}_b$ is the distance between the sublattice sites involved. Using Eqn. 3.65 and 3.68, we obtain the momentum space Hamiltonian for the honeycomb lattice $\hat{H}_{\text{TB}}^{\text{hc}}(\mathbf{k}) = \hat{\mathbf{v}}(\mathbf{k})^\dagger H^{\text{hc}}(\mathbf{k}) \hat{\mathbf{v}}(\mathbf{k})$, where $\hat{\mathbf{v}}(\mathbf{k}) = \left(\hat{a}(\mathbf{k}) \ \hat{b}(\mathbf{k}) \right)^T$, and

$$H^{\text{hc}}(\mathbf{k}) = -t \begin{pmatrix} 0 & e^{-i\mathbf{k} \cdot \mathbf{d}_1} + e^{-i\mathbf{k} \cdot \mathbf{d}_2} + e^{-i\mathbf{k} \cdot \mathbf{d}_3} \\ e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3} & 0 \end{pmatrix} \equiv -t \begin{pmatrix} 0 & f(\mathbf{k}) \\ f(\mathbf{k})^* & 0 \end{pmatrix}, \quad (3.69)$$

where the $\mathbf{d}$ vectors are given in Eqn. (3.46)⁵. This can be easily diagonalized using properties of Pauli matrices, and one immediately sees that the eigenenergies are given by

$$E_{\pm}^{\text{hc}}(\mathbf{k}) = \pm t |f(\mathbf{k})| = \pm t \sqrt{3 + 2[\cos(\mathbf{k} \cdot \mathbf{A}_1) + \cos(\mathbf{k} \cdot \mathbf{A}_2) + \cos(\mathbf{k} \cdot \mathbf{A}_3)]}. \quad (3.70)$$

We can similarly write down the real space tight-binding Hamiltonian of a slightly generalized version of the kagome lattice, called Lieb-kagome lattices (see Fig. 3.7), whose Hamiltonian is given by

$$\hat{H}_{\text{TB}}^{\text{Lk}} = -t \sum_m r \hat{a}_{\mathbf{R}_m}^\dagger \hat{b}_{\mathbf{R}_m} + \hat{b}_{\mathbf{R}_m}^\dagger \hat{c}_{\mathbf{R}_m} + \hat{c}_{\mathbf{R}_m}^\dagger \hat{a}_{\mathbf{R}_m} + r \hat{b}_{\mathbf{R}_m - \mathbf{A}_1}^\dagger \hat{a}_{\mathbf{R}_m} + \hat{c}_{\mathbf{R}_m - \mathbf{A}_2}^\dagger \hat{a}_{\mathbf{R}_m} + \hat{c}_{\mathbf{R}_m + \mathbf{A}_1 - \mathbf{A}_2}^\dagger \hat{b}_{\mathbf{R}_m} + \text{h.c.} \quad (3.71)$$

r is a parameter that interpolates between the kagome lattice and the Lieb lattice. $r = 1$ is the typical kagome lattice, and in this case I will also write the Hamiltonian as $\hat{H}_{\text{TB}}^{\text{kag}}$. $r = 0$

⁵ $\hat{H}(\mathbf{q})$ given in Eqn. (3.69) is complex. This might be somewhat confusing if one remembers that the Hamiltonians of lattices with $\mathcal{C}_2\mathcal{T}$ symmetry can be written as real operators [88, 89], and we have taken a very “nice” approach to write down the Hamiltonian. Nothing is really at odds here, since we can indeed find a basis where the Hamiltonian is real:

$$\mathcal{U}^\dagger \hat{H}(\mathbf{q}) \mathcal{U} = -t \begin{pmatrix} C(\mathbf{q}) & S(\mathbf{q}) \\ -S(\mathbf{q}) & -C(\mathbf{q}) \end{pmatrix},$$

where

$$\begin{aligned} C(\mathbf{q}) &= \cos(-\mathbf{q} \cdot \mathbf{d}_1) + \cos(-\mathbf{q} \cdot \mathbf{d}_2) + \cos(-\mathbf{q} \cdot \mathbf{d}_3) \\ S(\mathbf{q}) &= \sin(-\mathbf{q} \cdot \mathbf{d}_1) + \sin(-\mathbf{q} \cdot \mathbf{d}_2) + \sin(-\mathbf{q} \cdot \mathbf{d}_3), \end{aligned}$$

and the unitary matrix is found by the Takagi factorization of the operator that represents the $\mathcal{C}_2\mathcal{T}$ symmetry [88], which is σ_x in the sublattice basis in the case of honeycomb lattices:

$$\sigma_x = \mathcal{U} \mathcal{U}^T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}.$$

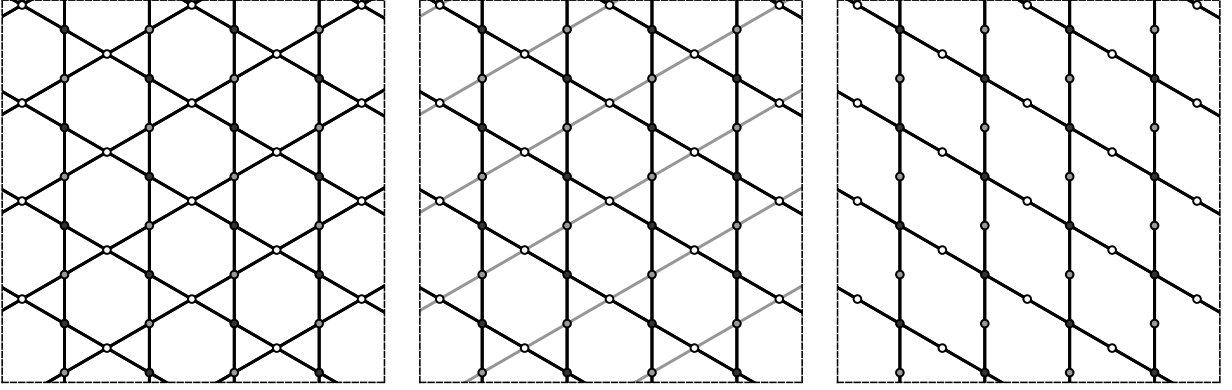


Figure 3.7: Lieb-kagome lattices. The lattice geometry is interpolated from the kagome lattice (left) to the Lieb lattice (right) by decreasing the value of r (represented by dimmer lines). This figure serves to visualize the tight-binding Hamiltonian defined in Eqn. (3.71), but we cannot produce a Lieb lattice in our experiment, due to the reason stated in the main text.

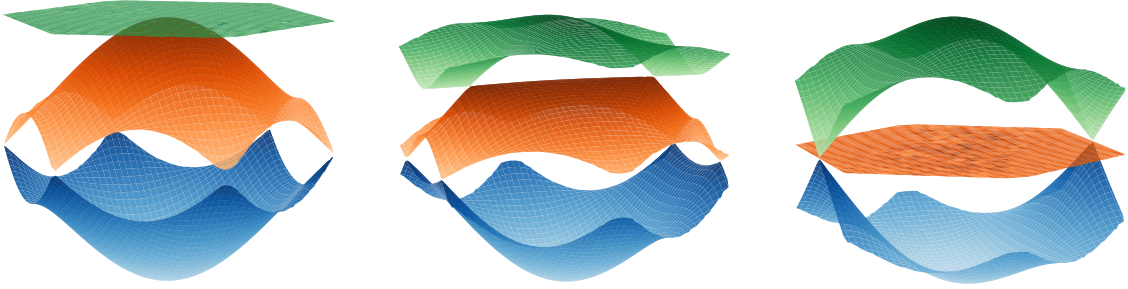


Figure 3.8: The band structures of Lieb-kagome lattices. $r = (1, 0.5, 0)$ from left to right. The left plot ($r = 1$) is the kagome lattice, and the right plot ($r = 0$) is the Lieb lattice (with a hexagonal Bravais lattice, instead of the usual square Bravais lattice).

gives the Lieb lattice. r can also be on the $\hat{b}^\dagger \hat{c}$ or the $\hat{c}^\dagger \hat{a}$ terms, which will change the axis of mirror symmetry. In our experiment, we can work with intermediate values of r by slightly imbalancing the 532 nm beams, but if the imbalance is too extreme, the lattice sites become strongly distorted, and the Wannier approximation breaks down, so we are not able to go all the way to $r = 0$.

The momentum space Hamiltonian of (3.71) is then given by $\hat{H}_{\text{TB}}^{\text{Lk}}(\mathbf{k}) = \hat{\mathbf{v}}(\mathbf{k})^\dagger H^{\text{Lk}}(\mathbf{k}) \hat{\mathbf{v}}(\mathbf{k})$,

where $\hat{\mathbf{v}}(\mathbf{k}) = \left(\hat{a}(\mathbf{k}) \ \hat{b}(\mathbf{k}) \ \hat{c}(\mathbf{k}) \right)^T$ ⁶, and

$$H^{\text{Lk}}(\mathbf{k}) = -2t \begin{pmatrix} 0 & r \cos(\mathbf{k} \cdot \mathbf{d}_3) & \cos(\mathbf{k} \cdot \mathbf{d}_2) \\ r \cos(\mathbf{k} \cdot \mathbf{d}_3) & 0 & \cos(\mathbf{k} \cdot \mathbf{d}_1) \\ \cos(\mathbf{k} \cdot \mathbf{d}_2) & \cos(\mathbf{k} \cdot \mathbf{d}_1) & 0 \end{pmatrix}. \quad (3.72)$$

The eigenenergies for generic $1 \geq r \geq 0$ can be written in terms of the cubic formula, but the expression is very long. See Fig. 3.8 for the band structure for different values of r . Setting $r = 1$ gives the Hamiltonian of the kagome lattice, $H_{\text{TB}}^{\text{kag}}(\mathbf{k})$. For the case of the kagome lattice, the eigenenergies are given by

$$E_{\text{flat}}^{\text{kag}}(\mathbf{k}) = 2t, \quad E_{\pm}^{\text{kag}}(\mathbf{k}) = E_{\pm}^{\text{hc}}(\mathbf{k}) - t. \quad (3.73)$$

In particular, the highest energy band is completely dispersionless, and the two dispersive bands share exactly the same dispersion relation as the honeycomb lattice. We note that the quantum geometry of the Bloch states is different, as we have alluded to in the introduction. An important difference, for example, is the existence of a quadratic band touching point between the flat band and the higher dispersive band at the Γ point, which is associated with a winding number of two. This is similar to the case of the honeycomb p -band touching point explored in chapter 5. Additionally, kagome lattice offer a simple model where there is nontrivial interband topology, as characterized by a topological invariant called the patch Euler class, $\chi_{23} = 1$ [90]. We will defer a more detailed discussion to Ref. [50].

3.4.3 Compact localized state

The dispersionless band in the kagome lattice band structure shown in Fig. 3.8 is known as a flat band. Flat bands are famous for hosting so-called compact localized states (CLS), which results from the geometric frustration of the lattice geometry. CLS are eigenstates of the Hamiltonian with finite amplitude only within a finite spatial region. It can be shown that CLS can be constructed in any flat band Hamiltonian with finite-range hopping [36]. In the kagome lattice, the CLS lives on hexagonal plaquettes (see Fig. 7.10 for a visualization of the state), with equal amplitudes on the six sites that alternate in the phase of the on-site wave function. Intuitively, this state cannot tunnel out of the lattice due to destructive interference.

More rigorously, we may define the CLS operator on plaquette $\diamond_{\alpha}$ for a particle with spin σ as

$$\hat{\diamond}_{\alpha,\sigma} = \frac{1}{\sqrt{6}} \sum_{i \in \diamond_{\alpha}} (-1)^i \hat{c}_{i,\sigma} \quad (3.74)$$

and the number operator associated with this CLS, $\hat{n}_{\diamond_{\alpha},\sigma} \equiv \hat{\diamond}_{\alpha,\sigma}^{\dagger} \hat{\diamond}_{\alpha,\sigma}$. From this definition, we find that $[\hat{H}_{\text{TB}}^{\text{kag}}, \hat{n}_{\diamond_{\alpha},\sigma}] = 0$, confirming that this state is an eigenstate.

⁶I am using the same notation as the honeycomb lattice — $\hat{\mathbf{v}}(\mathbf{k})$ is understood to have the right number of sublattice sites.

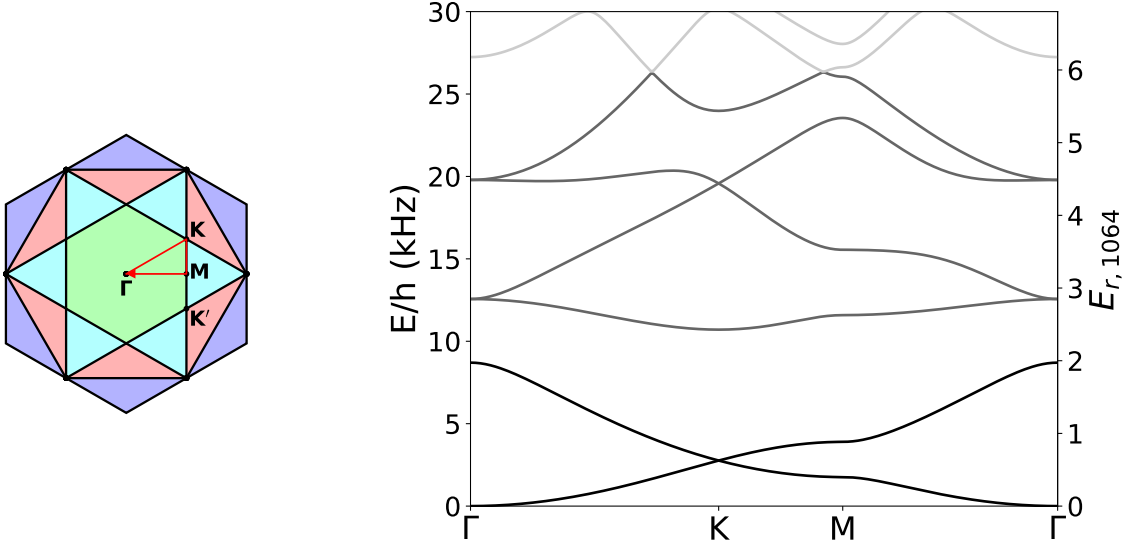


Figure 3.9: Band structure of the honeycomb lattice. Left: the quasimomentum trajectory used for the band structure plot to the right. Right: the band structure of the honeycomb lattice with lattice depth $V_{1064} = -9E_{r,1064}$. The left y -axis is evaluated for ^{40}K . The right y -axis is valid for both species. Black, gray and light gray indicates the band manifolds that would be associated to s -, p - and higher band manifolds in tight-binding models. In band structure plots, I set $E = 0$ to be at the ground state.

Note that the CLS remains an eigenstate of the system even if the lattice is not periodic, since the interference only depends on local hopping. One way to “delocalize” the CLS is by considering interactions. For example, by introducing the on-site Hubbard interaction term $\hat{U} = U \sum_i \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma}$, the CLS operator no longer commutes with the Hamiltonian:

$$[\hat{U}, n_{\alpha}] = \frac{U}{\sqrt{6}} \sum_{i \in \alpha} (-1)^i \hat{n}_{i,-\sigma} (\hat{c}_{i\sigma}^\dagger \hat{\alpha}_{\alpha,\sigma} - \hat{\alpha}_{\alpha,\sigma}^\dagger \hat{c}_{i\sigma}). \quad (3.75)$$

(But note that if $\hat{n}_{i,-\sigma}$ evaluates to a constant for all i , then the right hand side becomes zero.)

3.4.4 Honeycomb lattice band structure

Fig. 3.9 shows the numerically calculated band structure of the honeycomb lattice up to the sixth band for a typical lattice depth used in our experiments. One of the most striking feature are the linear band touching points (LBTP) at the high symmetry K and K' points, which are the well known Dirac points. These and the quadratic touching points (QBTP) in the p -bands are the main subjects of chapter 5. There are also van Hove points at the M and M' points, and the hexagons formed by them are constant energy lines, resulting in Fermi surface nesting [35].

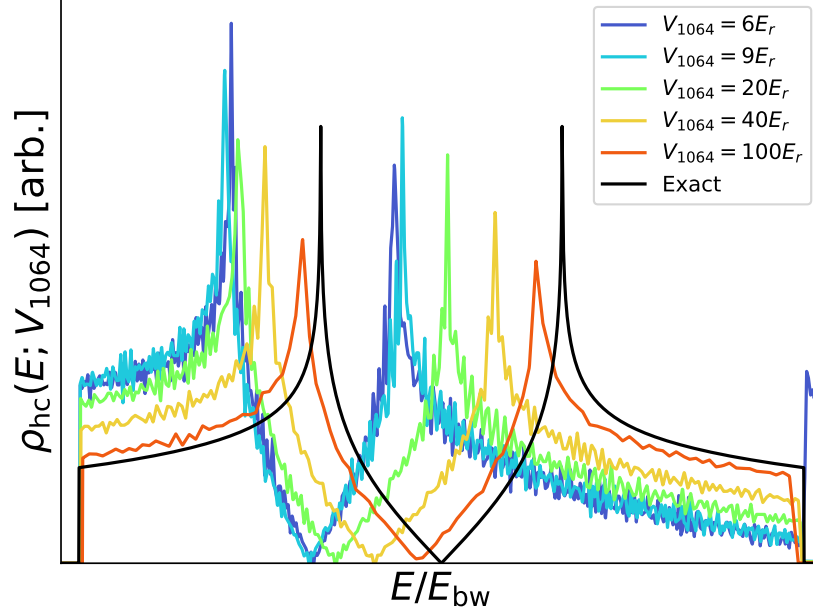


Figure 3.10: DoS of honeycomb lattices evaluated at different lattice depths, limited to the energy range that covers the s -bands. Each numerical DoS is obtained by sampling 11600 points in the first Brillouin zone. $\rho_{\text{hc}}(E; V_{1064})$ is normalized so that the bandwidths of the s -bands are the same in the figure, and that the areas under the curve are the same. At $V_{1064} = 6E_r$, the energy around Γ in the lowest p -band is lower than the energy around K in the higher s -band, so there is no (indirect) band gap between the s - and p -bands. At higher bandwidths, the number of bins assigned to the s -band is too few, resulting in the smooth round off at the band edges. The exact curve is from the lattice Green's function of the honeycomb lattice [91].

The potential barrier between neighboring lattice sites in a honeycomb lattice is only $V_{1064}/9$ [52]. This means that we expect some quantitative deviations from the tight-binding prediction. For example, the DoS of the system $\rho_{\text{hc}}(E; V_{1064})$ doesn't quite approach the tight-binding DoS until the lattice is very deep, see Fig. 3.10. $\rho_{\text{hc}}(E; V_{1064})$ is calculated numerically from the band structure: one first samples the Brillouin zone homogeneously on a fine grid, which yields the full two-dimensional band structure. By binning the resulting eigenenergies in a histogram of fine energy bins, we get a numerical approximation of the DoS. Note that $\rho_{\text{hc}}(E; V_{1064})$ only accounts for the dispersion relation in the lattice dimensions, which is taken to be the xy -plane in this thesis. We will discuss how to account for the weakly confining z -dimension in Sec. 3.4.6.

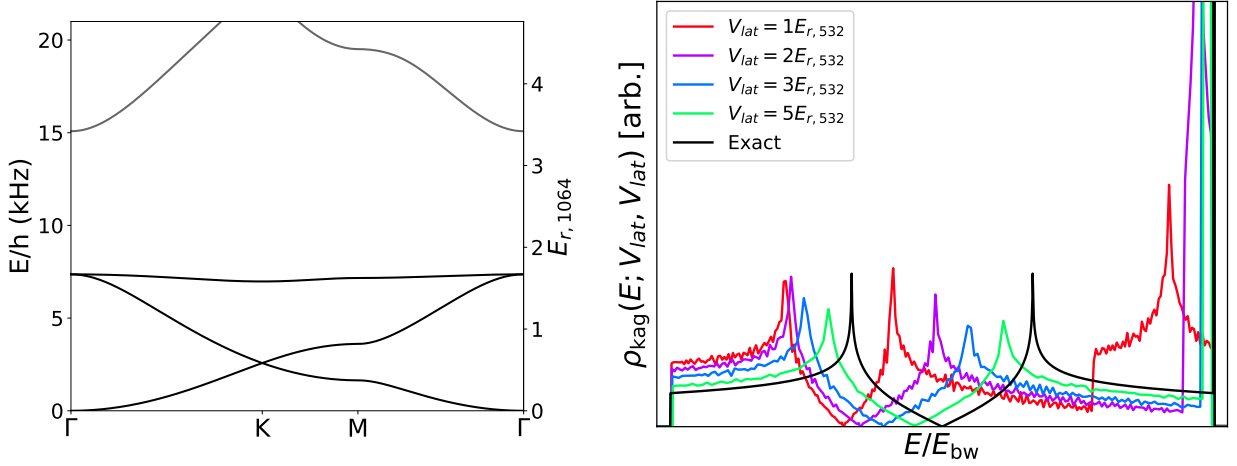


Figure 3.11: Left: band structure of the kagome lattice evaluated along the same quasi-momentum trajectory as shown in Fig. 3.9. The lattice depths are chosen to be $V_{532} = 2E_{r,532} = 8E_{r,1064} = -V_{1064}$. The left y -axis is evaluated for ^{40}K . Right: DoS of kagome lattices evaluated at different lattice depths, limited to the energy range that covers the s -bands. Each numerical DoS is obtained by sampling 11600 points in the first Brillouin zone. $\rho_{\text{kag}}(E; V_{\text{lat}}; V_{\text{lat}})$ is normalized so that the bandwidths of the s -bands are the same in the figure, and that the areas under the curve are the same. The s -bands are gapped from higher bands for all the lattice depths chosen. The exact curve is from the lattice Green's function of the kagome lattice [92, 93], with the delta function at the flat band replaced with a rectangular function with a width equal to 0.2% of the s -band bandwidth to help with visualization.

3.4.5 Kagome lattice band structure

The band structure of a kagome lattice is plotted in Fig. 3.11. The most striking feature of the band structure is the almost flat third band. This arises from the geometrical frustration of the kagome geometry (see Sec. 3.4.3). The third band is exactly flat in the tight-binding model involving only the s -orbitals, and the deviation from plane wave expansion can be understood as corrections from the s -band tight-binding model, such as non-vanishing hopping amplitudes to farther neighbors, coupling between s - and higher orbitals, and the coupling to the higher energy sublattice site D.

As we have seen in Sec. 3.4.2, the lower two bands share the same dispersion relation as the honeycomb lattice. Besides from the LBTP, the s -bands of kagome lattices also feature a QBTP between the flat band and the second band. In terms of the quantum geometrical structures around those singular points, they are similar to those found in the honeycomb lattices. There is also a Fermi surface nesting, with the constant energy lines forming a hexagon at the van Hove points at M and M' , but the main difference from that of the honeycomb lattice is that the sublattice population varies strongly at different quasimomenta, which modifies the nesting vectors [35].

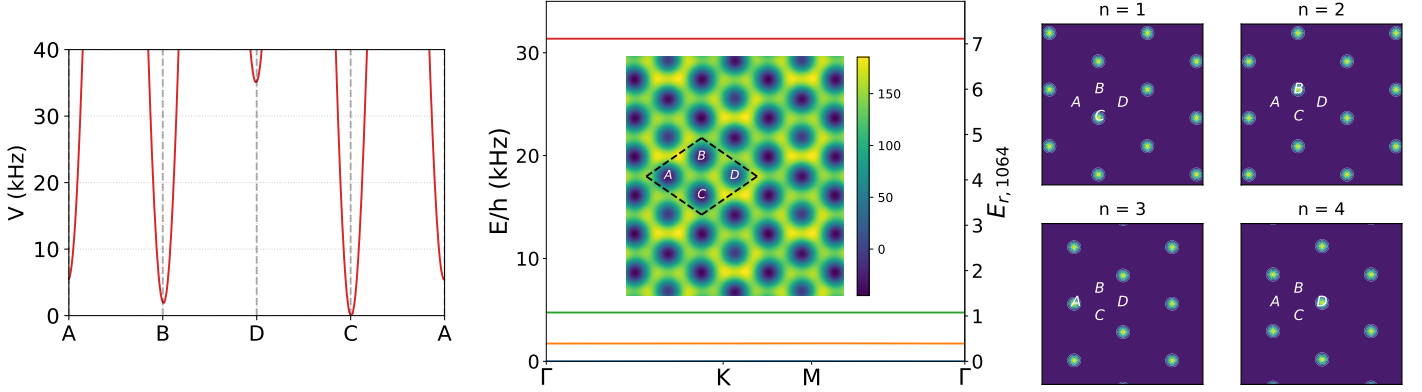


Figure 3.12: The “ABCD lattice” with the lowest four bands predominantly populating only one of the sublattice site. The lattice parameters are $V_{532} = 10E_{r,532}$, $V_{1064} = -10E_{r,1064}$, and $(\Phi_1, \Phi_3) = (\pi/4, \pi/5)$ for the 1064 nm lattice. Left: the potential of the ABCD lattice along a real space trajectory that pass through the center of the A-B-D-C-A sites, in that order. Middle: the band structure of the ABCD lattice, evaluated along the same quasimomentum trajectory as shown in Fig. 3.9. The dispersion is dominated by the on-site offsets. Inset: the real space potential of the ABCD lattice. Right: the density distribution $n_{\mathbf{q}}^{(n)}(\mathbf{r}) = |\psi_{\mathbf{q}}^{(n)}(\mathbf{r})|^2$ of the $\mathbf{q} = \mathbf{0}$ states for the four lowest bands. $n_{\mathbf{q}}^{(n)}(\mathbf{r})$ is essentially the same for any $\mathbf{q}$.

The DoS of the kagome lattice, $\rho_{\text{kag}}(E; V_{532}; V_{1064})$, can be numerically calculated in a similar way as described in the last section. The results are plotted in Fig. 3.11. Since the potential barrier between neighboring lattice sites in a kagome lattice is $(8/9)V_{532}$ [52], reaching the tight-binding limit requires lower potential depths when measured in units of recoil energies.

Hexagonal superlattices

To conceptually map the degrees of control we have over our lattice beams to the tight-binding model, we note that the 532 nm lattice mainly controls the hopping strengths t_{AB}, t_{BC} , and t_{CA} , between different sublattices. (It also changes U since it changes how localized the Wannier functions are, but U can be individually tuned with Feshbach resonances.) The 1064 nm mainly controls the on-site offsets, $V_{A,B,C,D}$. For example, with a carefully chosen relative displacement between the two lattices, it is possible to create a superlattice where each of the lower four bands has population mainly in only one of the sublattice, see Fig. 3.12. This can be useful for sublattice-resolved band mapping measurement when single-site resolution is not available, but one needs to ensure that the phase lock is sufficiently fast and precise so that the lattice potential can be quenched to this setting much faster than the tunneling time $\hbar/t$.

Understanding the superlattice potential can be tricky. At extreme power ratios $\varepsilon = V_{532}/V_{1064}$, the resulting lattice is not really a kagome lattice, but merely perturbed triangular

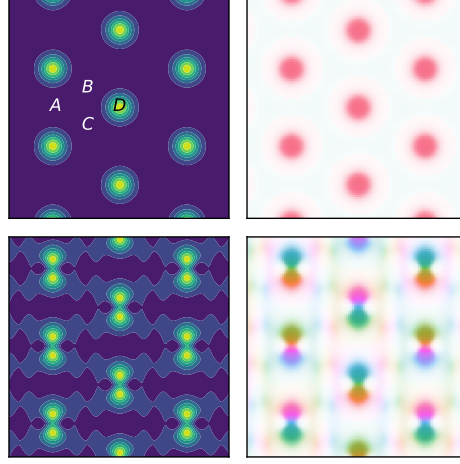


Figure 3.13: Examples of the non-trivial orbital nature of the higher bands in kagome lattices. Both states are selected from the seventh band. $\mathbf{q} = \mathbf{0}$ for the top row, and $\mathbf{q}$ is along the K-M high symmetry line. The left column and right column show density and phases of $\psi_{\mathbf{q}}^{(n)}(\mathbf{r})$, respectively.

or honeycomb lattices. Also, the higher bands in a kagome lattice at reasonable z (so that the s -bands are well-described by a kagome lattice tight-binding model) are typically not purely p -bands, but a mixture of the p -orbitals in the $\{A, B, C\}$ sites, and s -orbitals in the D sites. Exactly how they mix is determined by the on-site oscillator frequency of the 532 nm lattice sites (V_{532}), the potential offset between $\{A, B, C\}$ and D sites (V_{1064}), and the specific band and quasimomentum of the Bloch state. Example states that demonstrate this effect is shown in Fig. 3.13. In this sense, isolating p -orbital physics of kagome lattice is currently beyond reach.

3.4.6 Fermi energy in optical lattices

The optical potential used for the plane wave expansion calculation, Eqn. (3.51), is only two-dimensional. In reality, the third dimension in the z -direction is confined by the approximately harmonic potential with trap frequency ω_z due to the optical dipole traps and the lattice beams. The system can therefore be described as a lattice of cigar-shaped clouds of atoms, where the spatial extent is determined by ω_z . It is possible to create quasi-two-dimensional lattices by adding a deep one-dimensional lattice in the z -direction such that the hopping time scale $\hbar/t_z$ is much longer than the experimental time scales. We will not consider this additional lattice in this section since it is not used in the works reported in this thesis.

To account for the z -dimension, we need to combine $\rho_{\text{hc}}(E; V_{1064})$ with the DoS of a one dimensional harmonic oscillator. For independent degrees of freedoms, several densities of

states are combined using convolutions:

$$\rho(E) = \rho_1(E) * \rho_2(E) = \int_0^E d\varepsilon \rho_1(\varepsilon) \rho_2(E - \varepsilon). \quad (3.76)$$

We will take $\rho_2 = \rho_{\text{hc}}$, and for the z dimension we consider an infinitely large box (constant) potential in the z -direction. Although the DoS of a box potential diverges as inverse square root as energy approaches zero, $\rho_{\text{box}} \propto E^{-1/2}$, this is usually not a problem, since in a reasonable⁷ lattice the dispersion in the ground band is quadratic, and $\lim_{E \rightarrow 0} \rho_{\text{lat}}(E) \propto E$.

The Fermi energy can now be found by using the local density approximation, which assumes that at a position $\mathbf{r}$, the property of the gas is the same as a bulk gas in a uniform system with local chemical potential $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$. We have

$$N = \int d^3\mathbf{r} G_{\text{hc}, 3\text{D}}(E_F - V_{\text{ext}}(\mathbf{r})), \quad (3.77)$$

where $V_{\text{ext}}(\mathbf{r})$ is the external potential (usually the harmonic potential imposed by the trapping beams), and $G_{\text{hc}, 3\text{D}}(\mu)$ is the density of particles in the honeycomb lattice at chemical potential μ and zero temperature, assuming an infinite flat potential in the third dimension. We note a useful result when finding $G_{\text{hc}, 3\text{D}}(\mu)$:

$$\begin{aligned} G(\mu) &= \int_0^\mu dE \rho(E) = \int_0^\mu dE \int_0^E d\varepsilon \rho_1(E - \varepsilon) \rho_2(\varepsilon) \\ &= \int_0^\mu d\varepsilon \rho_2(\varepsilon) \int_\varepsilon^\mu dE \rho_1(E - \varepsilon) \\ &= \int_0^\mu d\varepsilon \rho_2(\varepsilon) G_1(\mu - \varepsilon) = \rho_2 * G_1(\mu). \end{aligned} \quad (3.78)$$

For the case where the z -dimension confinement is harmonic, which is the typical experiment situation, we can instead take ρ_1 to be the DoS of a harmonic oscillator. Nominally, the DoS is constant, $\rho_{\text{ho}}(E) = 1/\hbar\omega_z$, where ω_z is the trap frequency. However, when E_F is comparable in order of magnitude to $\hbar\omega_z$, it is more appropriate to replace the DoS with a Dirac comb, $\rho_{\text{ho}}(E) = \sum_{n=0}^\infty \delta(E - (n + 1/2)\hbar\omega_z)$. In this case, Eqn. (3.77) evaluates to a sum of two dimensional integrals instead of a big three dimensional integral. For harmonic confinement in the z direction, the two approaches agrees to better than 0.1% for large numbers ($O(10^5)$) of atoms.

⁷An example of an “unreasonable” lattice is the kagome lattice with negative hopping, whose flat band is the ground band.

Chapter 4

Experimental sequence

Before a description of the experimental sequence, it is instructive to understand why the sequence is designed as it is. The main change to the optical lattice experiment during my PhD is the introduction of a new atomic species, ^{40}K , which is a fermion. Due to the Pauli exclusion principle, identical fermions do not interact through s -wave scattering, and the lowest energy scattering process is p -wave scattering. This means that thermalization between ^{40}K atoms in the same internal states becomes very inefficient roughly around 100 μK and below [94]. To the best of the author’s knowledge, all of the degenerate fermi gas experiments still rely on evaporation cooling to achieve the phase space density required.

There are two main approaches to overcome the thermalization issue. The first is to trap the fermions in more than one internal states, so that atoms in different states can scatter with each other through s -wave scattering. This is how quantum degeneracy is first achieved in ultracold fermi gases, using magnetically trapped ^{40}K atoms in a mixture of $|F = 9/2, m_F = 9/2\rangle$ and $|F = 9/2, m_F = 7/2\rangle$ states [95]. The other approach is the so-called “sympathetic cooling,” where fermions thermalize with a spatially-overlapped cloud of bosons, and are indirectly cooled down as the bosons are cooled using traditional evaporative cooling methods. This is first achieved by sympathetically cooling ^6Li using ^7Li [96].

In our experiment, we opted to take the sympathetic cooling approach, where Rb is used as the coolant for ^{40}K . Rb and ^{40}K are known to be good evaporation cooling partners [58, 97], and they also share similar polarizabilities at the wavelengths of the existing optical lattice setup. While this section documents an established sequence from the creation of an ultracold quantum gas to details of everyday lattice beam calibrations, I also include an account of the challenges encountered during the design of the sequence.

4.1 Creating quantum degenerate gases

Similar to most of the optical lattice experiments, we need to first create a quantum degenerate gas before turning on the lattice. A brief overview of the cooling sequence is as follows: a 70 to 80 $^\circ\text{C}$ Rb and ^{40}K atoms are first cooled in two axes in a 2D magneto-optical

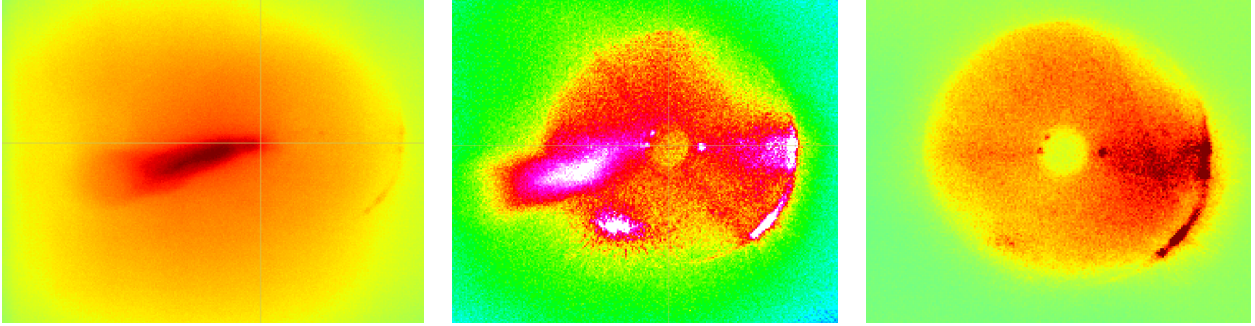


Figure 4.1: Fluorescence images of 2D MOTs of different species. Colormaps, ranges and exposure times are different for the three images. Left to right: Rb, ^{39}K , ^{40}K . The circular object in the three images is the front view of the differential pumping tube, through which we can see the fluorescence of the 3D MOT (not shown). For ^{40}K , the fluorescence strength changes as one changes the detuning of either the cooling or the repump beam, but there is no visible flux of atoms.

trap (MOT), forming a flux of atom with small radial velocity spread. This atomic flux goes through the hole in the differential pumping tube connecting the 2D MOT cell and the 3D MOT chamber and loads the 3D MOT. After loading enough atoms, we briefly switch to a compressed MOT (CMOT) configuration before optically pumping the atoms to the desired internal states and transferring to a magnetic trap. A series of coils then follow pre-programmed current ramp profiles to move the trap center to the science cell, where we achieve quantum degeneracy by radiofrequency (RF) evaporation cooling, followed by forced optical evaporation cooling in a crossed optical dipole trap (xODT). We look at each step in more detail in the sections below.

4.1.1 Magneto-optical traps

The experiment begins with loading a dual-species MOT. Due to the lower vapor pressure of potassium and low abundance of ^{40}K , the atomic flux of ^{40}K from 2D MOT is much smaller than Rb, and it takes much longer to load enough ^{40}K atoms for us. In fact, the number of ^{40}K atoms that we can load is so small that makes it difficult for us to characterize and optimize them in the 3D MOT chamber using our suboptimal MOT imaging system. Here we provide a account of how we optimize the MOT parameters, with a focus on ^{40}K .

Initial alignment of the 2D MOT

We have a camera imaging in the direction of the differential pumping tube for characterization purposes. (This camera is removed for everyday operation, since it blocks the 2D MOT push beams.) As seen in Fig. 4.1, we can easily see the beam of atoms from fluorescence imaging for Rb and ^{39}K , but we were never able to see a clear beam for ^{40}K . We confirm that we have a 2D MOT of ^{40}K indirectly through the successful loading of a ^{40}K 3D MOT. The

quarter-wave plates for each of the 2D and 3D MOT beams are first set to get the textbook configuration for MOTs, and once we have a MOT, they are adjusted empirically to get the brightest fluorescence, and finally the largest MOT we can achieve.

Our alignment procedure starts with loading a Rb 3D MOT. Due to the clearly visible atomic beam, we can easily align the beam to the hole of the differential pumping tube by adjusting the power splitting ratio in each direction, or the current going through each of the four 2D MOT coil. This was enough for us to load a 3D MOT of Rb successfully. We note that even without the 2D MOT, a very small 3D MOT can be loaded from the Rb atoms that make their way out of the 2D MOT cell into the UHV chamber. This small MOT is useful for identifying the position of the center of the quadrupole field on the security camera that monitors the 3D MOT.

We have found that we can increase the MOT loading rate by almost 50% by blocking a small portion of the 2D MOT beam near the differential pumping tube, and the loading rate is very sensitive to the position of this block. We are not entirely sure what is the cause, but suspicions include the scattered light from the tube disturbing the atomic flux, and an outward force imparted by the beam reflected by the slanted tube entrance surface. The beam blocks are pieces of papers taped to the coil mounts.

We aligned our ^{39}K MOT with the same procedure. After successfully loading a ^{39}K MOT, we were able to load a tiny ^{40}K MOT by changing the offset lock frequencies in the same afternoon, despite not being able to see a 2D MOT of ^{40}K .

Optimization of MOT loading

When switching from ^{39}K to ^{40}K MOTs, one thing to keep in mind is that the power splitting between different 3D MOT beams that optimizes ^{39}K MOTs most likely does not optimize ^{40}K MOTs. This is because the repump beams also contribute a lot to the trapping forces for ^{39}K MOTs (Sec. 2.1.2). The difference in power splitting ratio between cooling and repump beams (Sec. 2.3.1) then means that the trapping forces are very different for ^{39}K and ^{40}K . But after the ^{39}K MOT is optimized, we can usually load enough ^{40}K atoms in the MOT such that the optical densities in MOT absorption images are high enough to yield a reliable atom count. We can then optimize ^{40}K number using absorption images. (The fluorescence signal from trapped ^{40}K atoms is still too low for the shuttering technique described in the next paragraph to work.)

For initial optimization of MOT parameters, we have found a “shuttering” technique to be very useful, if the fluorescence signal from the MOT is strong enough to be monitored on a photodiode that is sufficiently blocked from the scattered light of MOT beams. For this technique, we have a MOT optimization sequence in which we load a MOT repeatedly, but only for a short duration each cycle, typically 0.5 s to 2 s. The 3D MOT cooling beam is shuttered off for 0.1 s between each cycle to allow all the trapped atoms to escape the trapping region, while the 2D MOT beams are kept on all the time. This results in a sawtooth-like fluorescence signal on the monitoring photodiode, and we try to maximize the signal amplitude while scanning parameters. This is a very useful technique given the large

parameter space of MOT loading, including current in each coil, power splitting ratio, total MOT beam powers, cooling and repump detunings, position of the 2D MOT beam block, etc.¹ The final optimization is done with absorption imaging, since the strength of the fluorescence signal also depends on parameters like detuning, and does not directly reflect the atom number in the MOT.

While the temperature of the gas during evaporation is effectively set by Rb atoms, eventually we find that we are mostly limited by the number of ^{40}K atom number when aiming for a degenerate fermi gas. Therefore, all the MOT optimizations prioritize maximizing the number of ^{40}K atoms. ^{39}K is currently mainly used as a helper species for sequence debugging should we lose ^{40}K MOT altogether and is not optimized in the end. We first use the shuttering technique to optimize ^{39}K MOT, which also makes the ^{40}K MOT loading better. We then use absorption imaging to optimize ^{40}K MOT, after which the parameters shared between K and Rb MOTs are fixed, such as coil currents and beam block positions. We have found that the MOT quadrupole field that maximizes the loaded atom number is lower for ^{40}K compared to Rb. Finally, we optimize Rb MOT loading using parameters that only affect Rb atoms, first using the shuttering technique, and then with absorption imaging. While the dual-wavelength wave plates are not perfectly full-order for the wavelength we don't want to change, usually we only need to re-optimize the power splitting once for each species. We have seen that revisiting the power splitting every few months improves the MOT loading by up to 20%.

We note that currently we don't have a separate molasses stage in our sequence. This is partially due to the group's previous experience that the energy gained from the expansion of the cloud during molasses partially cancels out the cooling we get, and partially because the Majorana loss rate scales as $(1/T)^2$ (see Eqn. (4.3)). We do, however, use a molasses sequence to help us cancel the stray magnetic field in the MOT chamber, which was helpful for setting up optical pumping. For this calibration, the sequence is very similar to the shuttering sequence, except that instead of shuttering off the cooling light between each run, we cut the current going through the MOT coils, leaving only the MOT beams on. When the stray fields are calibrated well and the optical pressure is well-balanced, the atoms slowly expands from the MOT position in a few seconds. We keep a record of the bias fields required to cancel the background fields from this calibration, but MOT beam balancing is optimized for largest atom cloud in the end.

The procedure so far doesn't include a push beam. The push beam is only installed in the experiment in October 2025, and it increases the MOT loading rate by more than a factor of two. Existing literatures have been divisive on the benefit of a push beam², with some groups seeing no benefit of push beams [55]. For the experiments that see improvements, resonant [98, 99], red- [100, 101, 102, 103] or blue-detuned [58] push beams have been used, and some

¹This works the best when the parameter can be tuned by hand. For things that are fully controlled digitally, e.g. DDS that drives MOT AOMs, a hack is to replace the DDS with analog VCOs temporarily so one can tune the control voltages by hand. Once ideal parameters are found, one records the optimal frequencies and beam power, and reproduce that on the DDS.

²References listed here are not limited to ^{40}K .

	Rb	⁴⁰ K
2D MOT		
Cooling power	270 mW	440 mW
Cooling detuning	−1.3Γ	−2.5Γ
Repump power	5 mW	350 mW
Repump detuning	0Γ	−0.2Γ
Push power	380 μW	140 μW
Push detuning	2.3Γ	1.2Γ
Field gradient (along cooled directions)	12 G cm ^{−1}	
3D MOT		
Cooling power	170 mW	107 mW
Cooling detuning	−3.3Γ	−3Γ
Repump power	5 mW	127 mW*
Repump detuning	0Γ	1.2Γ*
Field gradient (radial)	6.5 G cm ^{−1}	

Table 4.1: Optimized MOT loading parameters. Optical powers are the sums of all MOT beams. Field gradients are calculated from coil geometries and currents. $\Gamma = 2\pi \cdot 6 \text{ MHz}$ for both Rb and ^{40}K . *: ^{40}K loading is insensitive to 3D MOT repump parameters at the power we use, see main text.

groups additionally add a counterpropagating beam [100, 101, 102]. Our suspicion is that the benefit of a push beam is additionally affected by the geometry of the vacuum chamber, the size and capture velocity of the 3D MOT, collisions between atoms in the 2D MOT cell, and more. In our case, we were able to almost immediately see an improvement in the atom loading rate after scanning push beam detuning and intensity, and did not investigate further.

The important MOT parameters after the full optimization procedure are summarized in table 4.1. On a typical day, we first load a ^{40}K MOT for 15 s to 25 s, and then turn on Rb MOT loading for another 2 s to 5 s. The typical number of atoms we load is around $1 \cdot 10^9$ for Rb and $1 \cdot 10^7$ for ^{40}K . We have noticed that loading too many Rb atoms can reduce the atom number after RF evaporation (see below), and we control the Rb atom number by changing the loading time slightly. We note that at the repump power we use now, changing the repump power and detuning for ^{40}K 3D MOT does not have an observable effect within at least $\pm 2\Gamma$.

4.1.2 Optical pumping

Before ramping up a magnetic trap in the MOT chamber, we first run a compressed MOT (CMOT) by lowering the Rb repump power to $20\text{ }\mu\text{W}$ for 30 ms. We also lower the radial gradient to 2.3 G cm^{-1} and increase the detuning of the MOT cooling beam to -8.7Γ . This reduces the radiation pressure of the atoms trapped in the MOT, thereby reducing the size of the cloud. This is helpful for reducing the heating from the potential energy of the cloud in the magnetic trap [104, 105]. The ^{40}K cooling and repump parameters are not changed.

After CMOT, the atoms are optically pumped to the desired magnetically trappable state to improve the loading efficiency. Since we rely on the collision between Rb and K atoms in the sympathetic cooling stage that follows, we must choose the internal states that are “good collisional partners,” as explained in Sec. 4.1.4. In our case, this means using the $|F=2, m_F=2\rangle$ state for Rb, $|F=9/2, m_F=9/2\rangle$ for ^{40}K , and $|F=2, m_F=2\rangle$ for ^{39}K . We use a dedicated optical pumping beam that propagates along the magnetic transport axis for this purpose. A small bias magnetic field of around 0.8 G is applied along this axis using a single hand-wound coil, and σ^+ beams are turned on for 4 ms for Rb, and 2 ms for ^{40}K . These steps are the most time-sensitive steps in the sequence for preparing degenerate quantum gases, and sometimes changes on the order of a few 100 μs is required. This should be kept in mind if the laser table optics is modified and the delays of shutters are changed.

For each species, the repump beam $F-1 \rightarrow F$ drives the same transition as in the MOTs, but the $F \rightarrow F+1$ cooling transition is inappropriate for optical pumping to the stretched $m_F = F$ state, since the atoms in the correct state will keep scattering photons and get unwanted momentum kicks. Therefore, we use the $F \rightarrow F$ transitions instead. The hyperfine splitting of the $^2\text{P}_{3/2}$ term in Rb is large enough that a resonant $F=2 \rightarrow F'=2$ beam sufficiently far detuned from the $F'=1$ or 3 transitions, so it is possible to use the D2 transition. For K, we have to use the D1 transition due to the small $^2\text{P}_{3/2}$ hyperfine splitting.

4.1.3 Magnetic transport

Once atoms are pumped to the right states, we ramp up a magnetic quadrupole trap with a radial gradient of 32.8 G cm^{-1} in 20 ms. After a 5 ms blowaway pulse to remove atoms in the wrong hyperfine state, the remaining atoms are then transported to the science cell using the three magnetic transport coils and the Feshbach coil surrounding the science cell in 4.5 s. More details on the optimization of the transport sequence can be found in Ref. [50].

We note that magnetically trapped atoms are extremely sensitive to scattered near-resonant light, since it only takes one photon to pump the atom into an untrapped state. When we first transported Rb atoms to the science cell, we found that the lifetime of atoms was around one second. The culprit turned out to be cooling light that reflected from the laser table, to the wall, then finally to the science table. We easily got minute-long lifetime after closing the enclosures of both the science table and the laser table.

4.1.4 RF evaporation cooling

General evaporation concepts

The most important figure of merit is given by [106]

$$\gamma \equiv \frac{\log(\varpi_f/\varpi_i)}{\log(N_f/N_i)}, \quad (4.1)$$

where ϖ is the phase space density as defined in Eqn. (3.10), N is the number of atoms, and subscripts i and f represent initial and final values. This can be massaged to give $\varpi_f = (N_f/N_i)^\gamma \varpi_i$, which makes it clear that γ quantifies the proportional gain in ϖ as a function of fractional atom number loss. γ is a parameter that is affected by the evaporation time. For example, if there are no loss mechanisms and one is patient enough, one can trap the atoms in an extremely deep trap, and wait for an event where one atom carries all the energy of the sample and escapes the trap, in which case γ would be extremely large. This doesn't work in practice because this will take almost an infinite amount of time, and there are loss and heating mechanisms that competes with the evaporation process. This results in a tradeoff that limits the energy carried away by each particle, which is roughly given by the trap depth, conveniently written as $\eta k_B T$. The more slowly the trap depth is reduced during evaporation, the larger η is, and its exact value is measured experimentally.

For sympathetic cooling, there are two species involved, so we additionally define

$$\gamma_{Rb} \equiv \frac{\log(\varpi_{f,Rb}/\varpi_{i,Rb})}{\log(N_{f,Rb}/N_{i,Rb})}, \quad \gamma_K \equiv \frac{\log(\varpi_{f,K}/\varpi_{i,K})}{\log(N_{f,K}/N_{i,K})}. \quad (4.2)$$

It is important to use the right internal state combinations to prevent inelastic two-body collisions. Since the total m_F during the collision process is conserved, we only need to consider whether a m_F conserving process is energetically allowed. Additionally, for evaporation cooling in magnetic traps, the atoms must be prepared in a low-field seeking state, which limits our option to either $|F=2, m_F=2, 1\rangle$ or $|F=1, m_F=-1\rangle$ for Rb, and $|F=9/2, m_F=9/2 \sim 1/2\rangle$ or $|F=7/2, m_F=-7/2 \sim -1/2\rangle$ for ^{40}K . As it turns out, the only stable combination of magnetically trappable states is $|F=2, m_F=2\rangle$ for Rb and $|F=9/2, m_F=9/2\rangle$ for ^{40}K , since there are no other combinations with the same total m_F .

Evaporation cooling of Rb

After transport, the magnetic field gradient (in the weak radial direction, denoted as B'_r from now on for clarity) at the science cell is first ramped up to 103.3 G cm^{-1} in 50 ms to increase the density of the cloud to foster efficient thermalization. We note that this gradient is very low compared to most quantum gas experiments, and is limited by the (lack of) thermal dissipation of the Feshbach coil. The microwave knife is generated by mixing a 6.73 GHz carrier (ARTIQ Almazny) with a DDS signal (ARTIQ Urukul). In contrast to the old experiment, where the sideband used for evaporation is red-detuned from the bare

hyperfine level splitting at 6.835 GHz, we use a blue-detuned microwave knife, since the shift in the transition frequency between $|F = 2, m_F = 2\rangle$ and $|F = 1, m_F = 1\rangle$ is positive for non-zero magnetic field, which is the opposite of the $|F = 1, m_F = -1\rangle$ to $|F = 2, m_F = -2\rangle$ transition.

Starting at 120 MHz blue-detuned from resonance³, we decrease the detuning sequentially to (80, 40, 20, 8 and 0.7) MHz in a piecewise linear fashion⁴. The evaporation trajectory is optimized by varying the time between each intermediate detunings, and maximizing the figure of merit γ_{Rb} . We performed this optimization process without loading ^{40}K atoms. We start with a gas of temperatures $(T_x, T_y) \sim (280, 370)$ μK right after trap compression, where one temperature is cited in each direction, because the gas has not fully thermalized after the transport along the y -axis. The initial step is very inefficient due to the low density of the cloud, and we are limited to $\gamma_{Rb} \lesssim 1$. At below 100 μK , we have found that $\eta \sim 10$ results in the largest achievable $\gamma_{Rb} \lesssim 3$ in our experiment.

Sympathetic cooling of ^{40}K

Physically, cooling ^{40}K with Rb in a magnetic trap faces different challenges at high and low temperatures. At high temperatures of a few hundreds of μK , the s -wave scattering length between ^{40}K and Rb approaches zero due to the Ramsauer-Townsend effect. Thermalization between the two species thus relies on higher-wave scattering processes, and in particular is slower than what one would naïvely assume from the background scattering length. This effect was indeed observed in early attempts of sympathetic cooling between ^{40}K and Rb [107, 97].

At lower temperatures, while the scattering cross-section σ_{K-Rb} is larger than σ_{Rb-Rb} by roughly a factor of two so thermalization is efficient, ^{40}K is much more susceptible to Majorana spin flip losses. An intuitive scaling analysis of the lifetime due to spin flip τ_M is given in [108]. For an atom trapped in a magnetic trap with field gradient $\partial B_r / \partial r = B'_r$, the Larmor frequency is given by $f_L \sim \mu B'_r / \hbar$, where μ is the magnetic moment of the atom, and b is the minimum distance of the atom's trajectory from the center of the trap (the impact parameter). Losses due to spin flips can happen when $f_L \lesssim v/b$, where $v \sim \sqrt{T/m}$ is the speed of the atom. This defines a loss radius given by $b_0 \sim \sqrt{v\hbar/\mu B'_r}$.

We relate b_0 to a loss rate by finding the rate Γ_M at which an atom enters the surface that is defined by the loss radius. The density of atoms is given by $n = N/l^3$, which defines the radial extent of the gas l . This allows us to write $\Gamma_M \sim n v b_0^2 / N = v^2 \hbar / l^3 \mu B'_r$. We would like to get rid of the v and l in this equation. To this end, we first eliminate v^2 using the virial theorem $m v^2 \sim \mu B'_r l$, and then use the equipartition theorem $k_B T \sim \mu B'_r l$ to relate l to

³Note that when the detuning is ν , the trap depth of Rb atoms is given by $(2/3)\hbar\nu$, since the $|F = 1, m_F = 1\rangle$ state is also shifted but in the opposite direction. The microwave doesn't address any transition in K atoms, so the trap depth of K atoms doesn't change.

⁴The last detuning is changed from time to time to optimize the degenerate Fermi gas we get after the full evaporation sequence, and is usually between 0.7 to 1.5 MHz. The Rb BEC we get at the end, when no ^{40}K is loaded, is very insensitive within this range.

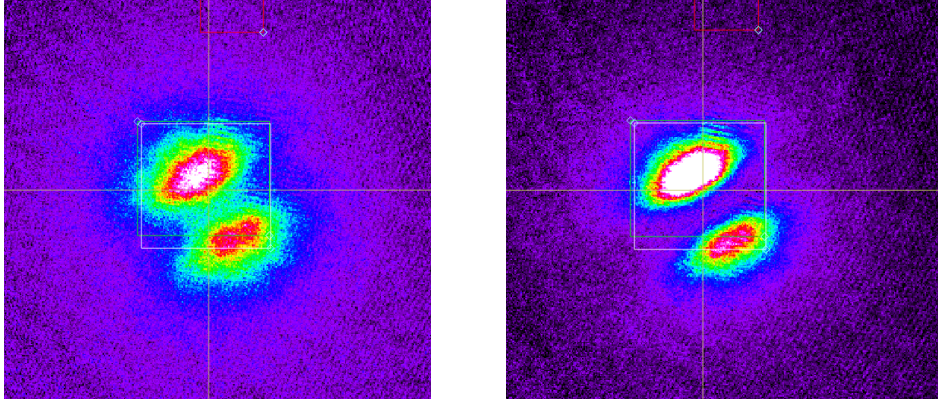


Figure 4.2: *In situ* images of ^{40}K atoms at the end of the RF evaporation. Left: the plug beam is misaligned, preventing efficient cooling of ^{40}K . There are also too many atoms in the lower half of the plugged trap. Right: the atom cloud is properly cooled with an aligned plug beam, and most of the atoms are in the upper half of the trap, which is where we align the xODT to.

T . This gives us

$$\Gamma_M = \frac{1}{\tau_M} \sim \frac{\hbar}{m} \left(\frac{\mu B'_r}{k_B T} \right)^2, \quad (4.3)$$

which shows that ^{40}K is more likely to suffer from Majorana losses due to its lower mass. Additionally, the larger F of ^{40}K means that it is more likely for a ^{40}K atom to leak to other m_F states, which we refer to as depolarization. The energy difference between the trapped state and the neighboring m_F state is given by $\hbar f_L/F$, and a more careful analysis show that depolarization rate scales as $\sqrt{F}$ [109, 110].

In practice, spin flips prevent us from cooling below a certain temperature, since the colder atoms are lost from the trap. This necessitated the installation of a plug beam, which was not required in the Rb machine. The 420 mW, 760 nm plug beam is focused to a waist of $36\mu\text{m}$. We have found that *in situ* images of ^{40}K atoms are useful tools for aligning the plug beam to the magnetic field zero, since the cloud appears much “fuzzier” at the same evaporation parameters when the plug beam is misaligned (Fig. 4.2)⁵. We obtained the first degenerate Fermi gas in our experiment two weeks after installing the plug beam.

Since ^{40}K atoms are not removed by the microwave knife, the number of ^{40}K atoms only decreases by around 20% due to losses from background gas collisions, and at later stages of the evaporation, Majorana spin flips and ^{40}K -Rb-Rb three-body losses. Experimentally, we have found that γ_K is not a very useful parameter, since the atom losses are very small, and γ_K is too sensitive to the small fluctuations in run-to-run atom numbers. Instead, it is more helpful for us to compare the temperature of K and Rb and make sure that the two species are properly thermalized, which required us to sweep detunings slower in the first

⁵Currently, instead of trying to align the plug to the trap center, we scan the bias fields to align the trap center to the plug, since it is easier to schedule in ARTIQ.

step, likely due to the Ramsauer-Townsend effect. Optimizing the final RF evaporation step in a plugged trap is also not very useful in the end, since the success of our sequence is also highly dependent on the transfer to the xODT and the evaporation efficiency therein, so the parameters for the last few steps are optimized while looking at the full evaporation sequence. We have also found that ramping down the gradient B'_x to 58.9 and 39.4 G cm⁻¹ in the last two steps helps with retaining more ⁴⁰K atoms, presumably due to reductions in three-body losses.

Evaporation cooling of fermions near degeneracy

While we achieve quantum degeneracy in an optical trap, we note that degenerate Fermi gases have been prepared in also Ioffe-Pritchard type magnetic traps, where there is no magnetic field zero [58, 97]. Regardless of the nature of the trapping force in the final step, here I would like to highlight the fundamental difficulties of the evaporation cooling technique when applied to fermions. A good review on this subject is given in [79].

Pauli blockade As the temperature of the fermi gas decreases, the low energy states are increasingly occupied. For a collision to happen, the momentum and energy must be conserved, so a lack of empty low energy state reduces the phase space available, and the collision rate between particles drops drastically due to this effect at low temperatures [111].

Hole heating Loss processes, such as collisions with background gases, can create holes deep inside the Fermi surface that adds $O(E_F)$ of energy to the system. If the single particle lifetime of trapped atoms is τ_L , it was shown in [112] that the temperature of Fermi gas increases to $T/T_F > 0.1$ within $0.07\tau_L$. Combined with the inefficiency of collision at lower temperatures, this poses significant challenges to cool the system with evaporative cooling. We note that going from a spin-polarized sample of fermions to a spin-balanced mixture necessarily increases the temperature of the system to around $T/T_F = 0.6$, since the RF pulses one would use to prepare the internal state is not momentum selective, and holes are created in the system [79].

The lowest temperature achieved for bulk Fermi gases is around $0.05T_F$ [113], given the difficulties of cooling Fermi gases using traditional means. The need to go to lower temperatures has led to effort to further cool the system in lattices through entropy redistribution, which will be the topic explored in chapter 7.

4.1.5 Forced optical evaporation

The xODT is ramped up to $(I_{ODTa}, I_{ODTb}) = (420, 1400)$ mW in 100 ms right after the end of the RF evaporation sequence, during which we also linearly lower the gradient B'_r to 20.2 G cm⁻¹. Once the xODT is at their maximum power, we further lower B'_r to 2.9 G cm⁻¹, at which the vertical gradient of the magnetic trap no longer support either species against

	Rb	^{40}K
Trap frequencies ($\omega_x, \omega_y, \omega_z$)	$2\pi \cdot (49.8, 70.7, 256.1) \text{ Hz}$	$2\pi \cdot (68.7, 97.4, 353.1) \text{ Hz}$
Atom numbers	$1.2 \cdot 10^5$ (no ^{40}K) $5 \cdot 10^4$ (with ^{40}K)	$1 \cdot 10^5$
Thomas-Fermi radii (R_x, R_y, R_z)	(8.8, 7.6, 4.6) μm (no ^{40}K)	(34.7, 24.5, 6.8) μm

Table 4.2: Typical experiment parameters after optical evaporation.

gravity, and all the remaining atoms are optically trapped. (These steps are called “predecompress” and “decompress” due to historical reasons.)

The transfer of atoms from the plugged trap to the xODT is very sensitive to bias fields, since if the trap center moves by more than the beam waist of the plug beam, atoms are quickly lost from the trap due to spin flips. Even if the atoms are not lost yet, if the global minimum of the plugged trap is not in the right half of the trap, more atoms will be on the wrong side of the plug, reducing the loading efficiency. To get a sense of scales, a 1 mG field moves the center of a magnetic trap with gradient 10 G cm^{-1} by $1 \mu\text{m}$, so the bias fields should be controlled on the order of a few 10 mG ⁶. We have found that occasionally scanning the bias field values at predecompress and decompress within a small range is very helpful for maintaining the working condition of the experiment.

Once atoms are trapped optically, we achieve quantum degeneracy using a simple exponential ramp to (45, 288) mW in 4 s. The main change in the sequence, compared to the old machine, is that we still keep the weak quadrupole trap potential after decompress in the first one-third of the evaporation. The center of the magnetic trap is above the ODT plane, and its main purpose is to provide a weak radial confinement along the direction of the two ODTs. When atoms are first transferred into the ODTs, there are still a lot of atoms in the non-overlapping region of the two ODTs from thermal distribution, and the radial confinement helps with making use of these atoms in the “arms” for evaporation cooling. Once all of the atoms are in the xODT region, we gradually ramp off the quadrupole in the middle one-third of the evaporation sequence.⁷ After reaching the minimum optical potential, we slightly increase the ODT powers to (47, 305) mW in 100 ms, which is intended to counteract the change in potential due to the lattice beams.

When ^{40}K atoms are trapped, care should be taken to make sure that the final trap depth is larger than the Fermi energy to prevent atom loss and heating [84]. The intensities of the two ODTs are scanned to optimize the phase space density of ^{40}K at the end of evaporation.

⁶The passenger elevator right across from our lab changes the bias field in the lab by as much as 20 mG, but when the bias fields are well-adjusted, the atom cooling sequence is not sensitive to the position of the elevator. So this estimation should be considered a pessimistic one that doesn’t consider the fact that the optical potential takes over at some point.

⁷The imaging bias field along the top-down direction is ramped to its final value during the same time. This ramp has no observable effect in atom cooling.

They are very imbalanced due to the different beam shapes of the two beams. For sequences that work with ^{40}K , Rb atoms are blown away with a 200 μs resonant pulse at the end of optical evaporation. Table 4.2 summarizes the final trap parameters in our system. Note that $\omega_{\text{K}}/\omega_{\text{Rb}} = 1.38$ (see Eqn. (3.33)).

We note that we have not tried to transfer the Rb atoms to the absolute ground state $|F = 1, m_F = 1\rangle$, which is a stable combination with ^{40}K atoms in any of the m_F state in the $F = 9/2$ manifold under a small and finite magnetic field, because the Landé g -factor is larger for Rb than ^{40}K , and spin-changing relaxation processes are energetically forbidden. This combination is used in some works, and ^{40}K loss rate seems to be lower in this case [110, 114], but working with the stretched states already works well enough for us at the moment.

4.2 Optical lattice calibration

The central idea of all the calibration procedures is that we must use the atoms themselves to determine whether the lattice beams are aligned and at the desired intensities. While we are now usually interested in using ^{40}K for lattice experiments, it is much more convenient to use Rb BECs for lattice alignment and calibrations, because

- with a BEC, we can use the same lattice balancing and calibration techniques that we have been using in our experiment, while Fermi gases don't give clear diffraction peaks and thus are not amenable to the same techniques.
- the Rb sequence runs almost twice as fast, since we don't have to load ^{40}K .

After calibrating using Rb, we adjust the lattice beam intensity setpoints according to differences in polarizabilities. We acknowledge that the trap positions of Rb and ^{40}K are not exactly the same due to the differences in polarizabilities and mass. For a even more precise calibration, one can instead use ^{39}K .

While the optical lattice optics are practically the same as the previous generation, we have implemented a few changes to the daily calibration procedure, which are documented in this section.

4.2.1 Cuts and anti-cuts

The “cut” method that our lab has been using is documented in Claire Thomas's thesis [51]. This is the method that we still use for the 532 nm lattice beams. For the 1064 nm lattice beams, we used to match their spatial modes to the 532 nm beams at two separated spatial positions before the lattice beams enter the cell, and rely only on the 532 nm cuts for alignment to the atoms. This procedure does not account for the differences in refractive indexes at the two wavelengths, which means that the two colors might not be spatially overlapped after the focusing lens and the glass cell.

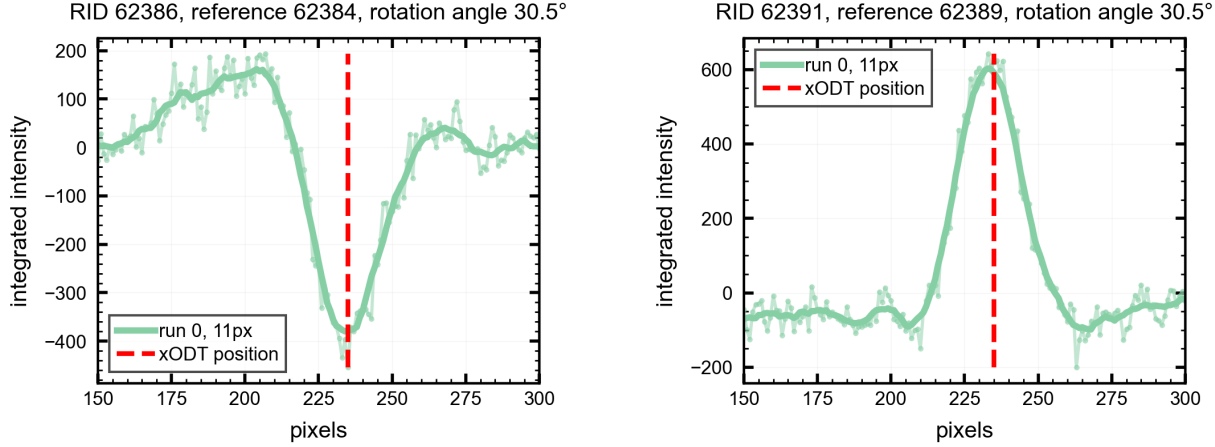


Figure 4.3: Typical cut and anti-cut data from November 5th, 2025.

We now perform what we call an “anti-cut” alignment for the 1064 nm beams, in which the same exact sequence for cuts is used, except that one of the 1064 nm lattice beams is turned on instead. This creates a bulge in the *in situ* Rb density in the ODT, which we try to match to the position of the xODT using horizontal degrees of freedom. The vertical knob is then used to maximize the amplitude of the bulge. Due to how the piezo mirror mounts are set up, we must first do the 532 nm cuts, followed by the 1064 nm anti-cuts. Empirically, we find that we have to revisit the cuts roughly once every one to two weeks.

4.2.2 Balancing and depth calibration

The procedures for balancing and calibration using Rb atoms are exactly the same as described in Claire’s thesis and will not be repeated here. The only difference we made is that when we are running a bichromatic lattice, we account for the confinement due to the lattice beams by turning both lattice beams on. This is because the position of atoms change when the lattice beams are turned on, and that changes the beam strengths seen by the atoms. The lattice beams for the wavelength not being balanced or calibrated are detuned by 300 kHz from each other so that the atoms only see an averaged potential. For experiments carried out with monochromatic lattices (which are all of the scientific works described in this thesis), only the lattice beams being used are turned on.

4.2.3 Signature of the kagome lattice geometry

While the procedure for searching for a kagome lattice is fundamentally the same as in the old machine, I would like to revisit the figure of merits that we have relied on for confirming a kagome geometry. We have also developed a way to systematically find a good initial

starting point when aligning a lattice from scratch, which is strongly inspired by the optical kagome lattice experiment in Cambridge [115].

Real space argument: matter wave interference

In our group, the indicator of the kagome geometry is usually taken to be [51, 116]

$$\tilde{P}_i \equiv \frac{P_{\mathbf{G}_i} + P_{-\mathbf{G}_i}}{2P_0} \left(\frac{2P_0}{P_{2\mathbf{G}_i} + P_{-2\mathbf{G}_i}} \right)^{1/4}, \quad (4.4)$$

where $P_{\mathbf{q}}$ is the population in the momentum peak $\mathbf{q}$, as defined in Sec. 3.4.1. $\tilde{P}_i$ can be thought of as an atom number-normalized population ratio between the first and second order peaks, and the power of 1/4 comes from the assumption that the Wannier functions are Gaussian-like.

This can be obtained by considering the system as an array of tiny BECs on each lattice site, whose relative phases are zero (namely, the quasimomentum is zero). The unit cell wave function of the Bloch state, assuming that the Wannier functions $w(\mathbf{r})$ are cylindrically symmetric Gaussian functions, can be written as

$$\psi_{\text{UC}}(\mathbf{r}) = \sum_{\alpha} \psi_{\alpha} w(\mathbf{r} - \mathbf{R}_{\alpha}) \quad (4.5)$$

where $\alpha \in \{A, B, C, D\}$ is the sublattice label, and $\mathbf{R}_{\alpha}$ is the basis vector of the sublattice α .

Since the Fourier transforms of Gaussians are also Gaussians, the Wannier function takes on the form $\tilde{w}(\mathbf{k}) = \tilde{w}_0 e^{-|\mathbf{k}|^2/k_0^2}$ in the momentum space, where k_0 is the extent of the Wannier functions in the momentum space and does not enter the final expression. The population of the momentum component $\mathbf{k}$ is then given by

$$P_{\mathbf{k}} = |\tilde{w}(\mathbf{k})|^2 |\psi_A e^{i\mathbf{k} \cdot \mathbf{R}_A} + \psi_B e^{i\mathbf{k} \cdot \mathbf{R}_B} + \psi_C e^{i\mathbf{k} \cdot \mathbf{R}_C} + \psi_D e^{i\mathbf{k} \cdot \mathbf{R}_D}|^2, \quad (4.6)$$

the phase terms coming from the familiar Fourier transform rules of translating $w(\mathbf{r})$.⁸

⁸We skipped a few steps here. For example, one may ask why we only consider $\mathbf{k} = \mathbf{G}_i$, and from what we wrote down in eqn. (4.6), any $\mathbf{k}$ would give some nonvanishing value. This is because we only wrote down the unit cell wave function, and the full wave function is given by repeating ψ'_{UC} for every lattice vectors $\mathbf{L}_u$, giving

$$\Psi(\mathbf{r}) = \psi_{UC}(\mathbf{r}) * \Delta(\mathbf{r}),$$

where $\Delta(\mathbf{r}) = (1/N) \sum_{u \in \text{U.C.}} \delta^{(2)}(\mathbf{r} - \mathbf{L}_u)$ is a 2D Dirac comb representing the triangular lattice. The Fourier transform $\tilde{\Delta}(\mathbf{k}) = \mathcal{F}[\Delta(\mathbf{r})]$ is again a triangular lattice, but with non-zero values only for $\mathbf{k} = \mathbf{G}_i$. It follows from the convolution theorem that

$$\mathcal{F}[\Psi(\mathbf{r})] = \mathcal{F}[\psi_{UC}(\mathbf{r})] \tilde{\Delta}(\mathbf{k})$$

is also only non-zero at the reciprocal lattice vectors. Eqn. (4.6) is just the $\mathcal{F}[\psi_{UC}(\mathbf{r})]$ part.

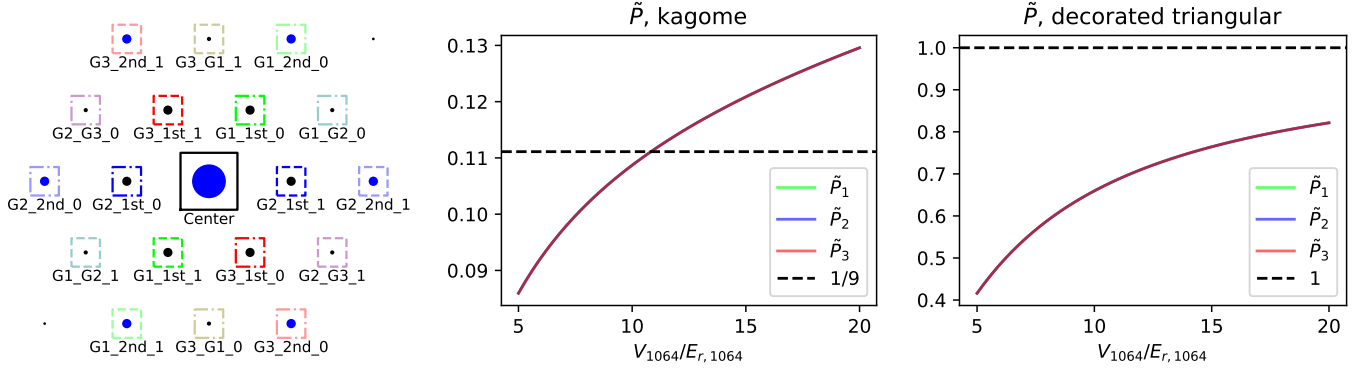


Figure 4.4: Numerical calculation of geometry indicators. Left: definition of peak labels. Middle and right: $\tilde{P}$ as a function of 1064 nm lattice depth for kagome and decorated triangular lattices, respectively. 532 nm lattice depth is set to $V_{532} = 5E_{r,532}$ for both plots.

We now evaluate eqn. (4.6) at the three lowest order diffraction peaks, which gives

$$\begin{aligned}
 P_0 &= |\psi_A + \psi_B + \psi_C + \psi_D|^2 \\
 P_{\pm \mathbf{G}_i} &= \mathbf{w} |\psi_A - \psi_B - \psi_C + \psi_D|^2 \\
 P_{\pm 2\mathbf{G}_i} &= \mathbf{w}^4 |\psi_A + \psi_B + \psi_C + \psi_D|^2
 \end{aligned} \tag{4.7}$$

where I wrote $\mathbf{w} = |\tilde{w}(\mathbf{G}_i)|^2$. Our goal is to find a useful relation of ψ_α 's by eliminating $\mathbf{w}$. This is done by noting that $\mathbf{w} = (P_{2\mathbf{G}_i}/P_0)^{1/4}$. The expression in eqn. (4.4) make use of the inversion symmetry and sum the two opposite momentum components together, and also include proper normalization. In any case, substituting eqn. (4.7) into eqn. (4.4) gives

$$\tilde{P}_i = \frac{|\psi_A - \psi_B - \psi_C + \psi_D|^2}{|\psi_A + \psi_B + \psi_C + \psi_D|^2}. \tag{4.8}$$

In particular, we use $\tilde{P}_i$ to distinguish the two geometries with six-fold rotational symmetry:

- kagome: $\psi_A = \psi_B = \psi_C = 1/3, \psi_D = 0 \Rightarrow \tilde{P}_i = 1/9$
- decorated triangular: $\psi_A = \psi_B = \psi_C = 0, \psi_D = 1 \Rightarrow \tilde{P}_i = 1$

Momentum space calculation

More quantitatively, one can follow the calculation in Sec. 3.4.1, and find the exact values of $\tilde{P}_i$'s (or any other possible indicators) for chosen lattice depths, which is perhaps an easier way to account for deviations from the real space argument than arguing using the ellipticity of the Wannier functions [51]. The results are shown in Fig. 4.4, where one sees that the

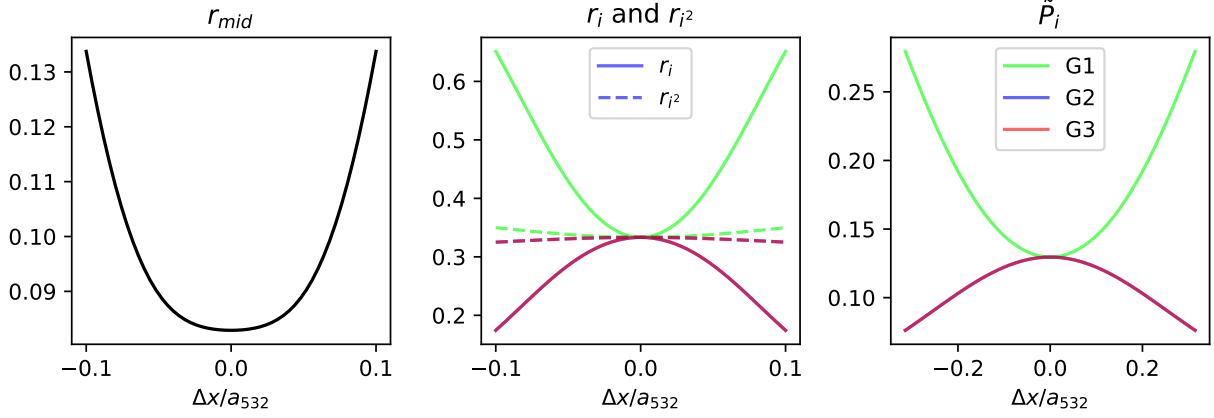


Figure 4.5: Geometry indicators as a function of 1064 nm lattice displacement in the direction of B1. Lattice depths: $V_{532} = V_{1064} = 20E_{r,1064}$.

real space argument works reasonably well for a wide range of V_{1064} for the kagome lattice. The agreement is not as good for the decorated triangular lattice, but $\tilde{P}_i$ is still much larger than the kagome lattice.

One may ask whether $\tilde{P}_i$'s are still the best indicators to look at when we are certain that we are closer to the kagome lattice instead of the decorated triangular lattice. Here we compare a few candidates for kagome signature. First of all, the diffraction peaks should be six-fold symmetric. To quantify this, we define

$$r_i = \frac{N_{\mathbf{G}_i} + N_{-\mathbf{G}_i}}{\sum_i N_{\mathbf{G}_i} + N_{-\mathbf{G}_i}}. \quad (4.9)$$

In a kagome lattice, $r_1 = r_2 = r_3 = 1/3$. (This is the same criterion used for balancing a monochromatic lattice.) We may similarly define the second order counterparts r_{i^2} by replacing $\mathbf{G}_i$'s with $2\mathbf{G}_i$ in Eqn. (4.9). Alternatively, one may look at the populations in the second order peaks in the middle (labeled as $\mathbf{G}_m\text{-}\mathbf{G}_n_0(1)$ in Fig. 4.4) and compare them to the second order peaks at the corners. For example, one may define

$$r_{mid} = \frac{\sum_{i \neq j} N_{\mathbf{G}_i - \mathbf{G}_j} + N_{-\mathbf{G}_i + \mathbf{G}_j}}{\sum_i N_{2\mathbf{G}_i} + N_{-2\mathbf{G}_i}}. \quad (4.10)$$

We now study how do the different indicators vary as we change the relative phase ϕ_{12} between B12, which displaces the lattice in the direction of B1. The results are plotted in Fig. 4.5. One sees that r_{mid} is very insensitive to displacements, and therefore is not a good indicator close to kagome geometry. r_{i^2} is very much useless compared to r_i . $\tilde{P}_i$ and r_i varies in a similar way, which is understandable, because they depend on the first order populations in the same way. For the indicators considered here, it seems like r_i is the best measure of “kagomeness.”

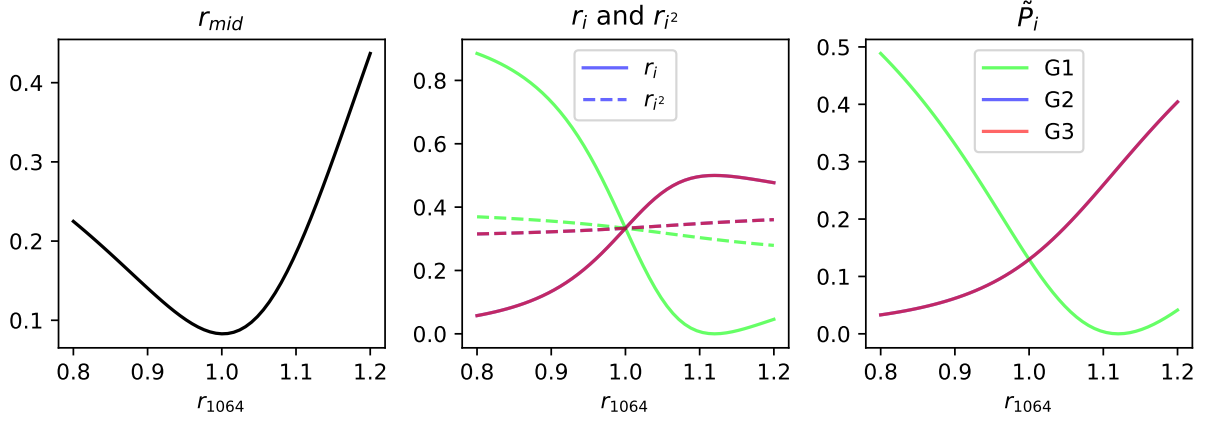


Figure 4.6: Geometry indicators as a function of 1064 nm lattice imbalance. The effect of imbalancing the 532 nm lattice is similar. Lattice depths: $V_{532} = V_{1064} = 20E_{r,1064}$.

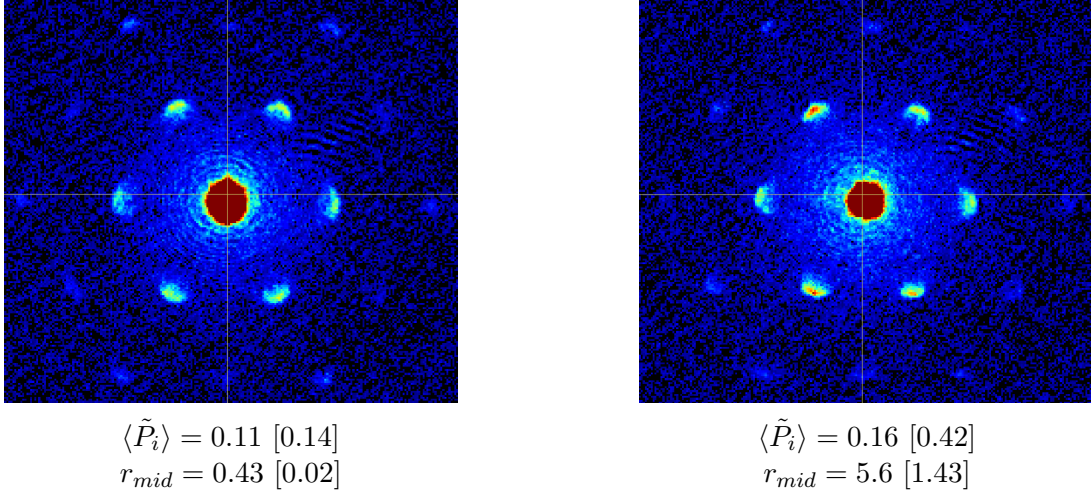


Figure 4.7: Diffraction images of Rb in kagome (left) and decorated triangular (right) lattices. r_i 's for both images are within 0.33 ± 0.01 . The lattice depths are $V_{532} = 20$ kHz and $V_{1064} = 25$ kHz, respectively. Numerically calculated values are in square brackets.

Note that in the discussion for kagome signatures so far, I have assumed that each monochromatic lattice is already balanced. None of the calibration procedure described in this section works if the monochromatic lattices are imbalanced, and in fact the rotational symmetry of the superlattice is linearly sensitive to beam imbalances, while it is only quadratically sensitive to lattice displacements. This is shown in Fig. 4.6, where one sees that the differences between different r_i 's change linearly as relative beam intensity is varied.

We now calculate the indicators of actual measured data shown in Fig. 4.7 for the two C_3 symmetric lattices. It appears that in contrast to what is shown in Fig. 4.4, $\tilde{P}$ is not a clear

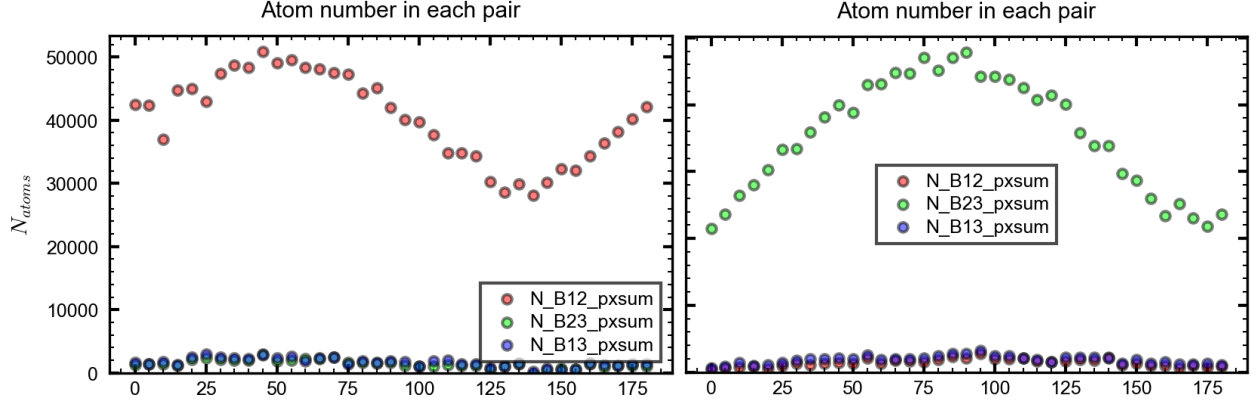


Figure 4.8: Number of atoms in the first order diffraction peaks as a function of the relative position between the 532 nm and 1064 nm 1D lattices. The x -axes are the set phase of the 1064 nm phase lock of the relevant beam pair. Left: B12. Right: B23. Data taken on December 11th, 2025.

indicator to tell which one is the kagome lattice, while r_{mid} does a much better job. The deviations from the numerically calculated values likely come from the nonlinear interaction between Rb atoms, which can be reduced by using ^{39}K and tuning to near-zero interaction strength. This may not have been a problem in the old machine, since the BEC was five times smaller, and the trap confinement was also much weaker.

Rough alignment using 1D superlattice scan

Historically, we haven't had a very systematic way to get a good initial guess for the relative phases between lattice beams. Since there are only two geometries with C_3 symmetry, kagome and decorated triangular, in principle we can try to get both of them experimentally, and the one with smaller r_{mid} is the kagome lattice. There is a more systematic way to do it, as described below.

In our new alignment procedure, we first do a 180° scan of the 1064 nm phase lock setpoint, which scans over the full range of relative position between the 532 nm and 1064 nm lattices. The setpoint that gives a kagome lattice is expected to be where the first order diffraction peaks of the 1D lattices are maximum. After scanning for the two lattice beam pairs, we then turn on all the lattice beams and fine-adjust the relative phases until we recover the six-fold rotational symmetry, which is, as far as we know, the most sensitive indicator. The results from 1D superlattice scans are usually good to within 10° .

4.2.4 Phase lock calibrations

The arbitrary phase lock setup is described in [53]. Since this is an essential component of the experiment, in this section I extend upon the calibration procedures already detailed therein.

To define the notations used in this paragraph, the essential equations are copied below. The two phase quadratures obtained from demodulated photodiode signals is given by $V_1 = V_0 \cos(\theta(t))$ and $V_2 = V_0 \sin(\theta(t))$, where $\theta(t)$ is the relative phase between the two lattice beams under consideration. Here, we do not include the imperfections in the relative intensities and phases for simplicity. Our goal is to lock $\theta(t)$ to a desired, possibly time-dependent, phase $\phi(t)$. This is done by making use of the trigonometric identity $\sin(A - B) = \sin A \cos B - \cos A \sin B$. By multiplying V_1 and V_2 by the scaling functions $S_1 = -\sin \phi$ and $S_2 = \cos \phi$ and adding the two resulting signals together, we get the desired error signal

$$V_{\text{err, no ff}} = V_1 S_1 + V_2 S_2 = V_0 \sin(\theta(t) - \phi(t)).$$

While our phase lock servo is not fast enough for the frequencies of interest, we implement a feedforward scheme such that the modulation voltage required to realize the relative phase $\phi(t)$ is also generated by our DAC (ARTIQ fastino). The feedforward voltage required is given in Sec. 5.3.2 as $V_{\text{ff}}(t) = K_{\text{VCO}}^{-1}(\text{d}\phi(t)/\text{d}t)$. By adding $V_{\text{ff}}(t)$ to the modulation port of the VCO, the remaining deviation from the desired phase $\phi(t)$ is now just phase noises in the system, which we will write as $n(t)$, and the error signal is now given by

$$V_{\text{err}} = V_1 S_1 + V_2 S_2 = V_0 \sin(n(t)), \quad (4.11)$$

as if it doesn't know about the change in the change of set phase ϕ .

For experiments that work with stationary superlattices, we don't need to further calibrate the phase lock, as long as we have confirmed that the lattice geometry is correct using the procedure described above. However, for experiments that translate the lattice, more care has to be taken. For a monochromatic lattice, we can in principle run lattice sequences without any active feedback, in which case the lattice translation is solely defined by the feedforward signal. The phase noise in the lattice beam pairs might heat up the atoms, but we have not found it to be a limiting factor for us for the experiments that we have done. Nonetheless, we usually run the experiment with phase stabilization, and for periodic modulations we have noticed that the error signal contains harmonics of the modulation signal (mainly first and second order harmonics) that vary slightly over timescales of an hour. This error signal directly corresponds to error in the lattice position⁹.

The effect of these harmonics is at least twofold. They correspond to excitation at well-defined frequencies, which can drive unwanted excitation, and is especially relevant for the experiment described in chapter 6. For superlattices there is a bigger issue, since if the harmonics of the two wavelengths are not matched exactly, the lattice geometry is distorted at the same time. To show that they can come from experimental imperfections, we show that a DC offset on the demodulated signal is one possible cause. Suppose that instead of the

⁹Alternatively, if $V_{\text{ff}}(t)$ is not chosen correctly, then we also expect to see first harmonics in the error signal, simply because the servo still has some residual error at frequency ω to correct, which it can't. This is not expected, since the DAC conversion delay of our VCOs is compensated to within 1 μs , and the required gain is set digitally. We have also confirmed that we cannot remove the first order harmonics by simply scanning around the phase delay and gain of $V_{\text{ff}}(t)$.

perfect quadratures of the relative phases, we get $V_1' = V_0 \cos(\theta) + c_1$ and $V_2 = V_0 \sin(\theta) + c_2$ in the demodulated signals. We focus on single frequency drives, $\phi(t) = M \sin(\omega t)$, and consider the case where $V_{ff}(t)$ accounts for the desired phase modulation. Eqn. (4.11) is then modified to

$$\begin{aligned} V_{err}' &= V_1' S_1 + V_2' S_2 \\ &= V_0 \sin(n(t)) - c_1 \sin(M \sin(\omega t)) + c_2 \cos(M \sin(\omega t)) \\ &= V_0 \sin(n(t)) + \epsilon \sin(\gamma - M \sin(\omega t)), \end{aligned} \quad (4.12)$$

where in the last line I reparametrized the offset by writing $c_1 = \epsilon \cos \gamma$ and $c_2 = \epsilon \sin \gamma$. The last term is an unwanted modulation signal. Similar imperfections have been considered in detail in different contexts, such as sideband locking using the Pound-Drever-Hall scheme [117].

There are many reasons why one can get such a DC offset:

- The simplest case is that the multiplier that we use in the phase lock circuit can have a small offset on the input side. AD835 specifies a typical offset of ± 3 mV on the input, with variations up to ± 25 mV within the operating temperature range (-40°C to 85°C).
- One can consider the case where somehow a phase-delayed signal is added to the detected quadrature. For example, if we add $p \sin(\omega t + \delta)$ to $V_2 = V_0 \sin(\theta)$, the demodulated signal will get an offset of $p \cos \delta$. This may happen if the cable that carries the photodiode signal picks up some unwanted noise, or if a small fraction of one of the lattice beam goes through a slightly different optical path but eventually also interferes on the photodiode.
- Residual amplitude modulation due to the electro-optical modulators (EOM) is known to be a cause of a DC offset [117, 118, 119] that is temperature dependent. For example, if the polarization of the input light is not aligned to the principal axis, then temperature fluctuations changes the birefringence of the EOM crystal, which turns into a temperature-dependent amplitude modulation after a PBS.

Experimentally, we can remove the first order harmonics by adding a small compensation offset to S_1 and S_2 , but we haven't been able to remove the second order harmonics. We have not identified a cause for second order harmonics so far, but they can come from e.g. nonlinearities of the ICs used in the feedback circuit. For example, we have noticed that driving the multiplier inputs close to the specified limits exacerbates these harmonics. This is a problem that has to be addressed in the future. From the amplitude of the error signal, we estimate that the spatial deviation from the programmed translation is at most 40 nm^{10} .

¹⁰Ideally one should characterize the actual deviation from the desired phase with an independent, out-of-loop interferometer setup, but this is very difficult in our setup due to space constraints.

Chapter 5

Quantum geometry of band touching points in honeycomb lattices

In this and the following chapter, we focus on the characterization of the quantum geometry of Bloch bands. Roughly speaking, in the context of solid state physics, quantum geometry is the study of how Bloch states (single or multiple bands) vary as a function of quasimomentum. On the other hand, topology studies the classification of the geometry of manifolds, for example, one to several Bloch bands across the whole Brillouin zone.

A famous example of Bloch band topology is the classification of energetically isolated bands through the Chern number, which underlies phenomena such as the quantum Hall effect [25, 26] and quantized optical response [29]. An example of a topological object that is not defined across the whole Brillouin zone is the winding number. It measures how many times the Bloch state of a certain band changes along a closed surface within the Brillouin zone. There is a strong interest to measure geometrical and topological quantities in cold atoms systems [120], which provides opportunities to implement novel measurement schemes [121, 20, 99] and engineer band geometry [122, 123, 124, 90].

We make the point that the resolution at which one can measure the changes in geometry is important, and can sometimes even affect one's ability to classify topological objects. A comical example is shown in Fig. 5.1, in which the topological feature (the hole) of the “donut” is small, so one needs good visions to see the hole. Our solid state counterpart of Fig. 5.1 is the winding number around band touching points, with either linear (LBTP) or quadratic (QBTP) dispersion near the singular point. In the case of LBTP, the Berry curvature is concentrated at the singular point, so any paths that encloses the LBTP would accumulate a Berry phase of π . This has been measured through interferometric measurements in [125], and can be understood as a measurement of the winding number of one around the LBTP. However, such interferometric style measurements are insensitive to the 2π Berry phase expected with the QBTP [45]¹.

¹This is true for our system, which has C_6 and time reversal symmetry. The Berry phase of a QBTP can be any value between 0 and 2π under general conditions [126].



Figure 5.1: A topologist's world. Left: a sphere. Middle: a donut. Right: a donut that looks like a sphere, because the topologist is nearsighted. Image credit: National Palace Museum.

In this chapter, we describe our work on measuring the variation of the Bloch states around band touching points in a honeycomb lattice. The variation is quantified by the quantum distance, which measures the (lack of) overlap between two quantum states. Since an infinitesimal change in the quantum distance gives the quantum metric [34], our work can also be seen as a measurement of the quantum metric in the polar coordinates. Our measurements are based on transporting a BEC in a well-defined Bloch state to the band touching points in the momentum space, where adiabatic evolution necessarily fails, and the final state of the BEC depends on the angle at which the atoms leave the singular point. Measuring the population in each Bloch bands for different turning angles reveals the quantum geometry around the touching points. Combining the results provides a measurement of the topological winding number along a closed contour that encloses the touching point.

As far as we know, this work is the first to characterize the geometry around the QBTP, which has attracted a lot of theoretical interest recently [36, 45, 34, 127]. The QBTP is shown to be protected by time reversal symmetry and four- or six-fold rotational symmetry, and can be broken into several LBTP depending on what symmetry is broken [45]. Our flexibility in tuning lattice geometry provides possibilities to study these effects experimentally.

This work was published at Ref. [49], and is the last publication from the old rubidium machine.

5.1 Two-band models for band touching points

While there are in principle infinite number of bands for a given periodic potential, it is often very useful to isolate a few of the relevant bands and study their properties, such as around a band touching point. In this approach, we expand the Hamiltonian around the vicinity of the band touching point, keeping only the lowest order terms in the magnitude of quasimomentum. We then diagonalize the Hamiltonian, and choose the two states that form the band crossing as an effective two-dimensional subspace.

A note on vector conventions: the orientation of all the vectors are rotated by 30° in the published work compared to the conventions in Sec. 3.3.1. To avoid confusion, I will follow the conventions in the paper for this chapter. This choice slightly simplifies the mathematical expressions².

5.1.1 s -bands and the linear band touching points

Let us first look at the specific cases studied in this work before studying a general two-band system. We may expand the tight-binding Hamiltonian of the honeycomb lattice given in Eqn. 3.69 around one of the Dirac points, which are located at $\mathbf{q}_K = (K, 0)$ and $\mathbf{q}_{K'} = (-K, 0)$ ($K = 2\pi/\lambda_{1064}$) (and equivalent quasimomenta). Writing $\mathbf{k} = \mathbf{q}_K + \mathbf{q}$, we find

$$H_K^{\text{hc}}(\mathbf{q}) \approx \hbar v_g \begin{pmatrix} 0 & q_+ \\ q_- & 0 \end{pmatrix}, \quad (5.1)$$

where $q_\pm = q_x \pm iq_y$, and $v_g = 3a_{\text{hc}}t/2\hbar$ is the group velocity at the Dirac points in the tight-binding picture [86]. We also call the Dirac points linear band touching points (LBTP).

The eigenstates of Eqn. (5.1) are given by

$$|u_{\mathbf{q}}^{K,(1)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -q_+/q \\ 1 \end{pmatrix}, \quad |u_{\mathbf{q}}^{K,(2)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} q_+/q \\ 1 \end{pmatrix}. \quad (5.2)$$

The eigenstates are only a function of the angular position with respect to the K point, and is independent of the magnitude $q \equiv |\mathbf{q}|$. To see this, we rewrite $\mathbf{q}$ in polar coordinates, $\mathbf{q} = q\boldsymbol{\rho}(\varphi_q)$, where $\boldsymbol{\rho}(\varphi) \equiv \cos \varphi \mathbf{x} + \sin \varphi \mathbf{y}$ is the radial unit vector. Then $q_x = q \cos \varphi_q$, $q_y = q \sin \varphi_q$, and

$$|u_{\mathbf{q}}^{K,(1)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\varphi_q} \\ 1 \end{pmatrix}, \quad |u_{\mathbf{q}}^{K,(2)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\varphi_q} \\ 1 \end{pmatrix}. \quad (5.3)$$

Eqn. (5.3) shows that $|u_{\mathbf{q}}^{K,(1)}\rangle$ and $|u_{\mathbf{q}}^{K,(2)}\rangle$ lies on the great circle of a Bloch sphere whose north pole and south pole are the $(1, 0)$ and $(0, 1)$ states in the sublattice basis, and is only dependent on φ_q .

Pseudospin picture of two-band models

The Hamiltonian in Eqn. (5.1) can be written as $-\mathbf{B}_{\text{LBTP}} \cdot \boldsymbol{\sigma}$, which is exactly the same as that of a spin-1/2 particle in a magnetic field if we identify the direction of this fictitious field to be $\boldsymbol{\rho}(\varphi_q)$, and the field strength to be qv_g . Drawing from this analogy, we will call a honeycomb s -band state a “pseudospin” in a two-dimensional Hilbert space. The state $|u_{\mathbf{q}}^{K,(1)}\rangle$ ($|u_{\mathbf{q}}^{K,(2)}\rangle$) can then be identified as a spin parallel (antiparallel) to the direction of

²For example, if we followed the conventions in Sec. 3.3.1 and expanded around $\mathbf{q}_K = (0, K)$ for the s -bands, we will have the same expressions for Eqn. (5.1) and (5.2), but with $q_\pm = q_y \pm iq_x$ and $\mathbf{q} = q\boldsymbol{\rho}(\varphi_q + \pi/2)$.

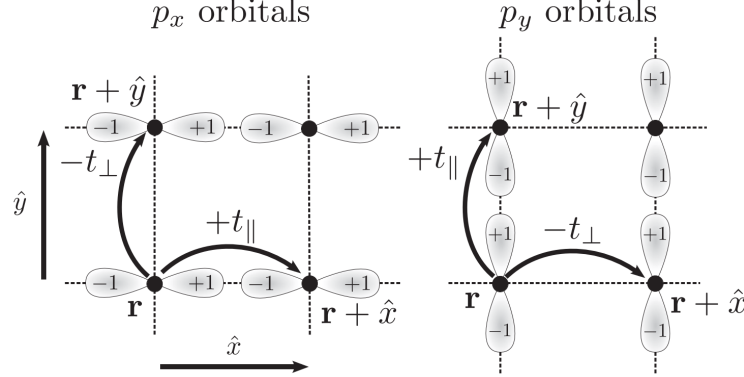


Figure 5.2: Visualization of p -orbitals and the two different kinds of bonds (illustrated on a square lattice). The hopping strengths of the σ -bond (π -bond) is denoted as $t_{\parallel}$ ($t_{\perp}$) in the figure. Figure reproduced from Ref. [128].

the fictitious field. The distance from the LBTP only affects the magnitude but not the direction of the fictitious field, which provides an intuitive way to understand Eqn. (5.3). We also see that the direction of $\mathbf{B}_{\text{LBTP}}$ changes by a full period as φ_q varies from 0 to 2π , which we associate with a winding number of one.

We note that in our case, the algebra that describes the pseudospin is actually just $SO(2)$ instead of $SU(2)$, since the fictitious field always points in the x - y plane. This is because the honeycomb lattice does not have site offsets. The connection will be made clear in Sec. 6.2.

5.1.2 p -bands and the quadratic band touching point

We will now study the quadratic band touching points (QBTP) at the Γ point in the p -band tight-binding model. The formalism and vector conventions here will follow [129] and the supplemental material of [49].

Each site now host two orbitals, and we will denote the annihilation operators of the two orbitals as $\hat{p}_x$ and $\hat{p}_y$, see Fig. 5.2. The wave functions are dumbbell-shaped with one node at the center, and the two lobes are of opposite signs. Depending on the relative orientation of the orbitals on neighboring lattice sites, the hopping strengths is given by either the “head-to-tail” σ -bonds, or the much weaker “shoulder-by-shoulder” π -bonds. For simplicity, we will only consider σ -bonds in this section, and hence there is only one hopping parameter t . If we stick to the convention where there is a negative sign in front of t in the tight-binding Hamiltonian, we have $t < 0$ due to the odd parity of the p -orbitals (i.e. a $+$ lobe faces a neighboring $-$ lobe).

To construct the tight-binding Hamiltonian, We must form the correct superposition of the p_x and p_y states such that the head-to-tail condition is met for each term. This is done by defining the following states:

$$\hat{p}_1 = \frac{\sqrt{3}}{2}\hat{p}_x + \frac{1}{2}\hat{p}_y, \quad \hat{p}_2 = -\frac{\sqrt{3}}{2}\hat{p}_x + \frac{1}{2}\hat{p}_y, \quad \hat{p}_2 = -\hat{p}_y, \quad (5.4)$$

which are the projections of the p -orbitals along the neighboring site vectors defined in Eqn. (3.46). Using these operators, the honeycomb p -band tight-binding Hamiltonian can be written as

$$H_p^{\text{hc}} = -t \sum_{\mathbf{r} \in A} \sum_{i=1,2,3} \hat{p}_{\mathbf{r},i}^\dagger \hat{p}_{\mathbf{r}+\mathbf{d}_i^{\text{hc}},i} + \text{h.c.} \quad (5.5)$$

The sum over $\mathbf{r} \in A$ means that $\hat{p}_{\mathbf{r},i}$ is a $\hat{p}_i$ -orbital on site A at location $\mathbf{r}$, and the other operator is implicitly a B-site, since all nearest neighbors of A-sites are B-sites.

Defining $\hat{\mathbf{v}}(\mathbf{k}) = (\hat{p}_x^A(\mathbf{k}) \hat{p}_y^A(\mathbf{k}) \hat{p}_x^B(\mathbf{k}) \hat{p}_y^B(\mathbf{k}))^T$, we can write the momentum space Hamiltonian as $\hat{\mathbf{v}}(\mathbf{k})^\dagger H_p^{\text{hc}}(\mathbf{k}) \hat{\mathbf{v}}(\mathbf{k})$, where the kernel is

$$H_p^{\text{hc}}(\mathbf{k}) = -t \begin{pmatrix} 0 & 0 & \frac{3}{4}(e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2}) & \frac{\sqrt{3}}{4}(e^{i\mathbf{k} \cdot \mathbf{d}_1} - e^{i\mathbf{k} \cdot \mathbf{d}_2}) \\ 0 & 0 & \frac{\sqrt{3}}{4}(e^{i\mathbf{k} \cdot \mathbf{d}_1} - e^{i\mathbf{k} \cdot \mathbf{d}_2}) & \frac{1}{4}(e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2}) + e^{i\mathbf{k} \cdot \mathbf{d}_3} \\ \text{h.c.} & & 0 & 0 \\ & & 0 & 0 \end{pmatrix} \quad (5.6)$$

$$\equiv -t \begin{pmatrix} 0 & h(\mathbf{k}) \\ h^\dagger(\mathbf{k}) & 0 \end{pmatrix} = -t (\tau_x \otimes \text{Re}[h(\mathbf{k})] - \tau_y \otimes \text{Im}[h(\mathbf{k})]).$$

In the last line, we have used the Pauli matrices in the sublattice basis, $\tau_{x(y)}$.

Since H_p^{hc} is invariant under $t \rightarrow -t$, $\hat{p}^A \rightarrow -\hat{p}^A$, the band structure is symmetric about zero energy. The dispersion relations of the p -bands are given by

$$E_{1,4} = \mp \frac{3}{2}t, \quad E_{2,3} = \mp \frac{t}{2}|f(\mathbf{k})|, \quad (5.7)$$

where

$$E_\pm^{\text{hc}}(\mathbf{k}) = \pm |f(\mathbf{k})| = \pm t \sqrt{3 + 2[\cos(\mathbf{k} \cdot \mathbf{A}_1) + \cos(\mathbf{k} \cdot \mathbf{A}_2) + \cos(\mathbf{k} \cdot \mathbf{A}_3)]}, \quad (5.8)$$

the same function that we defined for the honeycomb s -band in Sec. 3.4.2. The lowest and highest bands are exactly flat, and both of them crosses with the neighboring band at the high symmetry point Γ . We will refer to these two touching points quadratic band touching points (QBTP), since the band gap grows quadratically away from Γ .

In this work, we will focus on the lower QBTP between band 3 and 4. Our goal now is to find an effective two-band Hamiltonian for the lower QBTP to the lowest order in q . The first step is to find the basis states for the effective two band model. Let us first diagonalize $H_p^{\text{hc}}(\mathbf{k})$ at the QBTP to get some intuition. Exactly at $\mathbf{k} = \mathbf{0}$, the kernel takes on a particularly simple form, with $h(\mathbf{0}) = 3I/2$, and the eigenstates are given by

$$\psi_{\pm x} = \frac{1}{\sqrt{2}}(1, 0, \pm 1, 0), \quad \psi_{\pm y} = \frac{1}{\sqrt{2}}(0, 1, 0, \pm 1). \quad (5.9)$$

Physically, the states with a minus (plus) sign correspond to (anti-)bondings, with eigenenergies $\mp 3/2$. Indeed, the eigenstates near Γ are approximately given by the following expres-

sions to lowest order in q [129]:

$$\begin{aligned}\psi_{1,4}(\mathbf{q}) &= \frac{1}{\sqrt{2}q}(-q_y, q_x, \pm q_y, \mp q_x), \\ \psi_{2,3}(\mathbf{q}) &= \frac{1}{\sqrt{2}q}(q_x, q_y, \mp q_x, \mp q_y).\end{aligned}\tag{5.10}$$

Eqn. (5.10) show that around Γ , the p -orbitals of the four Bloch states are either both parallel or both perpendicular to the quasimomentum $\mathbf{q}$. We also already see that the eigenstates vary by two full cycles around Γ (since $\psi_n(-\mathbf{q}) = -\psi_n(\mathbf{q})$). Expecting that the lowest order corrections should be second order in quasimomentum around Γ , we expand Eqn. (5.6) to $O(q^2)$:

$$\begin{aligned}h(\mathbf{q}) &\approx \begin{pmatrix} \frac{3}{2} + i\frac{3}{4}q_y - \frac{3}{16}(3q_x^2 + q_y^2) & i\frac{3}{4}q_x - \frac{3}{8}q_xq_y \\ i\frac{3}{4}q_x - \frac{3}{8}q_xq_y & \frac{3}{2} - i\frac{3}{4}q_y - \frac{3}{16}(q_x^2 + 3q_y^2) \end{pmatrix} \\ &= \underbrace{\left[\left(\frac{3}{2} - \frac{3}{8}q^2 \right) I - \frac{3}{16}(q_x^2 - q_y^2)\sigma_z - \frac{3}{8}q_xq_y\sigma_x \right]}_{\text{Re}[h(\mathbf{q})]} + i \underbrace{\left[\frac{3}{4}q_y\sigma_z + \frac{3}{4}q_x\sigma_x \right]}_{\text{Im}[h(\mathbf{q})]}.\end{aligned}\tag{5.11}$$

Our goal now is to perturb away the $\{\psi_{+x}, \psi_{+y}\}$ subspace. We first rewrite the kernel in the bonding/antibonding basis, $(\hat{\psi}_{+x}(\mathbf{q}) \hat{\psi}_{+y}(\mathbf{q}) \hat{\psi}_{-x}(\mathbf{q}) \hat{\psi}_{-y}(\mathbf{q}))^T$. The unitary transformation is best done in block diagonal form:

$$\begin{aligned}U &= \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix} \\ \Rightarrow H_p^{\text{hc}}(\mathbf{q}) &= U^\dagger H_p^{\text{hc}}(\mathbf{q}) U = \begin{pmatrix} \text{Re}[h(\mathbf{q})] & -i \text{Im}[h(\mathbf{q})] \\ i \text{Im}[h(\mathbf{q})] & -\text{Re}[h(\mathbf{q})] \end{pmatrix}\end{aligned}\tag{5.12}$$

Given that the off-diagonal blocks are $O(q)$, we cannot simply “crop” the kernel to the lower bands manifold (the lower right block of Eqn. (5.12)). The coupling between the lower and higher bands can be accounted for using the Löwdin partitioning method [130, 131, 126], which is an expression for the second order perturbation theory for block Hamiltonians. for a block Hamiltonian of the form

$$H = \left(\begin{array}{c|c} H_{\alpha\alpha} & H_{\alpha\beta} \\ \hline H_{\beta\alpha} & H_{\beta\beta} \end{array} \right),\tag{5.13}$$

the effective Hamiltonian for the β block is given by

$$\mathcal{H}_\beta = H_{\beta\beta} + H_{\beta\alpha}(E_0 - H_{\alpha\alpha})^{-1}H_{\alpha\beta}.\tag{5.14}$$

Here, we choose $E_0 = -3/2$, the lower flat band energy. Using Eqn. (5.11), (5.12) and (5.14), we find

$$H_{\text{QBTP}}^{\text{hc}} \approx \frac{3}{8}t \begin{pmatrix} q_x^2 & q_xq_y \\ q_xq_y & q_y^2 \end{pmatrix} - \frac{3}{2}tI.\tag{5.15}$$

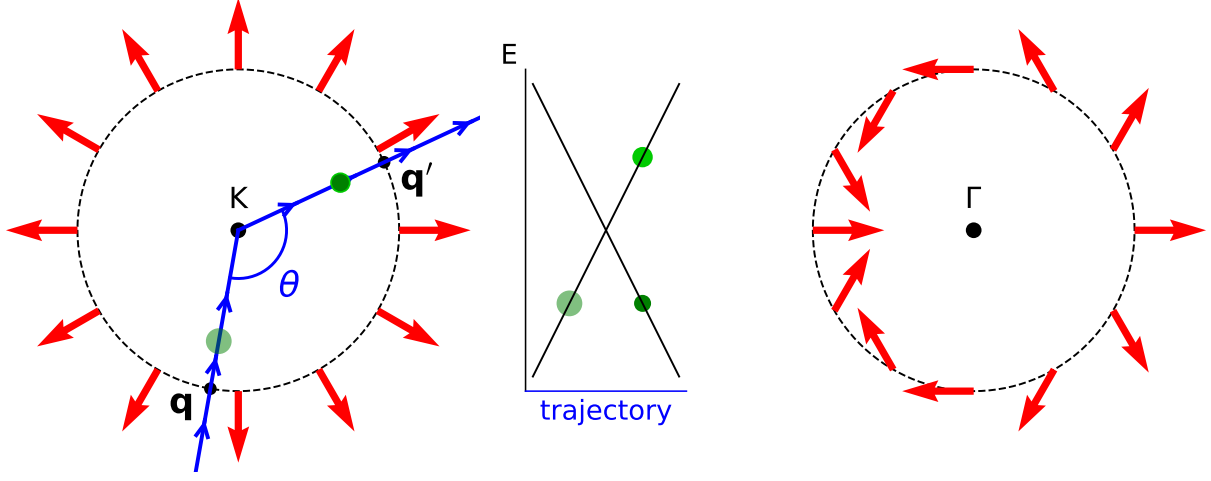


Figure 5.3: Illustration of the experiment protocol, zoomed in to the region near band touching points of interest. Left: a BEC (green circles) is translated in the quasimomentum space along trajectories (blue lines with arrow heads) that goes through the LBTP. The BEC is initially prepared in the lower band, which corresponds to a pseudospin pointing along the fictitious field (red arrows). After leaving the LBTP, the BEC is now in a superposition of the lower and upper band, and we measure the population in each band using band mapping. Right: The fictitious field around the QBTP.

We can drop the identity term, which simply sets the flat band energy to $-3/2$, and perform one last unitary transformation to the basis defined by

$$\psi_{\pm\chi} = \frac{1}{\sqrt{2}}(\psi_{-x} \pm i\psi_{-y}). \quad (5.16)$$

These are states with the on-site phase of the wave function winding in opposite handedness, with matching phases on the neighboring sites. Finally, we arrive at

$$H_{\text{QBTP}}^{\text{hc}} \approx \frac{1}{4m} \begin{pmatrix} q^2 & q_-^2 \\ q_+^2 & q^2 \end{pmatrix} \equiv \frac{1}{4m}(q^2 I + \mathbf{B}_{\text{QBTP}} \cdot (\sigma_x, \sigma_y)), \quad (5.17)$$

where $m \equiv 4\hbar^2/3ta_{\text{hc}}^2$ is the effective mass of the band with quadratic dispersion. The direction of the fictitious field around the QBTP $\mathbf{B}_{\text{QBTP}} = (q_x^2 - q_y^2, 2q_x q_y)$ is then given by $\boldsymbol{\rho}(2\varphi_q)$. The direction of $\mathbf{B}_{\text{QBTP}}$ varies by two full periods around the Γ point, which we associate with a winding number of two.

5.1.3 Summary of the published results

In this section, we briefly summarize the measurement scheme and the main findings published in Ref. [49]. We load a BEC with ignorable interaction strength into an optical

honeycomb lattice, which can be translated through arbitrary trajectories. The BEC is prepared in the lower Bloch band involved in the band touching with high fidelity. In the lattice frame, the BEC moves in the quasimomentum space towards either the LBTP or the QBTP, and then leaves the singular point at varying angles θ (see Fig. 5.3). We will use $\mathbf{q}$ ($\mathbf{q}'$) to label a quasimomentum close to the singular point on the trajectory before (after) the turn.

Using band mapping measurements, we find that the population of atoms are mainly split between the two crossing bands after the lattice translation sequence. The population transferred to the upper band is determined by the quantum distance between the initial and final Bloch state:

$$d(\theta) \equiv 1 - \left| \langle u_{\mathbf{q}'}^{(n)} | u_{\mathbf{q}}^{(n)} \rangle \right|^2 = \begin{cases} \frac{1}{2}(1 - \cos \theta) & \text{LBTP,} \\ \frac{1}{2}(1 - \cos 2\theta) & \text{QBTP.} \end{cases} \quad (5.18)$$

Indeed, we observe that Eqn. (5.18) correctly predicts the experimentally measured population transfer as θ is varied from 0 to 2π .

This result can be understood intuitively in pseudospin picture. From Sec. 5.1, we see that the direction of the fictitious field is independent of the distance from the singular point, as long as the two-band picture holds. Therefore, we expect no changes in band populations as the quasimomentum state approaches and accelerates away from the band touching point. Exactly at the band touching point, there is no band gap, so the sudden approximation holds exactly, and the population in each band is simply given by the projection of the original state onto the new basis, determined by the direction of the fictitious field. From Fig. 5.3, we see that periodicity of the quantum distance in Eqn. (5.18) reflects the winding number of one and two³ of the LBTP and QBTP fictitious fields, respectively.

5.2 Cold atoms

Since this work was performed using the old rubidium machine, there are some crucial system parameters that are different from the values reported in chapter 2 and 4. In particular, our previous work has shown that the band structure is renormalized by the mean-field interactions of bosons [132], and furthermore the time scale in which we observed coherent diffraction peaks is affected by various instabilities when the BEC is in a Bloch state that is close to the band edges [53]. These effects put a fundamental limit on the time scale of the experiments, which determines the momentum resolution of how precisely we can locate the singular points.

In this work, we worked with a small Rb atom number of $1-2 \cdot 10^4$ in the $|F = 1, m_F = -1\rangle$ state. The trap frequencies at the end of evaporation is also much smaller ($\omega_{x,y,z} = 2\pi \cdot$

³In principle, observing that the band occupation varies by two periods as a function of θ is not enough to claim that we measure a winding number of two — the contrast of the variation in band population must be one. Our claim that we measure $w = 2$ rely on the fact that the Berry phase associated with a QBTP is 2π if a system exhibits both C_6 and time-reversal symmetry, which ensures that the winding number is two [126].

(23, 41, 46) Hz) compared to our current experiment. Using these parameter and Eqn. (3.24), we find that the peak density of the BEC is within the range $1.7 \cdot 10^{13}$ to $3.4 \cdot 10^{13} \text{ cm}^{-3}$. The maximum mean-field energy is then given by $U_0 n_{\text{TF}} \approx 264 \text{ Hz}$. This is much larger than the on-site offset 33 Hz due to the vector polarizability of Rb, but small enough that the modification in the band structure does not have a measurable effect in our experiment. The weak mean-field energy also means that effects such as dynamical instabilities are less problematic. We note that unlike the optical acceleration pulse method used in [132], the lattice translation technique used in this work does not compress the atom cloud, so the density is roughly constant throughout the sequence.

Instead of a typical ToF measurement in which the atoms are free falling due to gravity during the free expansion, we turn on a quadrupole field whose trap center is above the cloud position, with the z -gradient just enough to compensate for the gravitational pull. The atoms then evolve in an approximately harmonic confining magnetic potential, whose frequency is determined by the proximity of the magnetic field trap center. By evolving in the trap for a quarter period, which was 50 ms for the parameter used in the experiment, the momentum operator at the time atoms are released evolve exactly to the position operator in the Heisenberg picture. We refer to this technique as “momentum space focusing,” which is not very crucial in this work, because atoms in different bands are mapped to different plane waves with momenta differing by $\hbar \mathbf{G}$, where $\mathbf{G}$ is some reciprocal lattice vector. As long as these plane waves are well separated, whether the final images are exactly momentum measurements or an approximation thereof in the far-field regime does not really matter. We do, however, benefit slightly from the long ToF enabled by gravity compensation, which allowed better atom counting due to slightly lower optical densities.

5.3 Lattice translation

In this section we derive the analog signal required to generate the lattice translation sequence. We also document the hardware setup used in producing this work. While the National Instrument PXI box described in this section is replaced when we switched to ARTIQ for our control system, this section explains the design choice of using an ARTIQ fastio module (fast DAC) for phase lock control in our current setup.

We note that it is not necessary to stabilize the relative phases of the lattice beams if one is only working with monochromatic lattices. Phase noise might heat up the atoms and result in more uncertainty in the trajectory traversed by atoms, but is not destructive for the experiment scheme. However, phase stabilization is crucial for superlattice experiments for maintaining the correct lattice geometry. In this work, all the data were taken with the phase feedback loop engaged.

5.3.1 From phase to displacement

Let us first consider a one dimensional optical standing wave for simplicity. We consider two plane waves given by

$$E_1(x, t) = e^{i(kx - \omega t - \phi)}, \quad E_2(x, t) = e^{i(-kx - \omega t)}, \quad (5.19)$$

where $k = 2\pi/\lambda$ is the wave number, and ϕ is a phase. E_1 (E_2) propagates to the right (left). The sum of the two plane waves gives a standing wave pattern,

$$\begin{aligned} I(x, t) &\propto |E_1(x, t) + E_2(x, t)|^2 \\ &= 2(1 + \cos(2kx - \phi)) \\ &= 2 \left(1 + \cos \left[g \left(x - b \cdot \frac{\phi}{2\pi} \right) \right] \right), \end{aligned} \quad (5.20)$$

where $b = \lambda/2$ is the lattice constant, and $g = 2k = 2\pi/b$ is the primitive “vector.” I will drop the constant offset from now on. In the last line, $I(x, t)$ is rewritten to directly connect ϕ to the displacement of the standing wave pattern. As expected, the intensity is the same for $\phi = 0$ and $\phi = 2\pi$, and the standing wave is displaced by one lattice constant. If the two beams are not exactly counterpropagating, then one replaces k with $k_{\parallel} = k \sin(\theta/2)$, where θ is the angle between the two wave vectors. The resulting lattice is still one dimensional, with a larger lattice constant $a = \lambda/2 \sin(\theta/2)$.

Now, let us consider a time-dependent relative phase, $\phi(t)$. The simplest case is a phase that accumulates linearly, which I will suggestively write as $\phi(t) = 2\pi\delta_{12}t$. Substituting this into Eqn. (5.19), we see that δ_{12} corresponds to the frequency detuning between plane waves E_1 and E_2 . Eqn. (5.20) now becomes

$$I(x, t) \propto \cos [g (x - b\delta_{12}t)], \quad (5.21)$$

which corresponds to a moving standing wave with velocity $+b\delta_{12}$. There is a nice way to understand this using Doppler shifts: consider $\delta_{12} > 0$ (blue detuned E_1). For an observer moving to the right at speed v , E_1 (E_2) is red (blue) shifted, so there must be some value of v that shifts the two waves into resonance, and the standing wave appears stationary for the moving observer. v is then given by

$$f \frac{v}{c} = \frac{\delta}{2} \Rightarrow v = b\delta. \quad (5.22)$$

A more general time-dependent phase can always be written as a time-dependent detuning,

$$\phi(t) \equiv 2\pi \int dt \delta_{12}(t) \Rightarrow \delta_{12}(t) = \frac{d\phi(t)}{dt}. \quad (5.23)$$

And the velocity of the lattice is given by $b\delta_{12}(t)$. Reading Eqn. (5.23) backwards, we see that that the velocity of the lattice is always proportional to the detuning, and the accumulated

phase is found by integrating the detuning. This is a useful fact given that what we directly control in experiments is the detuning between lattice beams (through VCOs).

Let us finally consider the optical potential of hexagonal lattices, which is given in Eqn. (3.50). In our experiment, we treat B2 as the reference beam, so we only change the detunings of B1 and B3. While it is not straightforward to see how the lattice is displaced by looking at Eqn. (3.50), it is clear from the Doppler shift picture that detuning B1 (B3) displaces the lattice in the direction $\mathbf{k}_{1(3)}$ ⁴. For example, if an observer moving against $\mathbf{k}_1$ finds that B1 is blue-shifted by Δ , both B2 and B3 are red-shifted by $\Delta/2$. The resonance condition is then modified as

$$f\frac{v}{c} = \frac{2\delta}{3} \Rightarrow v = a_{\text{lat}}\delta, \quad (5.24)$$

where $a_{\text{lat}} = 2\lambda_{\text{lat}}/3$ is the lattice constant defined in Sec. 3.3.1. Since this work only uses the 1064 nm lattice, I will use $a_{\text{lat}} = A = 710$ nm. Combining everything together, we find that the velocity of the lattice as a function of detunings is given by

$$\mathbf{v} = A(\delta_1(t)\hat{\mathbf{K}}_1 + \delta_3(t)\hat{\mathbf{K}}_3), \quad (5.25)$$

where $\delta_{1(3)}(t)$ is the detuning between B1(3) and B2, and $\hat{\mathbf{k}}_{1(3)}$ is the unit vector in the direction of B1(3). As a sanity check, we can substitute $\phi_{1(3)} = -2\pi\delta_{1(3)}t$ into Eqn. (3.50), and confirm that it is the same as (taking $r_1 = r_3 = 1$)

$$I(\mathbf{r}) = I_0 [3 - \cos(\mathbf{G}_3 \cdot (\mathbf{r} - \mathbf{v}t)) - \cos(\mathbf{G}_1 \cdot (\mathbf{r} - \mathbf{v}t)) - \cos(\mathbf{G}_2 \cdot (\mathbf{r} - \mathbf{v}t))], \quad (5.26)$$

5.3.2 Output functions required for the phase lock

For this work, we will entirely be interested in controlling the velocity of the lattice, which determines the quasimomentum of atoms in the lattice frame. Therefore, Eqn. (5.25) means that our goal is to generate the desired detunings $\delta(t)$, and the required phase lock setpoint is determined from $\delta(t)$. For this section, I drop the lattice beam subscripts 1(3), and the discussion applies to both beams.

In our experiment, the detunings between lattice beams are controlled by DDS waveform generators (Keysight 33600A) that act as voltage controlled oscillators (VCO). The output frequency is modified by $\Delta f = K_{\text{VCO}}V_m$ when a modulation voltage V_m is applied. Here, K_{VCO} is the gain of the VCO, with dimensions of Hz V^{-1} . This gives us the feedforward voltage required to generate the desired detuning as $V_{\text{ff}} = \delta(t)/K_{\text{VCO}}$, and the required phase setpoint is given by integrating the detuning (Eqn. (5.23)). The signals multiplied to the detected phase quadratures are then simply given by $\sin(\phi(t))$ and $\cos(\phi(t))$ (see Sec. 4.2.4).

The working principle is very simple, but the actual implementation requires a lot of care. As an example, let us first consider how would one implement the lattice translation of the QBTP sequence, see Fig. 5.4. In the simplest implementation, this would require piecewise

⁴Based on this argument, it should become clear that if the three beams are not C_3 symmetric, the displacement might not be along the direction of the detuned beam.

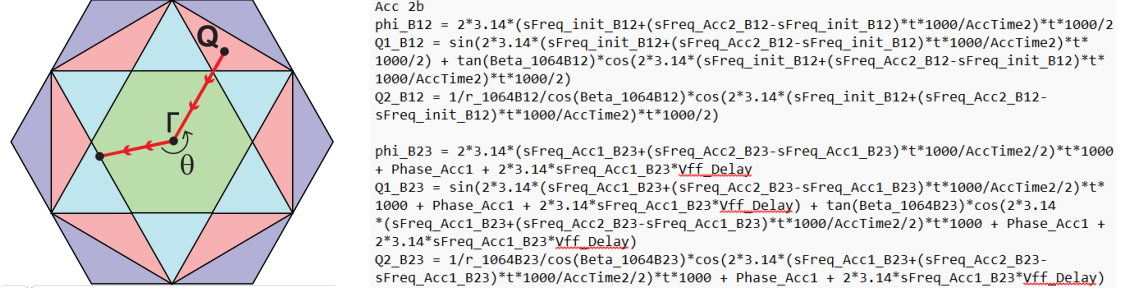


Figure 5.4: Example of the analog control for phase-stabilized lattice translation. Left: an example of the QBTP lattice translation sequence consisting of three segments. Right: the functions that generate the required phase lock signals for the last segment. The text box in Cicero GUI that displays at most ~ 20 letters is not quite large enough for these functions.

linear ramps in the two detunings, where the acceleration in each line segments is constant. We then have $\delta(t) \propto t$ and $\phi(t) \propto t^2$. Logically, the sequence contains the following steps:

$$\underbrace{[\Gamma \rightarrow \mathbf{Q}] \Rightarrow [\text{hold at } \mathbf{Q}]}_{\text{Load into the 3rd band}} \Rightarrow \underbrace{[\mathbf{Q} \rightarrow \Gamma] \Rightarrow [\Gamma \rightarrow \mathbf{q}(\theta)]}_{\text{Turn at the QBTP}} \Rightarrow \underbrace{[\text{hold at } \mathbf{q}(\theta)]}_{\text{Band mapping}}$$

In each of the steps, we need to account for the following:

- The VCOs have an DAC conversion delay of around $14 \mu\text{s}$, while the multipliers used for the phase locks are analog, and have no delay. Therefore, the feedforward signal must output $14 \mu\text{s}$ earlier than the phase lock signals.
- For the signals to be continuous, the accumulated phase $\phi(t)$ from all previous steps must be accounted for. This is somewhat annoying to set up in Cicero (see the next section).

Therefore, the resulting output functions become very long (see Fig. 5.4 for an impression), even for this relatively simple three-step translation sequence.

5.3.3 Generating the signals

One can consider using arbitrary waveform generators (AWG) to generate the signals required for all the channels. However, given the large number of channels we need (twelve channels in total: each of the four lattice beam pairs needs two quadrature modulation signals and one feedforward for each lattice beam pair), we will need several AWGs to be able to do arbitrary lattice translation. The communication between Cicero and AWGs can also add a lot of experimental complexity.

Given that the lattice translation sequence is only a few ms long, we don't really need the large output buffer offered by AWGs. The first alternative that we consider are the DAC channels. The control system of the old machine is Cicero, which generates all the

outputs before an experiment run. Therefore, the smallest timestep that can be used is limited by the size of the buffer storing the outputs. Since our experiment cycle time was tens of seconds long, we had to use a large time step of $25\text{ }\mu\text{s}$, corresponding to a Nyquist frequency (frequency at which only two points are sampled each period) of 20 kHz . Since this is comparable to the largest frequency used in our lattice translation sequence, this means that the DAC output of Cicero would severely undersample our desired output.

We end up using DAC channels of a standalone PXI box from National Instrument to output phase lock signals. This PXI box runs its own copy of Cicero, and was the control PC of the lithium-rubidium mixture experiment in the group. The main difference of this Cicero implementation is that the output is generated in real time, similar to ARTIQ. Therefore, we don't encounter the same memory issue as long as the outputs are generated at the same rate as the output. The time step used in this experiment was $1.6\text{ }\mu\text{s}$, which is short enough. This Cicero was set to the “wait for retrigger” mode, and output upon receiving a trigger from the main Cicero⁵.

5.4 Details on the band mapping procedure

The band mapping procedure is done by ramping down the lattice depth exponentially and slowly enough, such that each Bloch state is adiabatically mapped to a plane wave state. Since the band gaps between neighboring bands are larger for a deeper lattice, it is intuitive that the ramp can be more aggressive initially. The ramp down times were chosen to be 0.6 ms for the LBTP measurements, and 1 ms for the QBTP measurements, which are informed by numerical simulations (see Ref. [50] for more detail).

However, band mapping is unreliable when the final quasimomentum of the atoms is close to Brillouin zone edges, regardless of how slow the ramp is, because the Bloch states for certain bands are connected to more than one plane wave states when the lattice is turned off. To see what bands are affected for a given quasimomentum, it is the easiest to work in the extended zone scheme, as shown in Fig. 5.5. For a chosen final quasimomentum, let us label all the equivalent quasimomentum points. If the quasimomentum is exactly on the edge between band n and m , then the Bloch state is simultaneously connected to two free particle states. For the example shown on the left in Fig. 5.5, we would not be able to differentiate between the population in band 1 and 2, since the red equivalent quasimomentum points are exactly on the boundary between the first and second Brillouin zones. However, since the blue points do not cross any Brillouin zone edges, atoms in band 3 and 4 can be faithfully mapped to a single plane wave state. Therefore, this quasimomentum choice was used for the characterization of the QBTP.

⁵Output module: two PXI-6713 (using six out of the eight channels on each module). The sampling resolution $1.6\text{ }\mu\text{s}$ was partially limited by the number of channels used. $1\text{ }\mu\text{s}$ steps were found to work when only one channel on each module is outputting. FPGA: Opal Kelly XEM3001. `OnBoardMemoryHalfOrLess` and `DMA` in Atticus buffer setting should be set to `True`. The total delay between trigger to signal output was found to be about 760 ns .

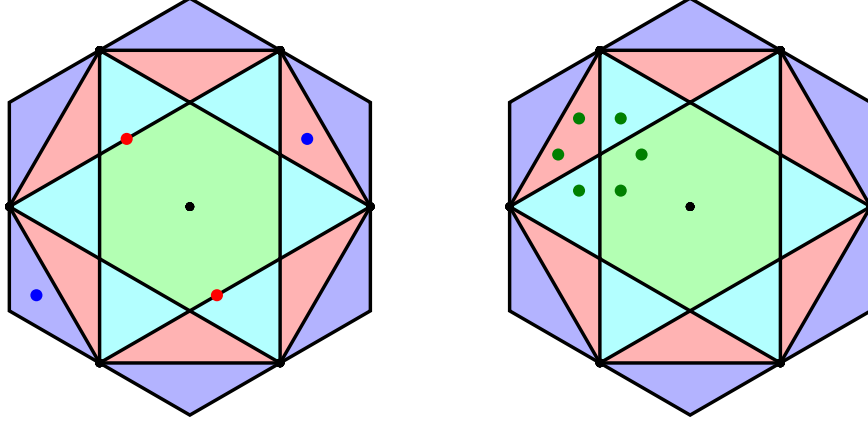


Figure 5.5: Choices of final quasimomenta for band mapping. Left: one example of the quasimomentum chosen for the QBTP measurement. The other eleven final quasimomenta used in the experiment are related by six-fold rotations and inversion. Right: the six quasimomenta chosen for the LBTP measurement.

Similarly, for the LBTP, we need to avoid the Brillouin zone edges of the first and second Brillouin zones. We are not concerned with the Brillouin zones of higher bands, since in the end we will simply sum the population in all the other bands as a measure of nonadiabaticity of the sequence. Out of the 24 values of θ used in the LBTP, we choose six of the angles that places the final quasimomentum away from Brillouin zone edges as the band mapping points, as shown in Fig. 5.5. After the turn at the LBTP, the atoms are then adiabatically accelerated to the closest of the six points before band mapping.

The band mapping technique is also used for initial state preparation for the QBTP measurements. For the QBTP measurements, the atoms are loaded in a running lattice, which requires us to ramp up the lattice rapidly to avoid displacing the atoms (see Sec. 5.5). We use the time-reversed version of the band mapping sequence to prepare higher band states from a non-zero quasimomentum. This is referred to as “inverse band mapping” in Ref. [49].

There is an important technical detail in the implementation: since the lattice beams themselves are also Gaussian beams, the position of the trap minimum can be different with and without the lattice. This is not a problem for the LBTP measurements, since the slow loading deforms the trapping potential adiabatically. But for the QBTP measurements, the atoms are placed at a slope of the final trapping potential, which exerts an unwanted force to the atoms. Therefore, in the “fast loading” sequence that was implemented, the atoms were first loaded into the ground state of a stationary lattice with a slow lattice ramp up, smoothly displacing the atoms to the new trap minimum. We then performed a fast band mapping to recover a plane wave, and then reloaded the atoms into a running lattice using inverse band mapping. See Fig. 5.6 for an example of the time sequence. We observe no

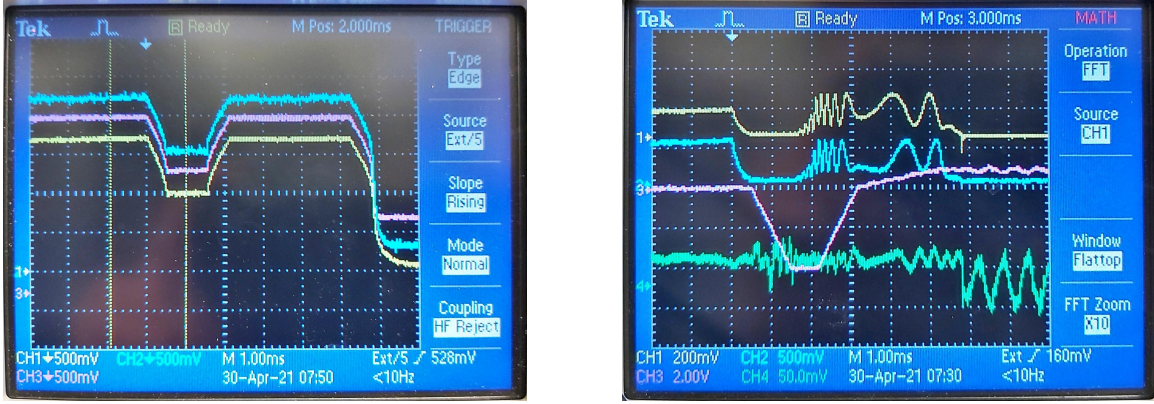


Figure 5.6: The lattice beam oscilloscope traces for the fast loading sequence. Left: intensities of the three lattice beams. Each trace is the signal from a logarithmic photodiode with a gain of around 10 dB every 0.4 V. Right: phase-related signals for one of the lattice beam pairs. Purple: modulation signal (proportional to lattice velocity). Green: error signal. Yellow and blue: the in-phase and out-of-phase quadratures of the relative phase between the lattice beam pair. The lattice translation begins after the first fast band mapping.

detectable population in the excited states after the first fast band mapping. We were able to achieve around 92% loading fidelity into the third band with this sequence.

5.5 Displacements due to lattice acceleration

Finally, we note that as the lattice accelerates, the atoms are also dragged along in the lattice [133]. In the lab frame, the velocity of the atom is given by

$$\mathbf{v}_{\text{lab}} = \mathbf{v}_{\text{lat}} + \mathbf{v}_g(\mathbf{q} = -m\mathbf{v}_{\text{lat}}), \quad (5.27)$$

where $\mathbf{v}_g(\mathbf{q})$ is the group velocity. The extreme cases are no lattice ($\mathbf{v}_{\text{lat}} = -\mathbf{v}_g(\mathbf{q})$) and extremely deep lattice ($\mathbf{v}_g = \mathbf{0}$). Integrating Eqn. (5.27) then gives the displacement of atoms throughout the sequence. Ideally, we don't care about the spatial position of atoms, since the final measurement is in the momentum space. However, since the trap potential is approximately harmonic, the displacement means that atoms are now accelerated in the opposite direction of the velocity of the lattice. This acceleration means that the actual quasimomentum trajectories taken by the atoms deviates from the programmed trajectory, and also poses a challenge in interpreting the results from band mapping, since the uncertainty in quasimomentum breaks down our peak-band number association scheme.

For the LBTP measurements, the displacements are around $1\mu\text{m}$, which is much less than the previous ODT beam waists of $43\mu\text{m}$. Therefore, the effect of lattice dragging can be safely ignored compared to other imperfections, such as an initial momentum fluctuation of around $0.05\hbar K$ [53]. However, for the QBTP measurements, the displacements can be as

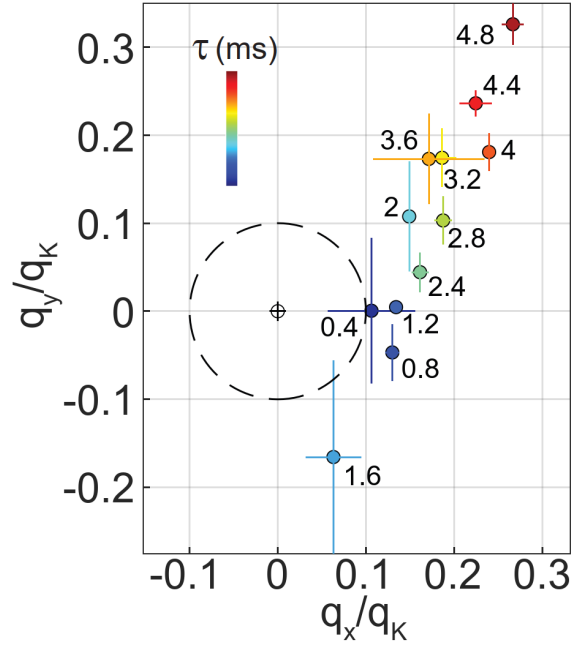


Figure 5.7: Unwanted acceleration of atoms in the confining potential due to the lattice dragging effect. The black dashed circle is centered at zero momentum, whose position in absorption images is measured using a stationary BEC. Here, $q_K = K$. Reproduced from [49].

large as around $6\mu\text{m}$, and the resulting acceleration from the external confinement can be on the order of $0.2\hbar K$ or more for long sequences. Fig. 5.7 shows this effect, measured by tracking the center of mass position of one of the peak after band mapping. We note that if we decide to perform similar measurements in the future, this problem can be alleviated by creating a flat box potential using a projected optical potential.

Chapter 6

Simulating optical excitations in honeycomb lattices

In chapter 5, we mentioned that the Bloch band structure plays a crucial role in understanding optical properties of materials. However, this cannot be the full story, because the excitation rate of a perturbation is also dependent on its matrix element between the states of interest. An important example is that the matrix element can vanish due to symmetry considerations, which leads to selection rules for excitations. We therefore expect that the optical response of material reveals certain relations between the involved Bloch states, and as we will see, the central quantity of interest is the interband Berry connection.

In this chapter, we establish the relation between periodic lattice translation, or lattice shaking, and optical excitations in solids. This relation has been used in previous proposals to devise novel ways to measure the Chern number [134] and quantum metric [135] using atoms in optical lattices. But as far as we know, no existing works directly relate the interband Berry connection to experiment observables. I will describe how we were able to observe optical selection rules that originate from the interband Berry connection. The main finding of this project, which is the measurement of the full interband Berry connection field and Dirac strings, will be covered in Malte Schwarz's PhD thesis [50]. This work is reported at Ref. [136].

6.1 Lattice shaking as optical probes

We will first briefly review the formulation of optical excitations in solids. We will find that under certain approximations and gauge choices, the perturbation Hamiltonian is proportional to the position operator. This will allow us to directly map lattice shaking to optical excitations. The evaluation of the position operator matrix element is rather nontrivial due to the extended nature of Bloch states, and a careful treatment relates the matrix element to the interband Berry connection, establishing the connection between optical excitation and quantum geometry promised in the introduction.

6.1.1 Optical excitation in solids

The Hamiltonian of an electromagnetic wave interacting with single particles in a periodic potential is given by the minimal coupling Hamiltonian as [137]

$$\hat{H} = \frac{1}{2m} \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(\hat{\mathbf{r}}, t) \right)^2 + q\Phi(\hat{\mathbf{r}}, t) + V(\hat{\mathbf{r}}), \quad (6.1)$$

where q is the charge of the particle ($q = -e$ for electrons), $\mathbf{A}$ and Φ are the vector and scalar potential of the electromagnetic fields, respectively, and $V(\hat{\mathbf{r}})$ can in general be any potential, but we will eventually be interested in $V = V_{\text{lat}}$, the periodic lattice potential.

We will begin with the Coulomb gauge, $\nabla \cdot \mathbf{A} = 0$. For a single frequency electromagnetic field, this is given as

$$\begin{aligned} \mathbf{A}(\hat{\mathbf{r}}, t) &= A_0 \boldsymbol{\epsilon} e^{i(\mathbf{k} \cdot \hat{\mathbf{r}} - \omega t)} + \text{h.c.} \equiv \mathbf{A}_0(t) e^{i\mathbf{k} \cdot \hat{\mathbf{r}}} + \text{h.c.} \\ \Phi(\hat{\mathbf{r}}, t) &= 0, \end{aligned} \quad (6.2)$$

and the resulting electromagnetic fields are given by

$$\begin{aligned} \mathbf{B}(\hat{\mathbf{r}}, t) &= \nabla \times \mathbf{A} = iB_0(\mathbf{n}_k \times \boldsymbol{\epsilon}) e^{i(\mathbf{k} \cdot \hat{\mathbf{r}} - \omega t)} + \text{h.c.} \\ \mathbf{E}(\hat{\mathbf{r}}, t) &= -\nabla \Phi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} = iE_0 \boldsymbol{\epsilon} e^{i(\mathbf{k} \cdot \hat{\mathbf{r}} - \omega t)} + \text{h.c.} \end{aligned} \quad (6.3)$$

Here, $\boldsymbol{\epsilon}$ is the polarization vector, which we will elaborate on later. $\mathbf{n}_k$ is the direction of the wave vector. The amplitudes of the electric and magnetic fields are given by $E_0 = \omega A_0$ and $B_0 = k A_0 = E_0/c$.

The vector potential commutes with the canonical momentum under the Coulomb gauge, which allows us to simplify Eqn. 6.1 as

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{q}{mc} \mathbf{A}(\hat{\mathbf{r}}, t) \cdot \hat{\mathbf{p}} + \frac{q^2}{2mc^2} \mathbf{A}(\hat{\mathbf{r}}, t)^2 + V(\hat{\mathbf{r}}). \quad (6.4)$$

We will make two approximations. First, we assume that the optical excitation is weak, so we can drop the $\mathbf{A}^2$ term. Second, we take the electric dipole approximation, $e^{i(\mathbf{k} \cdot \hat{\mathbf{r}})} \approx 1$, which in the context of solids amounts to saying that the wavelength of the perturbation is much larger than the spatial dimension of a unit cell. Writing the Hamiltonian without optical fields as $\hat{H}_0 = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{r}})$, we arrive at

$$\hat{H} = \hat{H}_0 - \frac{q}{mc} \mathbf{A}(\hat{\mathbf{r}}, t) \cdot \hat{\mathbf{p}} \quad (6.5)$$

$$\approx \hat{H}_0 - \frac{q}{mc} \mathbf{A}(t) \cdot \hat{\mathbf{p}} = \hat{H}_0 - \left[\frac{qA_0}{mc} \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} e^{-i\omega t} + \text{h.c.} \right]. \quad (6.6)$$

Therefore, the perturbation Hamiltonian of a weak optical probe is proportional to the canonical momentum operator. This is sometimes referred to as the velocity gauge [138].

For our purposes, however, it is more relevant to work in the “length gauge,” which is obtained by performing a unitary transformation on Eqn. (6.1):

$$\hat{U} = \exp \left(-\frac{i}{\hbar} \frac{q}{c} \hat{\mathbf{r}} \cdot \mathbf{A}(t) \right). \quad (6.7)$$

$\hat{U}$ represents a boost. Note that we have already applied the dipole approximation, so $\mathbf{A}$ is independent of $\hat{\mathbf{r}}$. The transformed Hamiltonian reads

$$\hat{H} \equiv \hat{H}_0 + \hat{H}_I = \hat{H}_0 - q\hat{\mathbf{r}} \cdot \mathbf{E}(t) = \hat{H}_0 - (\boldsymbol{\mu} \cdot E_0 \boldsymbol{\epsilon} e^{-i\omega t} + \text{h.c.}) \quad (6.8)$$

Where we have dropped the i in Eqn. (6.3) (corresponding to changing the phase of the fields), and defined the dipole operator $\boldsymbol{\mu} \equiv q\hat{\mathbf{r}}$. This is sometimes referred to as the “length gauge” [138], and this is the gauge choice that we will use.

We note that the unitary transformation Eqn. (6.7) is equivalent to performing a gauge transformation defined by $\chi(\mathbf{r}, t) = -\hat{\mathbf{r}} \cdot \mathbf{A}_{\text{Coul}}(t)$ from the Coulomb gauge:

$$\begin{aligned} \mathbf{A}' &= \mathbf{A} + \nabla \cdot \chi \Rightarrow \mathbf{A}_{\text{len}} = 0 \\ \Phi' &= \Phi - \frac{1}{c} \frac{\partial \chi}{\partial t} \Rightarrow \Phi_{\text{len}} = \hat{\mathbf{r}} \cdot \frac{1}{c} \frac{d\mathbf{A}_{\text{Coul}}(t)}{dt} = \mathbf{r} \cdot \mathbf{E}(t). \end{aligned} \quad (6.9)$$

Substituting these equations into Eqn. (6.1) gives the same results. For the vector potential term to cancel out, we must work under the dipole approximation. (Otherwise, we will get higher order electric and magnetic multipole terms.)

The polarization vector

The polarization vectors follow the normalization condition $\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon} = 1$. We only consider polarized light here, and in this case $\boldsymbol{\epsilon}$ ’s are also called Jones vectors [139]. In particular, for linearly polarized light (which is the only case studied in this chapter), they are simply the radial unit vector, $\boldsymbol{\epsilon}(\theta) = \boldsymbol{\rho}(\theta) = \cos \theta \mathbf{x} + \sin \theta \mathbf{y}$. In this thesis, we only consider in-plane polarization vectors, which is native to our modulation scheme.

$\boldsymbol{\epsilon}(\theta)$ and $\boldsymbol{\epsilon}(\theta + \pi) = -\boldsymbol{\epsilon}(\theta)$ represent the same optical polarization with a π phase difference, and this phase is inconsequential for the excitation rate. However, we will keep track of this sign difference in this chapter, since it in principle results in observable coherence effect in our measurement scheme (see Sec. 6.3.2). There is also a small but observable difference in the center of mass after the shake between the two cases (see Sec. 5.7).

6.1.2 Excitation rate in time-dependent perturbation theory

Now, we follow standard time-dependent perturbation theory treatment for a time-periodic perturbation [137]. We will write $\hat{H}_I$ in Eqn. (6.8) as

$$\hat{H}_I = -\boldsymbol{\mu} \cdot E_0 \boldsymbol{\epsilon} e^{-i\omega t} + \text{h.c.} \equiv \hat{K} e^{-i\omega t} + \hat{K}^\dagger e^{i\omega t}. \quad (6.10)$$

We will only be interested in the positive frequency term $\hat{K}e^{-i\omega t}$ that is resonant with an absorption from the initial state $|i\rangle$ to the final state $|f\rangle$. Then, to first order in perturbation theory, the transition probability is given by

$$P_{fi} = \frac{4}{\hbar} \left[\frac{\sin^2(\delta t/2)}{\delta^2} \right] |\langle f | \hat{K} | i \rangle|^2 = \frac{4}{\hbar} (qE_0)^2 \left[\frac{\sin^2(\delta t/2)}{\delta^2} \right] |\boldsymbol{\epsilon} \cdot \langle f | \hat{\mathbf{r}} | i \rangle|^2$$

$$\xrightarrow{\delta t \rightarrow 0} \frac{t^2}{\hbar} (qE_0)^2 |\boldsymbol{\epsilon} \cdot \langle f | \hat{\mathbf{r}} | i \rangle|^2 \quad (6.11)$$

where $\delta \equiv \omega - \omega_{fi}$ is the detuning (in angular frequency). Therefore, we expect that for a resonant excitation, the excitation probability is quadratic in t (as long as the excited fraction remains small).

The matrix element that appear in Eqn. (6.11), $\langle f | \hat{\mathbf{r}} | i \rangle$, is innocent if $|i\rangle$ and $|f\rangle$ are localized states, such as atomic orbitals. But for spatially extended states such as Bloch states, say $|i\rangle = |\psi_{\mathbf{q}}^{(n)}\rangle$ and $|f\rangle = |\psi_{\mathbf{q}'}^{(n')}\rangle$, this is a rather tricky quantity. It can be shown that for $n \neq n'$, the matrix element is given by [140, 141]

$$\langle \psi_{\mathbf{q}}^{(n)} | \hat{\mathbf{r}} | \psi_{\mathbf{q}'}^{(n')} \rangle = i\delta(\mathbf{q} - \mathbf{q}') \mathbf{A}_{nn'}(\mathbf{q}), \quad (6.12)$$

where

$$\mathbf{A}_{mn}(\mathbf{q}) \equiv i \langle u_{\mathbf{q}}^{(m)} | \nabla_{\mathbf{q}} | u_{\mathbf{q}}^{(n)} \rangle \quad (6.13)$$

is the interband Berry connection. Eqn. (6.11) can then be expressed as (focusing on the resonant case, $\delta = 0$)

$$P_{mn}(\mathbf{q}) = \frac{t^2}{\hbar} (qE_0)^2 |\boldsymbol{\epsilon} \cdot \mathbf{A}_{mn}(\mathbf{q})|^2 \quad (6.14)$$

for transitions from band n to band m in solids.

6.1.3 Fictitious force from lattice shaking

Now, we study how periodic translations in lattice potential map to the optical excitation Hamiltonian in Eqn. (6.8). The Hamiltonian of a particle in a moving lattice is given by

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}} - \mathbf{r}(t)) \quad (6.15)$$

where $\mathbf{r}(t)$ is the time-dependent displacement, from which we find the velocity $\mathbf{v}(t) = d\mathbf{r}/dt$ and acceleration $\mathbf{a}(t) = d^2\mathbf{r}/dt^2$ of the lattice.

First, we transform the Hamiltonian using the time-dependent translation operator (note the positive sign),

$$\hat{U}_T(t) = \exp \left(+\frac{i}{\hbar} \hat{\mathbf{p}} \cdot \mathbf{r}(t) \right), \quad (6.16)$$

from which we find

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) - \hat{\mathbf{p}} \cdot \mathbf{v}(t) = \hat{H}_0 - \hat{\mathbf{p}} \cdot \mathbf{v}(t). \quad (6.17)$$

This is formally identical to Eqn. (6.6) if we identify $\mathbf{A}(t) \equiv (mc/q)\mathbf{v}(t)$, so we can think of Eqn. (6.17) as the Hamiltonian in the velocity gauge. We also see that the dipole approximation is exact for lattice shaking, since $\mathbf{v}(t)$ is independent of location.

It is now clear that we may similarly apply a boost to find the length gauge representation. Transforming $\hat{H}'$ under $\hat{U}_B(t) = \exp[-(i/\hbar)m\hat{\mathbf{r}} \cdot \mathbf{v}(t)]$, we find

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) + m\mathbf{a}(t) \cdot \hat{\mathbf{r}} - \frac{1}{2}m\mathbf{v}(t)^2. \quad (6.18)$$

We see that there is a time-dependent energy offset that is proportional to the kinetic energy in the lattice frame. This term is the “ $\mathbf{A}^2$ -like” term that is missing in lattice shaking compared to Eqn. (6.1). We will drop this term, since it only contributes to a global phase. Finally, we find

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) - \mathbf{F}(t) \cdot \hat{\mathbf{r}}, \quad (6.19)$$

where the fictitious force is defined as $\mathbf{F}(t) \equiv -m\mathbf{a}(t)$ [124]. This is in direct analogy to Eqn. (6.8). We see that the direction of the displacement corresponds to the polarization of the electromagnetic wave, and the acceleration of the lattice is proportional to the electric field strength.

6.2 The Berry connection matrix of two band systems

The s -bands of the honeycomb lattice provide a minimal system that demonstrates the effect of the interband Berry connection on optical transitions. We will first work out the expression for the Berry connection matrix in a generic two-state system, and then apply the result to the case of honeycomb lattice.

In terms of Pauli matrices, a general two-level system Hamiltonian can be written as

$$H_{\text{TLS}} = \mathbf{s} \cdot \boldsymbol{\sigma} = \begin{pmatrix} s_3 & s_1 - is_2 \\ s_1 + is_2 & -s_3 \end{pmatrix} = |\mathbf{s}| \begin{pmatrix} \cos \theta & e^{i\phi} \sin \theta \\ e^{-i\phi} \sin \theta & -\cos \theta \end{pmatrix}, \quad (6.20)$$

where $\mathbf{s} = s_1\mathbf{x} + s_2\mathbf{y} + s_3\mathbf{z}$ ($s_i \in \mathbb{R}$), and $\boldsymbol{\sigma} = \sigma_x\mathbf{x} + \sigma_y\mathbf{y} + \sigma_z\mathbf{z}$ is the Pauli vector. We have ignored the identity s_0I , since it only contributes to an energy offset without affecting any of the following results. In the second line we parametrized the Hamiltonian in a way similar to the Bloch sphere formalism,

$$\cos \theta = \frac{s_3}{|\mathbf{s}|}, \quad \sin \theta = \frac{\sqrt{s_1^2 + s_2^2}}{|\mathbf{s}|}, \quad \phi = -\arctan \frac{s_2}{s_1}. \quad (6.21)$$

With this parametrization, the eigenstates are given by

$$|u_+\rangle = \begin{pmatrix} e^{i\phi} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}, \quad |u_-\rangle = \begin{pmatrix} -e^{i\phi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix}. \quad (6.22)$$

Under the requirement that the eigenstates should be normalized as $\langle u_i | u_j \rangle = \delta_{ij}$ ($i, j \in \{+, -\}$), we can still multiply each of the state by an arbitrary phase factor $e^{i\Phi_{\pm}}$.

If the parameters ϕ and θ depend on some parameter(s), say $\boldsymbol{\xi}$, then we may define the Berry connection matrix (indexed by the state $+$ and $-$, with each entry a vector of the same dimension as $\boldsymbol{\xi}$) as¹

$$\mathbf{A}_{mn} \equiv i \langle u_m(\boldsymbol{\xi}) | \nabla_{\boldsymbol{\xi}} | u_n(\boldsymbol{\xi}) \rangle. \quad (6.23)$$

The diagonal terms are the intraband Berry connections of the two levels, given by

$$\mathbf{A}_{++} = -(\nabla_{\boldsymbol{\xi}} \phi) \cos^2 \frac{\theta}{2}, \quad \mathbf{A}_{--} = (\nabla_{\boldsymbol{\xi}} \phi) \sin^2 \frac{\theta}{2}, \quad (6.24)$$

and the off-diagonal terms are the interband Berry connection, given by

$$\mathbf{A}_{+-} = \mathbf{A}_{-+} = \frac{1}{2}(-i\nabla_{\boldsymbol{\xi}} \theta + \sin \theta \nabla_{\boldsymbol{\xi}} \phi). \quad (6.25)$$

Note that since both $\theta(\boldsymbol{\xi})$ and $\phi(\boldsymbol{\xi})$ are $\boldsymbol{\xi}$ -dependent, we have actually made the gauge choice $\Phi_{\pm}(\boldsymbol{\xi}) = 0$ for all values of $\boldsymbol{\xi}$ in writing down Eqn. (6.24) and (6.25). We see that when the diagonal terms in Eqn. (6.20) are zero, $\theta = \pi/2$ is a constant, and $\mathbf{A}_{+-}(\mathbf{q}) = \frac{1}{2}\nabla_{\boldsymbol{\xi}} \phi$ is purely real¹.

Let us apply what we derived to the honeycomb lattice Hamiltonian, Eqn. (3.69):

$$H^{\text{hc}}(\mathbf{q}) = -t \begin{pmatrix} 0 & f(\mathbf{q}) \\ f(\mathbf{q})^* & 0 \end{pmatrix} \quad (f(\mathbf{q}) = e^{-i\mathbf{q} \cdot \mathbf{d}_1} + e^{-i\mathbf{q} \cdot \mathbf{d}_2} + e^{-i\mathbf{q} \cdot \mathbf{d}_3} \equiv |f|e^{i\phi}), \quad (6.26)$$

and we identify $\boldsymbol{\xi}$ with $\mathbf{q}$ here². Since $H^{\text{hc}}(\mathbf{q})$ does not have diagonal terms, we only need to find $\nabla_{\mathbf{q}} \phi$. This is given by

$$\nabla_{\mathbf{q}} \phi = \frac{\text{Im}[f^* \nabla_{\mathbf{q}} f]}{|f|^2} = \frac{1}{2i|f|^2} (f^* \nabla_{\mathbf{q}} f - f \nabla_{\mathbf{q}} f^*). \quad (6.27)$$

Using Eqn. (6.25) and (6.27), we finally find

$$\mathbf{A}_{+-}(\mathbf{q}) = \frac{1}{2} \nabla_{\mathbf{q}} \phi = \frac{1}{2|f(\mathbf{q})|^2} \sum_j A_j(\mathbf{q}) \mathbf{d}_j, \quad (6.28)$$

¹Some people omit the i in the definition (Eqn. (6.23)), so that $\mathbf{A}$ is real when the eigenstates are chosen to be real, when allowed by $\mathcal{C}_2\mathcal{T}$ or $\mathcal{PT}$ symmetry. The nice thing about including the i is that $\mathbf{A}_{mn}$ becomes a Hermitian (, vectorial) matrix in band index:

$$\begin{aligned} \langle m | n \rangle &= \delta_{mn} \Rightarrow \langle \nabla m | n \rangle = -\langle m | \nabla n \rangle \\ &\Rightarrow (i \langle m | \nabla n \rangle)^* = -i \langle \nabla n | m \rangle = i \langle n | \nabla m \rangle. \end{aligned}$$

Note that under this definition, there is still nothing to prevent psychopaths from making $\mathbf{A}$ purely imaginary by using a different gauge choice, e.g. $\Phi_+(\mathbf{q}) = \pi/2$. $|u_+(\mathbf{q})\rangle$ simply becomes imaginary too. We have made a similar choice to make $\mathbf{A}$ purely real with the i in our definition, and indeed, the eigenstates are not real.

²We could have included other parameters, such as the intensity of the lattice beams (not periodic) and the relative phases between lattice beams (periodic), provided that the two-band model is still valid.

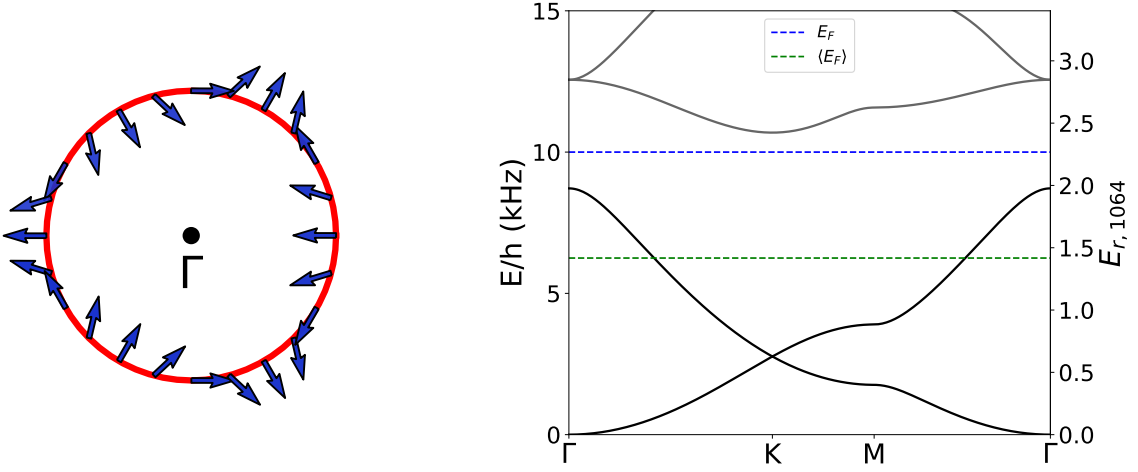


Figure 6.1: Left: the direction of $\mathbf{A}_{+-}$ evaluated at the center of the annular region in Fig. 6.3 (for a particular gauge choice). Right: the band structure of a honeycomb lattice with lattice depth $V_{1064} = -39.5$ kHz. Blue (green) dashed lines label the (averaged) Fermi energy.

where

$$A_j(\mathbf{q}) = \sum_i \cos[\mathbf{q} \cdot (\mathbf{d}_i - \mathbf{d}_j)]. \quad (6.29)$$

This is real, as expected from the $\mathcal{C}_2\mathcal{T}$ symmetry of the honeycomb lattice.

6.3 Observation of quasimomentum-dependent selection rules

From Eqn. (6.14), we see that the excitation rate vanishes when

$$\boldsymbol{\epsilon} \cdot \mathbf{A}_{mn}(\mathbf{q}) = 0, \quad (6.30)$$

which can be seen as a quasimomentum-dependent selection rule for optical excitations. Another immediate consequence is that there is no circular dichroism for a system with $\mathcal{C}_2\mathcal{T}$ or $\mathcal{PT}$ symmetry, since there exists a gauge where $\mathbf{A}_{mn}$ is completely real, and $|\boldsymbol{\epsilon} \cdot \mathbf{A}_{mn}|^2 = |\boldsymbol{\epsilon}^* \cdot \mathbf{A}_{mn}|^2$.

Let us see what this implies for the s -bands of the honeycomb lattice. Since the interband Berry connection is real, Eqn. (6.30) can only hold for real (linear) polarizations, which we will write as $\boldsymbol{\epsilon}(\theta_{\text{PM}})$. Substituting Eqn. (6.28) into Eqn. (6.30) gives

$$\cos(\theta_{\text{PM}} + 2\varphi_q) = 0 \Rightarrow \varphi_q = \left(\frac{m}{2} + \frac{1}{4}\right)\pi - \frac{\theta_{\text{PM}}}{2} \quad (m \in \mathbb{Z}) \quad (6.31)$$

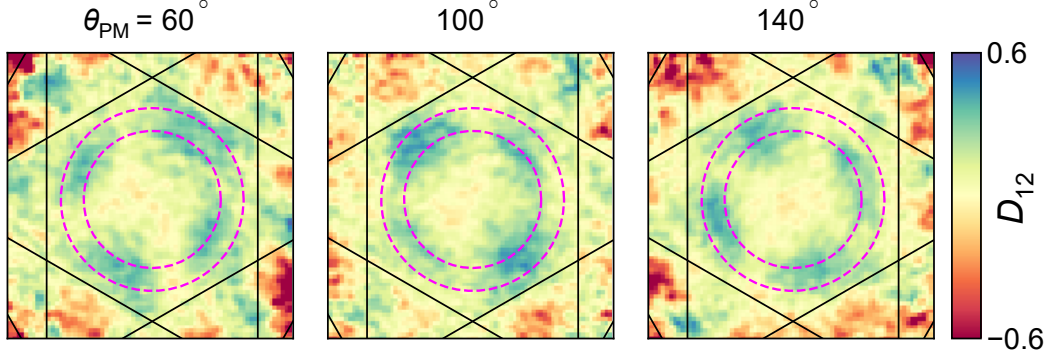


Figure 6.2: Examples of experimentally measured depletion ratios for selected shaking angles. Each image is averaged over three runs at $\epsilon(\theta_{\text{PM}})$ and three runs at $\epsilon(\theta_{\text{PM}} + \pi)$. Black solid lines label the Brillouin zone. Magenta dashed circles delimit the annular region used for data analysis (see Fig. 6.3).

to lowest order in q , where $\mathbf{q} = q\boldsymbol{\rho}(\varphi_q)$. We see that for small q , there are four rays stemming from the Γ point with zero excitation rate, and as such we call them “transparency lines” of optical excitations.

In this section, we demonstrate direct experimental evidence of transparency lines. We first briefly summarize the results. A spin-polarized degenerate Fermi gas is adiabatically loaded into the honeycomb lattice. The lattice is then modulated with different polarizations at a fixed frequency f_{PM} that drives resonant transitions from the ground band to the higher s -band of the honeycomb lattice. We then suddenly turn off all the lattice and trapping potentials, and measure the column density of atoms n_c after a long time-of-flight, which measures the momentum distribution of atoms. By comparing with reference runs without lattice modulation, we quantify the change in the momentum distribution within the first Brillouin zone by the depletion ratio, defined as

$$D(\mathbf{q}) \equiv \frac{n_{c,\text{ref}}(\mathbf{q}) - n_c(\mathbf{q})}{n_{c,\text{ref}}(\mathbf{q})}. \quad (6.32)$$

As the polarization is varied, we observe corresponding changes in the position of the transparency lines in the quasimomentum space, where $D(\mathbf{q})$ vanishes. See Fig. 6.2 for selected examples.

In the subsections, we describe the details of the experiment, and in particular the difficulty of making quantitative measurements in band manifolds with small energy separations.

6.3.1 Practical considerations

In the experiment described in this section, we adiabatically load around $8 \cdot 10^4$ ^{40}K atoms into the honeycomb lattice with a depth of 39.5 kHz. This corresponds to a Fermi energy of

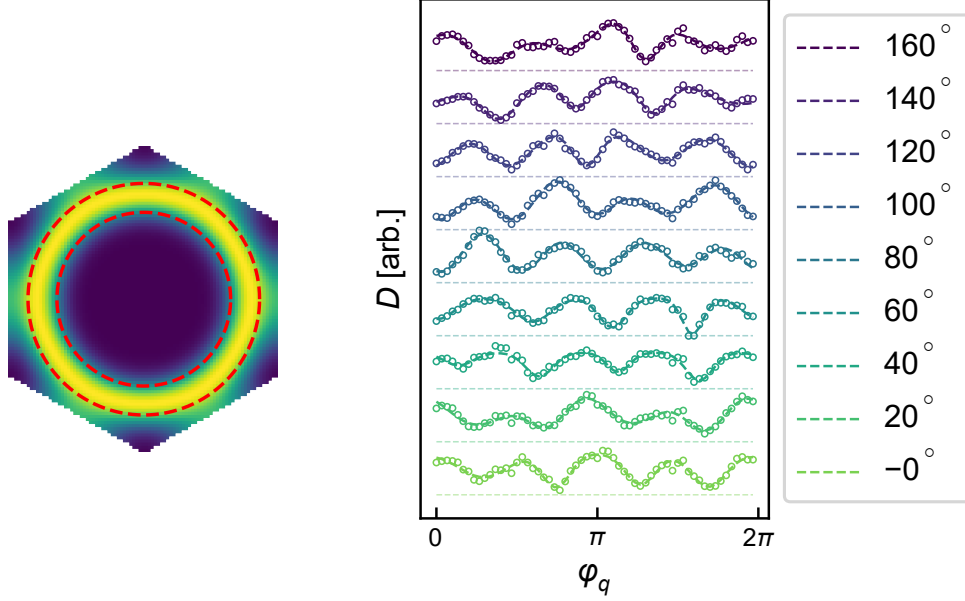


Figure 6.3: Left: the region that is resonant to the modulation within the first Brillouin zone. The width of the region is chosen to be 1 kHz, given by the inverse of the total modulation time. The red rings label the annular region used for data analysis. Right: results of the angular fit within the annular region for different polarizations $\epsilon(\theta_{\text{PM}})$. Scattered points are the angle-integrated depletion ratio. Each trace is vertically offset from each other for clarity.

around 10 kHz, or an average local Fermi energy of around 6.3 kHz (see Fig. 6.1). Loading more atoms initially increases the signal-to-noise ratio (at the quasimomentum of interest), but also increases the Fermi energy, eventually leading to a decrease in contrast if the second band state becomes occupied. The number of ^{40}K atoms is controlled by varying the loading time of the ^{40}K MOT.

One of the most limiting factor in our current experiment is the dynamics of the holes in a nonuniform trapping potential, a phenomenon we refer to as “hole diffusion” [142]. To understand this at an intuitive level, note that the excitation rate is uniform across the trapping potential, since the Thomas-Fermi radius is much smaller compared to the beam waists of lattice beams, and the lattice depth is approximately constant in the system. The holes generated by excitations then evolve along equal-energy orbits in the phase space, which is determined by the spatially-dependent trapping potential. We have found that hole diffusion currently limits our modulation time to around 1 ms, beyond which the measured depletion ratio at a certain $\mathbf{q}$ no longer faithfully represent the amount of excitation at the same $\mathbf{q}$.

An important consequence of hole diffusion is that we are not able to see zero excitation at the angular positions predicted by Eqn. (6.31). Even if there truly is no excitation at a

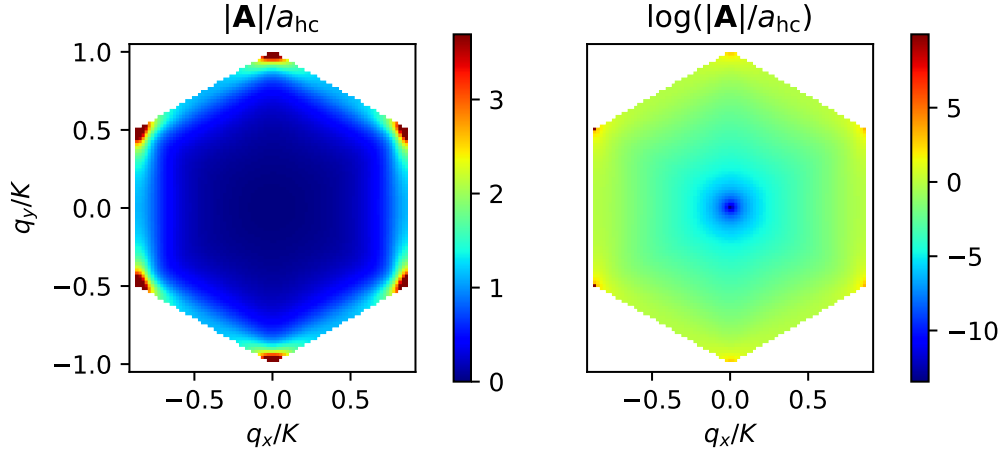


Figure 6.4: The magnitude of $\mathbf{A}_{+-}$ in units of a_{hc} , plotted in linear scale and log scale.

particular quasimomentum, say $\mathbf{q}_0$, the holes generated at neighboring quasimomenta diffuse to where we expect transparency lines, resulting in a finite value of $D(\mathbf{q}_0)$. Since the direction of $\mathbf{A}_{+-}$ varies continuously, the excitation rate near $\mathbf{q}_0$ is also small. As a result, we still expect to measure four minima in $D(\mathbf{q})$ centered around the angles predicted in Eqn. (6.31), although not diminishing to zero, as shown in Fig. 6.3.

To extract the positions of the transparency lines, we first restrict the analysis to the region resonant to the modulation (annular region labeled in Fig. 6.3). The measured values of $D(\mathbf{q})$ within the annulus are then fitted to a trial function $w(\varphi)$. The choice of the function is somewhat arbitrary, and we only require that it is a smooth function (as expected from the diffusion) with four minima (predicted by Eqn. (6.31)). $w(\varphi)$ is given by the sum of four Gaussians, each centered around φ_i with width σ_i and amplitude B_i , plus a constant offset A :

$$w(\varphi) = A + \sum_{i=1}^4 B_i \exp \left[\frac{\text{mod}_{(-\pi, \pi]}[\varphi - \varphi_i]^2}{2\sigma_i^2} \right] \quad (6.33)$$

$\text{mod}_{(-\pi, \pi]}[\varphi - \varphi_i]$ means that we take the modulo of $\varphi - \varphi_i$ such that $-\pi < \varphi - \varphi_i \leq \pi$ for each φ_i . The angular positions of the transparency lines are then taken to be $\{\varphi_1, \varphi_2, \varphi_3, \varphi_4\}$.

Another difficulty of probing $\mathbf{A}_{+-}$ is that the Berry connection is vanishingly small near zero quasimomentum, but strongly diverging near the Dirac points, see Fig. 6.4. By expanding Eqn. (6.28) around Γ , we see that the magnitude of the connection is exactly zero at Γ , and increases quadratically as q . From Eqn. (6.14), we see that the excitation rate is proportional to q^4 . A smaller modulation frequency f_{PM} is resonant at larger q , which yields much stronger signals. The value used in the experiment, $f_{PM} = 3$ kHz was chosen such that the signal strength is measurable, while still large compared to the 1 kHz Fourier width of the hole diffusion-limited modulation time.

The $P \propto q^4$ scaling also means that the signal almost vanishes at where the transparency condition we obtained in Eqn. (6.31) is a good approximation. This is not a major restriction,

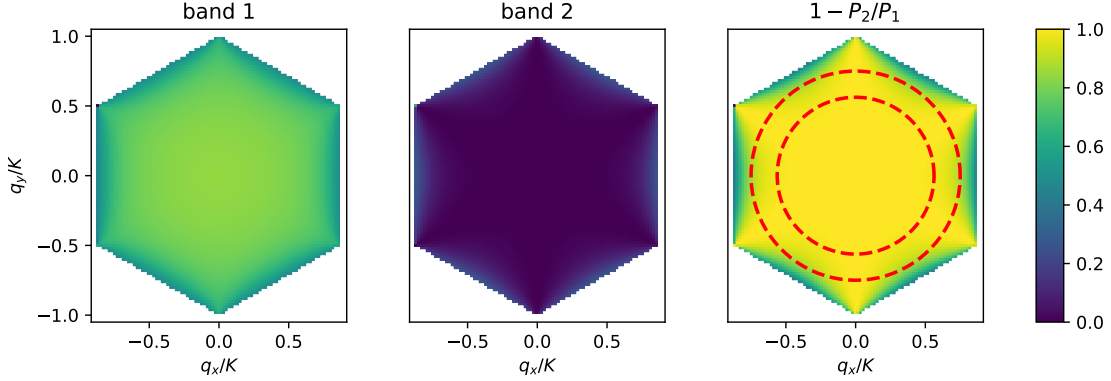


Figure 6.5: The participation ratio of the two bands and their differences within the first Brillouin zone.

since the transparency lines extends all the way to the K and K' points, and the expected positions of the transparency line can be computed using plane wave expansion. In fact, we find that even at $q = 0.66K$, the deviation from Eqn. (6.31) is only around $\pi/30$.

6.3.2 Interpretation of the depletion ratio

Ideally, we would like to measure the change in the Bloch state population in the ground band. The ideal way to do this is through band mapping. However, we have found that the dynamics during band mapping (0.3 ms) results in significant diffusion. This effect will be discussed more quantitatively in Malte Schwarz's thesis [50]. To maintain the quasimomentum resolution of our measurements, we therefore decided to perform diffraction imaging instead, in which the lattice is snapped off, and the Bloch states are projected to the plane wave basis. We then restrict our analysis to the first Brillouin zone, and use the depletion ratio defined in Eqn. (6.32) as a proxy of the change in ground band population.

Two concerns arise with this method. First, the momentum distribution of the ground band state is not entirely within the first Brillouin zone, and similarly the excited state may have nonzero amplitude in the first Brillouin zone. Let us call the population in this component the “participation ratio,” P . The numerically calculated values of P are shown in Fig. 6.5. We see that the change in the participation ratio between the two bands is slightly angle dependent within the ring of resonance, which results in a systematic measurement bias. The fact that P in the ground band is smaller than unity also means a reduced contrast.

Second, since the excitation between $|u_{\mathbf{q}}^{(1)}\rangle$ and $|u_{\mathbf{q}}^{(2)}\rangle$ is driven coherently, the relative phase between the two states should also affect our measurement results. To quantify this contribution, let us write the two states as (dropping the $\mathbf{q}$ dependence for brevity)

$$|u^{(1)}\rangle = \sum_{\mathbf{G}} a_{\mathbf{G}} |\mathbf{G}\rangle, \quad |u^{(2)}\rangle = \sum_{\mathbf{G}} b_{\mathbf{G}} |\mathbf{G}\rangle, \quad (6.34)$$

where $|\mathbf{G}\rangle$ is the plane wave state with wave vector $\mathbf{G}$, and we make the phase choice so that a_0 and b_0 are real positive numbers for this calculation.

The state after optical excitation is written as

$$|\Psi\rangle = A |u^{(1)}\rangle \pm B e^{i\gamma} |u^{(2)}\rangle, \quad (6.35)$$

where A and B are positive real numbers, and $B = \sqrt{1 - A^2}$. $+$ and $-$ signs correspond to shaking along θ_{PM} and $\theta_{\text{PM}} + \pi$, respectively. Then

$$|\langle \mathbf{0} | \Psi \rangle|^2 = a_0^2 (A^2 + r^2 B^2 \pm 2rAB \cos \gamma), \quad (6.36)$$

where $r = b_0/a_0$. The last term results from the coherence between the ground and excited states. We were fortunate that we averaged the θ_{PM} and $\theta_{\text{PM}} + \pi$ images in data analysis. The initial intention was to cancel out the lattice drag effect not accounted for by shifting the images by the center of mass drifts, but it turned out that this also resolved the complication from coherence.

Chapter 7

Flat band thermodynamics

As pointed out in the introduction, the particles in lattices have to be cooled to very low temperatures in order to access correlated phases of interest. In real materials this can be achieved in cryogenic systems, but it is a significant challenge for quantum simulation experiments using ultracold atoms. The typical technique used for reaching degeneracy is evaporation cooling, and as discussed in Sec. 4.1.4, pushing the limit of evaporation cooling for fermions is exceptionally challenging. This challenge has led to a class of entropy redistribution techniques, which are able to leverage different capabilities of modern cold atom experiments to cool the system beyond what can be typically achieved through laser cooling and evaporation cooling.

So far, one very successful approach for entropy redistribution in optical lattices is to create two partitions of the system (“joint system”), with a large density of states (DoS) in one of the region $\mathcal{R}$ (“reservoir”), and a small DoS in the other $\mathcal{S}$ (“system”). In this arrangement, the entropy per particle is lower in the system region under thermal equilibrium. Most of the implementations consider spatially separated regions [143, 144, 145, 146, 44], but it is also possible to use different atomic species [147] as the two partitions. For fermions, the band insulating state is a natural choice for the low DoS phase, since it has exactly zero entropy, and is relatively easy to prepare by tuning the local chemical potential of the system. The high DoS phase is often chosen to be a metallic state, whose charge degrees of freedom is available, and therefore has a large entropy capacity. Recent developments in holographic techniques for generating arbitrary potentials have allowed precise control over the trap shape required to realize such protocols, and have inspired new schemes for preparing nontrivial target states [148].

Following the same strategy, we ask whether the diverging DoS in lattice geometries that host a flat band can be used as a resource for efficient cooling. Several lattice geometries with flat bands have been realized in cold atom systems [149, 150, 151, 116]. An attractive feature of this proposal is that a flat band, having a diverging DoS (when interaction is ignored), should be able to cool any system with a finite DoS, including gapless many-body states such as metallic states. While studying the many-body ground states at flat band filling is one of the main goal of such experiments, there can also be other features of interest in the

dispersive part of the band structure at different filling factors, as discussed in Sec. 1.3 for the kagome lattice. This idea has been explored in Ref. [152], where the transport of holes to a fully filled flat band is facilitated with a weak resonant drive.

In contrast, current state-of-the-art schemes use gapped states e.g. a band insulator (BI) as the system, which is fully filled. In the latter case, it is easy to prepare an ultralow entropy BI, since particle excitations have a large energy gap. However, all the states in a BI is occupied, which makes the bulk of a BI generally somewhat boring. Making use of the ultralow entropy BI thus requires additional machineries. For example, a second lattice potential with a smaller spatial periodicity was used to split each lattice site of the original BI into two, without introducing additional entropy [44] (a simple adiabatic expansion proved to add too much entropy [43]). This procedure may not be possible for all the flat band systems of interest.

The first part of this chapter will take a thermodynamical approach, where one assumes that thermal equilibrium is established, so that the joint system is described by thermodynamical variables such as temperature T (equivalently, the thermodynamic beta $\beta \equiv 1/k_B T$) and chemical potential μ . Additionally, the relevant extensive quantities are number of orbitals L , particle number N and total entropy S . Given the DoS of the system and reservoir, we can then calculate the properties of the two subsystems, and determine if the system is cooled by the reservoir. We will first confirm the thermodynamic picture of flat band cooling for noninteracting systems, where we can study a large system size. To account for interactions, we then repeat the same calculations using numerical DoS obtained from tensor network calculation of smaller systems, and study how interaction modifies our previous conclusions.

Finally, we aim to address two assumptions required for the conclusions from thermodynamics to apply to real experiments: (i) the thermalization process is assumed to be isentropic, and (ii) the system must thermalize over an experimentally practical time scale. A strong motivation for inspecting the dynamics carefully is that flat bands are also famous for hosting compact localized states (CLS) [36] (see Sec. 3.4.3). These states have non-zero wave function amplitude only on a few sites, are exact eigenstates of the system if there is no interaction, and do not propagate in the system. It is not obvious how the situation changes when interaction is introduced in the system. Naïvely, the CLS will no longer be eigenstates when there are spatial overlaps with other particles, which promotes thermalization. However, simulation of the dynamics of interacting fermions in the kagome lattice is notoriously difficult due to the exponentially large Hilbert space, the fermion sign problem, and geometric frustration. To account for dynamics, we will therefore take a mean-field approach and simulate the time evolution of the proposed experimental realization using time-dependent Hartree-Fock theory, and calculate the relevant thermodynamical variables as the system evolves. This is an ongoing work that will be reported in future publications.

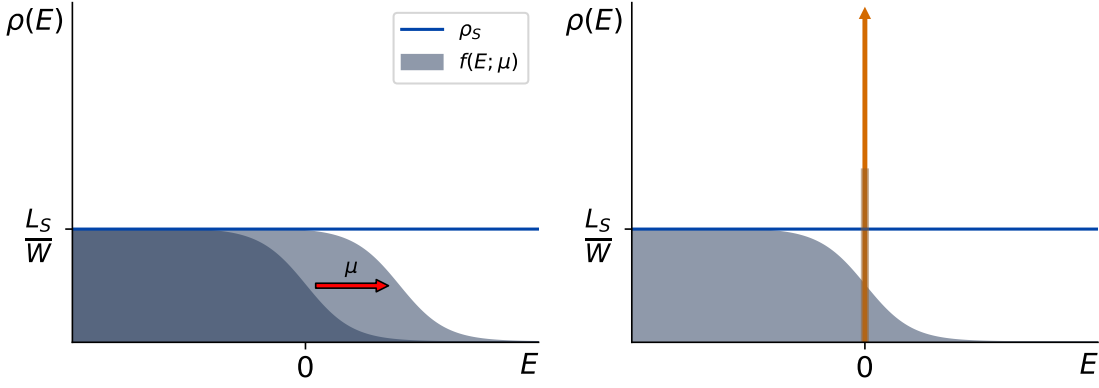


Figure 7.1: Schematics of the toy model. Left: the constant DoS of the system. The DoS extends to $E \rightarrow (-\infty, \infty)$. The filling at energy E is represented by gray shadings. Changing the chemical potential μ only displaces the distribution horizontally. Right: The joint DoS of the toy model. The Dirac function DoS of the reservoir is represented by an orange arrow.

7.1 A toy model for flat band cooling

To see how the idea of flat band cooling works in a purely thermodynamical setting, here we consider a toy model that reproduces the expected results qualitatively, and highlight questions raised by these studies. We will go to the thermodynamical limit, i.e. consider $N, L_{S(R)} \rightarrow \infty$ while holding $N/L_{S(R)}$ constant.

We consider a simplified model where the DoS of the joint system is separated into a system part $\rho_S(E)$ and a reservoir part $\rho_R(E)$, given by [153]

$$\rho_S(E) = \frac{L_S}{W}, \quad \rho_R(E) = L_R \delta(E), \quad (7.1)$$

where L_S, L_R are the number of orbitals in the system and in the reservoir, respectively, and W is the band width of the system. $E = 0$ is set at the energy of the reservoir flat band¹. A visualization of the DoS and its filling factor is given in Fig. 7.1. The system and the reservoir are assumed to be in thermal equilibrium, so T and μ are the same for both regions.

A note on notation: L is the number of **SITES** (not unit cells). Uppercase letters (N, S) are extensive and scale with L . Lowercase letters (n, s) are per **SITE**. σ is entropy per **PARTICLE**. Values without subscripts are properties of the joint system, and $S(R)$ means properties of the system (reservoir).

¹The absence of energy bounds in the system is justified by the fact that at low T , the states are completely filled deep below the Fermi sea, and completely empty high above, so beyond some energy cutoff, those states don't contribute to the properties of the system. We will take appropriate bounds when evaluating integrals as necessary.

7.1.1 Equation of state

We first solve the equation of state (EoS) of the model by considering the system and the reservoir separately. The particle number $N_{S(R)}$ and entropy $S_{S(R)}$ in the system (reservoir) can be found using²

$$\begin{aligned}
 N &= \int_{-\Lambda}^{\infty} dE \rho(E) f(E) \\
 S &= -\text{Tr}[\rho \ln \rho] \\
 &= -\sum_i \text{Tr}[\rho^{(i)} \ln \rho^{(i)}] \\
 &\xrightarrow{L_S \rightarrow \infty} -\int_{-\Lambda}^{\infty} dE \rho(E) \text{Tr}[\rho(E) \ln \rho(E)],
 \end{aligned} \tag{7.2}$$

where

$$f(E; \mu) = \frac{1}{1 + e^{\beta(E-\mu)}} = \frac{1}{1 + z^{-1} e^{\beta E}}$$

is the Fermi-Dirac distribution (or $f(E)$ for simplicity where no confusion arises), $z = e^{\beta\mu}$ is the fugacity, and we write the thermal state as the direct product $\rho = \bigotimes_i^{L_S} \rho^{(i)}$, where

$$\begin{aligned}
 \rho^{(i)} &= f(E_i) |1^{(i)}\rangle \langle 1^{(i)}| + (1 - f(E_i)) |0^{(i)}\rangle \langle 0^{(i)}| \\
 &= \begin{pmatrix} f(E_i) & 0 \\ 0 & 1 - f(E_i) \end{pmatrix}
 \end{aligned}$$

is the density matrix of a single orbital. Finally, we write $\rho^{(i)} = \rho(E)$ for a continuum of states in the thermodynamic limit.

Evaluating these equations gives

$$\begin{aligned}
 N_S(\mu, T) &= N_S(\mu) = N_{0,S} + \frac{L_S}{W} \mu \\
 \frac{S_S(\mu, T)}{k_B} &= \frac{S_S(T)}{k_B} = \frac{\pi^2}{3} \frac{L_S}{W} T,
 \end{aligned} \tag{7.3}$$

where $N_{0,S}$ is the number of particles in the system at $\mu = 0$ (the area of the darker shaded region in Fig. 7.1). $N_{0,S}$ serves as a reference for the changes in particle number, since the number of particles diverges from summing over the particles deep in the Fermi sea in this model. Note that N_S only depends on μ , and S_S only depends on T .

Calculating Eqn. (7.2) for the reservoir is very straightforward due to the delta function, yielding

$$\begin{aligned}
 N_R(\mu, T) &= L_R n_R \\
 \frac{S_R(\mu, T)}{k_B} &= L_R [-(1 - n_R) \ln(1 - n_R) - n_R \ln n_R],
 \end{aligned} \tag{7.4}$$

²For now, we argue that the exact value of the energy cutoff Λ is unimportant, since most of the changes in occupation happens near the Fermi surface. We will revisit this argument in Sec. 7.2. Λ makes sure that N and $N_{0,S}$ do not diverge, and the correction to Eqn. (7.3) is $O(e^{-\beta\Lambda})$. I can then take $\Lambda \rightarrow \infty$ to get the result in the main text.

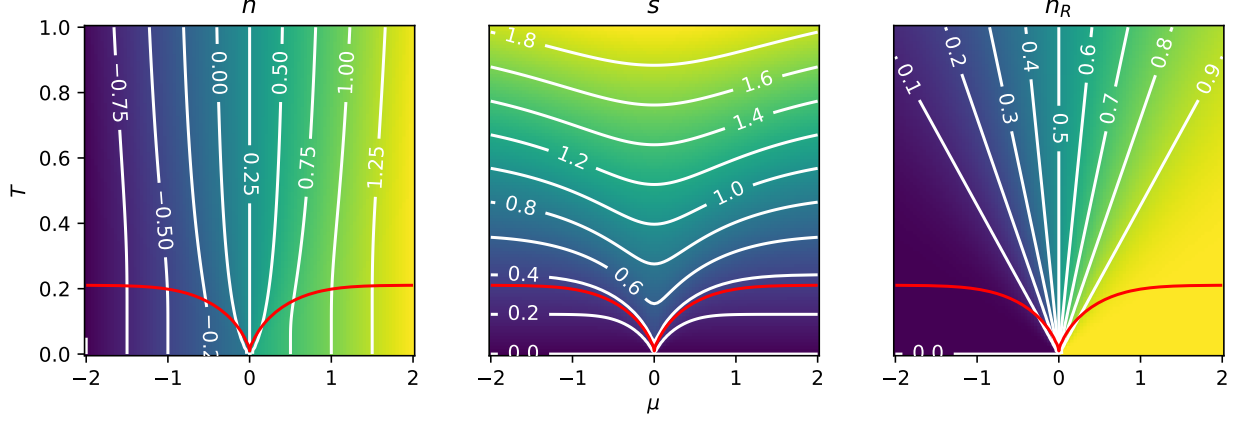


Figure 7.2: Constant n , s , and n_R curves in the $\mu - T$ space for the simplified model given in Eq. (7.2). n goes to negative values because it is referenced with respect to $n_{0,S}$. The red lines label the isentropic contour $s = \bar{S}_R/2L = \ln 2/2 \approx 0.347$ in all three plots.

where $n_R = f(0; \mu)$ is the filling in the reservoir determined by the Fermi-Dirac distribution. Importantly, we note that the entropy and particle number in the flat band do not depend on μ and T independently, but are rather determined by their ratio $\mu/k_B T$ through n_R .

We now add Eqn. (7.3) and Eqn. (7.4) together to find the EoS of the joint system (where for N_S I subtract the $N_{0,S}$ term):

$$\begin{aligned} N(\mu, T) &= \frac{L_S}{W} \mu + L_R n_R \\ \frac{S(\mu, T)}{k_B} &= \frac{\pi^2}{3} \frac{L_S}{W} T + L_R [-(1 - n_R) \ln(1 - n_R) - n_R \ln n_R]. \end{aligned} \quad (7.5)$$

Now let's see what we can learn from Eqn. (7.5). We consider $L_S = L_R = L' = L/2$, and plot $n \equiv N/L'$ and $s \equiv S/L'$ in Fig. 7.2. Focusing first on the entropy plot, we see that there is a family of isentropic contours that converges at $\mu = 0, T = 0$ as μ is varied. This can be interpreted as a flat band induced cooling in an isentropic process. To see this, let us start with a point on the red curve with $\mu < 0$. The red curve is defined by $s = \bar{S}_R/L$, where $\bar{S}_R = k_B L_R \ln 2$ is the maximum amount of entropy that can be stored in the reservoir. As μ is increased in the system, or equivalently, the energy of the system flat band is decreased with e.g. an external potential, the temperature goes down following the red isentropic curve. This is because the filling in the flat band n_R gradually approaches one half, as shown in the rightmost panel in Fig. 7.2. Finally, when μ is tuned to zero, the flat band is exactly half-filled, exactly taking up all the entropy in the joint system. If μ is increased further, then the entropy in the reservoir decreases again, leading to a finite T .

For higher initial entropies (points above the red line), the temperature does not go to zero at $\mu = 0$, and the flat band just accommodates as much entropy as it can. Interestingly, one might guess that if the system is initially prepared anywhere in the region below the

red line in Fig. 7.2, one can tune the chemical potential to $\mu = 0$, and the system would be cooled to $T = 0$ following the isentropic contours.

But now let us turn to the n plot on the left, and something weird happens. When $s = \bar{S}_R/L$ exactly, the $\mu = 0, T = 0$ point is single valued with $n = 0.25$, since the reservoir only takes up all the entropy at a single value of n_R ($= 0.5$). However, we notice that at $\mu = 0, T = 0$, there is a convergence of a range of constant particle number contours. This points out an oddity of the flat band cooling phenomena: for the family of isentropic curves that converge at $\mu = 0, T = 0$, only the red curve is single-valued in the n plot. To see how this statement works in action, let us now follow the same argument along a different isentropic curve, say $s = 0.2$. T similarly decrease to zero as μ is tuned to zero, but at this point the flat band is not half-filled yet. There are two values of n_R at which the flat band takes exactly all the entropy of the joint system, which is found by solving the S_R equation in Eqn. (7.4) to be $n_1 = 0.137$ and $n_2 = 0.863$. (We note that they represent two rays in the n_R plot that are tangent to the $s = 0.2$ isentropic line.) So when μ is increase to zero, initially we find $n_R = n_1$, and before μ can be increased further, more particles must be added to the flat band until $n_R = n_2$, while the system stays at $\mu = 0, T = 0$. But when $n_1 < n_R < n_2$, the system seems to be “running out of entropy,” and $S_R(n_R)$ grows beyond the total entropy in the joint system. We will take a closer look below, where find that this description is not accurate (particle number in the system also changes), but the system is indeed running out of entropy.

7.1.2 Cooling to zero temperature?

To get a closer look at what happens at $T = 0$, let us explicitly solve the EoS of the joint system for some low entropy $S < \bar{S}_R$ and different particle numbers. We first invert Eqn. (7.5) to get $\mu(N, S)$ and $T(N, S)$, from which we use the individual EoS Eqn. (7.3) and (7.4) to find the particle density and entropy per site in each subregion. The result is plotted in Fig. 7.3. From this calculation, because just relying on using T and μ to describe the joint system results in unphysical results.

One might first ask if it is possible to stay within the grand canonical approach, namely, assign a global μ and T to the joint system. Focusing at the μ plot, as μ is increased from below zero, perhaps the particle number jumps to a higher value at the inflection point of μ (vertical gray dashed line). One would then predict a bistability, since if μ is decreased from above instead, the jump to a lower N will happen at a different inflection point, and for some values of μ there are two possible values of N . This solution is questionable, as the entropy in the system already becomes negative before the inflection point. Therefore, we conclude that the system cannot be described by a grand canonical ensemble, at least not uniformly throughout the system.

A possible resolution is to have two “phases” in coexistence. There are two values of n_R at which the temperature is exactly zero, with the flat band fillings at n_R^{c1} and n_R^{c2} , respectively. By separating the joint system into two parts with these two filling factors, and changing the ratio of the sizes of the two parts, it is possible to put more particles into the joint

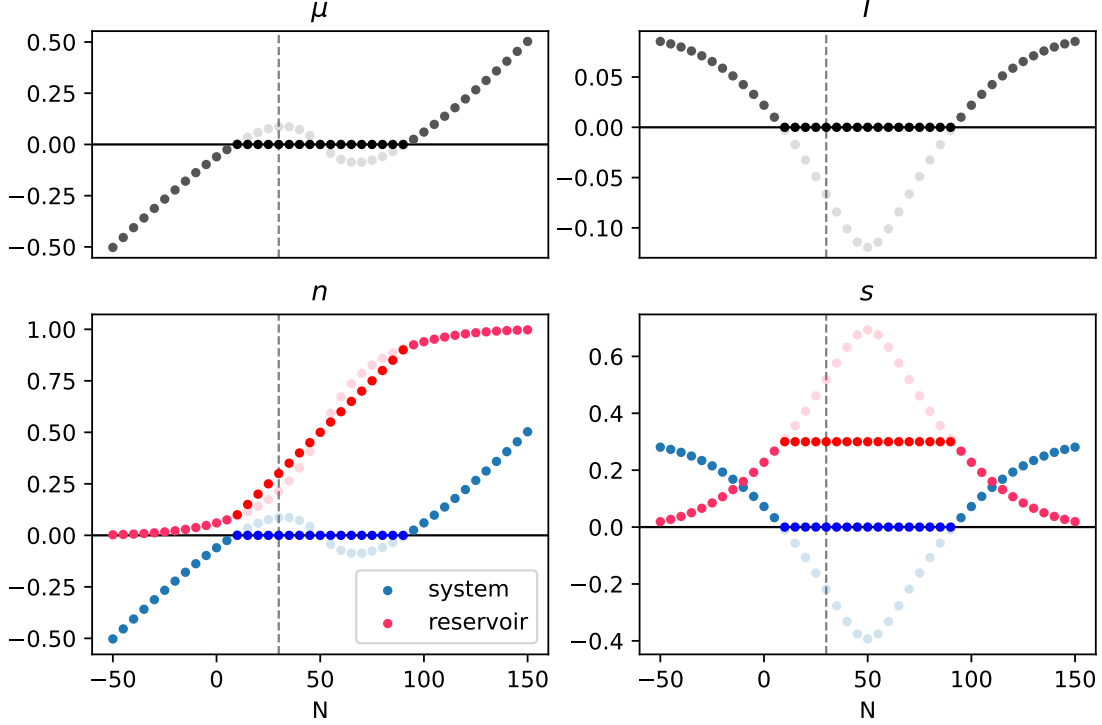


Figure 7.3: μ and T as a function of N , and the corresponding values n and s in the system and reservoir, for $s = 0.15$. In the unphysical region where $s_s < 0$, the original solution is made transparent, and the values of the proposed two phase mixture is plotted instead.

system without changing either μ or T . This is reminiscent of the coexistence curve that one learned in the standard treatment of the van der Waals equation of gases, where the isothermal contours in the $P-V$ plots becomes non-monotonic below a critical temperature. The phase that is actually realized is given by the Maxwell construction, where the system undergoes a first order phase transition, throughout which there is a mixture of gas and liquid [154], and the free energy is minimized. In this sense, a realization of the toy model might provide an opportunity to study a first order transition with microscopic resolution. It is unclear if a clear phase boundary should exist given the small system size that we will be able to create in our experiment. It should also be noted that this argument assumes thermal equilibrium.

7.1.3 Multiband considerations

Eventually, we are interested in studying flat band systems, which may also have (potentially several) dispersive bands in the energy spectrum. By also considering the number of dispersive bands below the flat band in the reservoir, we can get a rough estimate on the entropy per particle $\sigma \equiv S/N$ below which the zero temperature discussion becomes relevant.

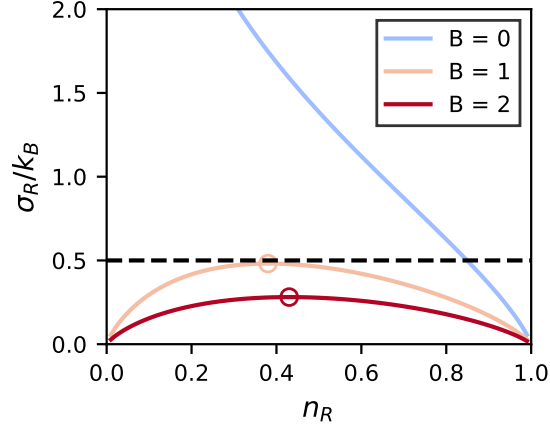


Figure 7.4: Entropy per particle in the reservoir for different B , number of bands below the flat band. For $B = 1$ and 2 , the point with maximum σ_R is labeled with an open circle, which is at $\sigma_R/k_B = 0.48$ and 0.28 , respectively.

We will again focus on the $T = 0$ case. If there are B dispersive bands below the flat band, the average entropy per atom in the reservoir $\sigma_R \equiv S_R/N_R$ is reduced by atoms in the dispersive bands to

$$\sigma_R = \frac{-(1 - n_R) \ln(1 - n_R) - n_R \ln n_R}{n_R + B}. \quad (7.6)$$

We plot σ_R for different values of B in Fig. 7.4. If σ is above these curves, then we don't expect to reach $T = 0$ for any choice of reservoir sizes and energy offset. This should be compared to typical experimentally realizable values with evaporation cooling, which is around $s/k_B \approx 0.5$ [147]. The actual σ required will be lower than this, because at $T = 0$ the atoms in the system region will carry zero entropy. This suggests that to investigate the region where cooling to $T = 0$ is predicted in the toy model, the atoms must first be cooled down using other cooling schemes. Alternatively, the band structure needs to be inverted so that the flat band is the first populated band using techniques such as Floquet engineering or negative temperature states.

7.2 Calculation of thermodynamic variables using numerical equations of state

In this section, we try to support the intuition that we have developed from studying the toy model in Sec. 7.1 with numerical calculations. In particular, we point out two qualitative differences between the toy model and a realistic model:

- By taking the lower energy bound Λ to infinite in the system region, the number of particles is infinite. While the change in the total particle number compared to some

reference chemical potential ($\mu = 0$) does not depend on Λ , values such as the entropy per particle σ and the (local) Fermi energy $T_{F,S}$ ³ do. This is problematic, since these are the typical measures of useful cooling. Therefore, we need to abandon the convenient unbounded DoS construction to evaluate cooling. The multiband consideration in the previous section provided another reason why σ is an important quantity.

- The total entropy in the system only depends on the temperature. This means that even if we did not define σ or T_F , we are satisfied to learn that the temperature is lowered when the chemical potential is tuned to be at the energy of the reservoir flat band. For a general DoS, a lower temperature does not necessarily imply a lower σ .

These questions are addressed in this section by considering DoS that are bounded below in energy. For this section, we continue to restrict ourselves with equilibrium properties.

7.2.1 Noninteracting system

The benefit of studying noninteracting systems is that analytic solution exists for infinite systems, and for finite size systems we can easily find solutions for large systems. I will use the exact DoS of the kagome lattice $\rho_{kag}(E)$ for system sizes that approach the thermodynamical limit, and numerically solve for a finite size system with expected imperfections to understand how they affect the cooling performance. (The hopping strength will be set to $t \equiv 1$ from now on.)

Thermodynamical limit

For the numerical simulation, we begin with a set of energy levels $\{E_{orbs}\}_{S(R)}$. Given $\{E_{orbs}\}_{S(R)}$, we can now calculate atom number and entropy by brute force [154]:

$$N_{S(R)}(\mu, T) = \sum_{E \in \{E_{orbs}\}_{S(R)}} f(E)$$

$$\frac{S_{S(R)}(\mu, T)}{k_B} = -N_{S(R)} \ln z + \sum_{E \in \{E_{orbs}\}_{S(R)}} \beta E f(E) + \ln(1 + ze^{-\beta E}). \quad (7.7)$$

³ $T_{F,S}$ should be defined as the Fermi energy in the system region when it is isolated from the reservoir, and using the global Fermi energy T_F leads to wrong interpretations. For example, let us consider what happens as we lower the reservoir energy to $-\infty$. The reservoir is already in the band insulating state when $|V_{offset}|$ is much larger to the temperature, and lowering V_{offset} further increases T_F but not T . Then T_F can be arbitrarily high, and $T/T_F \rightarrow 0$. This is also not an extreme case — this is just what is implemented in the system region in experiments described in, for example, Greiner's group [44].

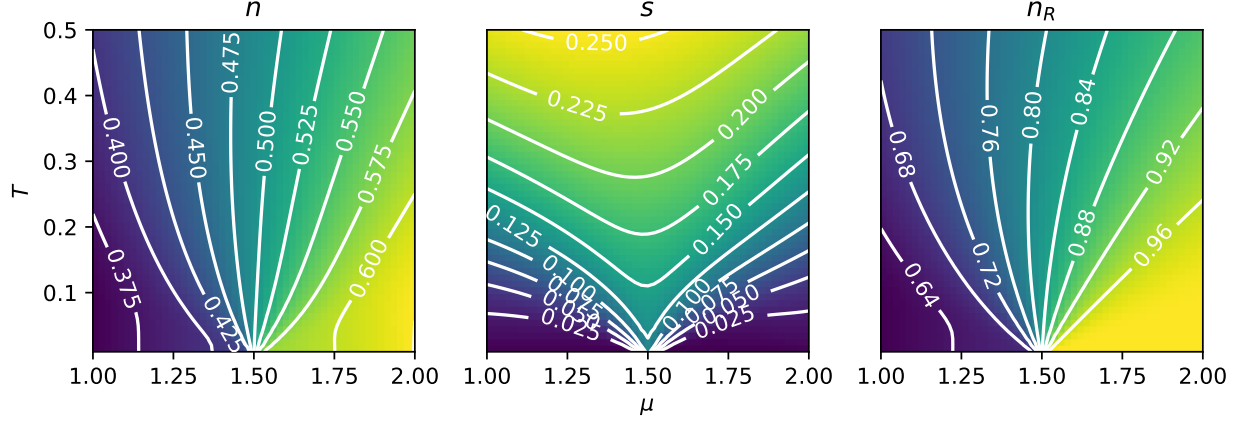


Figure 7.5: Constant n , s , and n_R curves in the $\mu - T$ space for the noninteracting kagome lattice.

$\{E_{orbs}\}_{S(R)}$ should be chosen such that their distribution faithfully reproduces $\rho_{kag}(E)$, the DoS of the kagome lattice s -bands⁴. To achieve this goal, we generate $\{E_{orbs}\}_{S(R)}$ by sampling the DoS in the system and reservoir region⁵, which is now written as

$$\begin{aligned}\rho_S(E) &= L_S \rho_{kag}(E) \\ \rho_R(E) &= L_R \rho_{kag}(E - V_{offset}).\end{aligned}\tag{7.8}$$

We will mostly be interested in cases where the chemical potential is close to the energy of the flat band. Therefore, the value of V_{offset} should be chosen such that the reservoir flat band is at the Fermi energy when the desired filling factor is achieved in the system. In the results shown below, we will choose $V_{offset} = -4.5$, so that the reservoir flat band is not at the same energy as the Dirac point (zero DoS) or the van Hove point (logarithmically diverging DoS).

Let us first look at the EoS of the noninteracting kagome lattice. The size of the reservoir is chosen to be the same as the system ($L_R = L_S = 3.75 \cdot 10^5$) to allow a direct comparison with the EoS of the toy model plotted in Fig. 7.2. For $V_{offset} = -4.5$, the energy of the

⁴ $\rho_{kag}(E)$, as shown in Fig. 3.11, is given analytically by the imaginary part of the lattice Green's function of the kagome lattice. $\rho_{kag}(E)$ is the sum of a Dirac delta function and the DoS of the honeycomb lattice, $\rho_{kag}(E) = \rho_{hex}(E) + \delta(E)$ [92, 93]. Proper normalization requires that $\int dE \rho_{hex}(E) = 2$. $\rho_{hex}(E)$ can be written down in terms of complete elliptic functions, but we will not be concerned with its exact form. Rather, we will just note that it is available in the python package `gftool` [155].

⁵Within the interval where $\rho(E)$ is non-zero, I generate $N_{bin} = 500$ energy bins, with weights determined by $\rho(E)$. N_{bin} is chosen such that the bin width is fine enough to reproduce fine features in the DoS, such as the weak divergences at the van Hove points, while still allocating enough levels for where the DoS approaches zero, such as near the Dirac point. Within each bin, energy levels are generated by linearly sampling the bin, such that the number of levels in each bin is proportional to the weight of the bin. The total number of energy levels $L = 7.5 \cdot 10^5$ is chosen such that no noticeable changes is seen by repeating the calculation with a larger system.

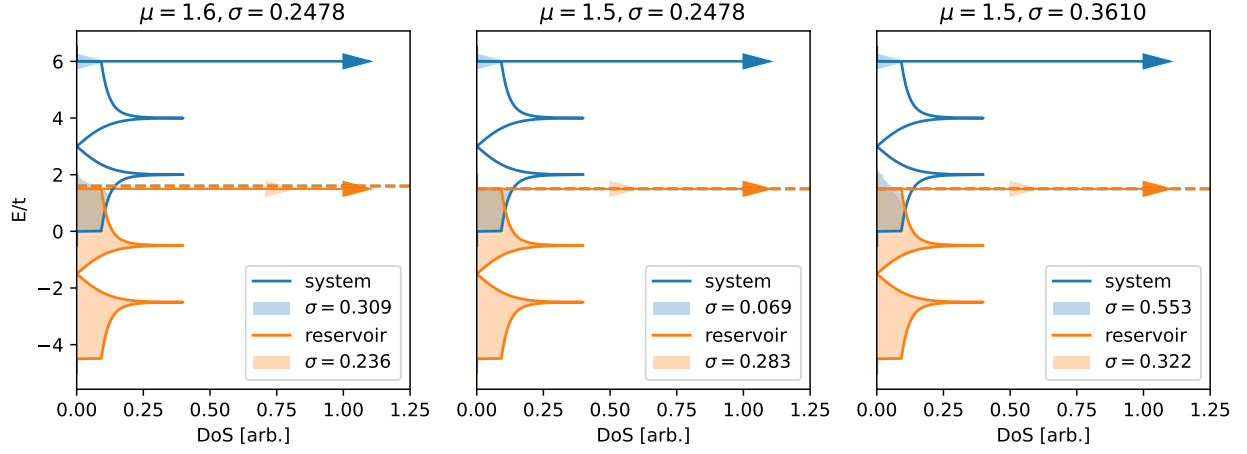


Figure 7.6: Visualization of filling factors for selected parameters. Left: $\mu = 1.6$, slightly higher than the flat band energy. Middle: $\mu = 1.5$, exactly at the flat band energy. The reservoir flat band is now almost exactly half filled, and we observe the expected flat band cooling effect. Right: $\mu = 1.5$, but at a higher entropy per particle. We see that even though the flat band is still almost exactly half-filled, the entropy stored in the flat band is not sufficient to cooling the system. The cooling figure of merit given in Eqn. (7.9) evaluates to $\varsigma = 0.247, -0.722, 0.532$, respectively.

reservoir flat band is at 1.5. We see that the EoS plots are qualitatively similar to the toy model, such as the families of constant- N and isentropic lines that roughly converge at $T = 0$ and $\mu = 1.5$ (flat band energy). This shows that the toy model indeed captures important aspects of the thermodynamics of the joint system. We notice that the largest value of s for which the system can be cooled to zero temperature⁶ is now at around $0.1k_B$, about three times smaller than the toy model. This can be explained by the existence of the two dispersive bands below the flat band. We thus expect that the flat band cooling argument in Sec. 7.1 still applies to this model.

Next, let us focus on the entropy per particle in each subregion. Examples of the result is shown in Fig. 7.6. We note that we still work with grand canonical ensembles here, and we vary μ and σ , so the number of particles and the total entropy is different in the three subfigures. First, we compare the first two subfigures in Fig. 7.6, where σ is the same, and we compare different chemical potentials. For the case where μ is slightly larger than the reservoir flat band energy, we see that the flat band is more than half filled, and as a result the reservoir does not store as much entropy as it can. σ in the system is even higher than the reservoir in this case, because for larger μ the reservoir approaches a band insulator, and eventually all the entropy will be in the system. This is in stark contrast to the case where

⁶The family of isentropic curves that converged at $T = 0$ does not seem to converge exactly. This is most likely a numerical artifact, because the lowest temperature in the plot is at 0.01 (below which we encounter an overflow error).

the chemical potential is exactly at the flat band, and we see much lower σ in the system.

Now we compare the middle and right subfigures in Fig. 7.6. The chemical potentials are the same in both cases, and the reservoir flat bands are both half-filled, meaning that they store the same amount of entropy. However, we see on the right subfigure that when the entropy in the joint system is too high, we actually find that $\sigma_S > \sigma_R$. This can be understood as follows. Once the entropy reduction due to flat band is accounted for, the remaining entropy must be distributed between the dispersive bands of the system and the reservoir, and in this case the system not only has a larger DoS, but also has states available above the chemical potential, so more excess entropy reside in the system than the reservoir. σ must be below a threshold value for $\sigma_S < \sigma_R$ to hold, and the threshold roughly agrees with the value obtained using Eqn. (7.6).

Let us now consider what this implies for a system with the same N and S as the rightmost figure, but where we are free to choose V_{offset} . From the flat band cooling picture we developed, we might guess that cooling would be achieved when μ is at the reservoir flat band. While the temperature goes down following the flat band cooling argument, the result in Fig. 7.6 showed that the entropy per particle in the system is actually *higher* compared to the case $V_{offset} = 0$. This example highlights the importance of clarifying what the meaning of cooling is.

This motivates us to use the reduction of entropy per particle as the figure of merit for cooling. I will measure the cooling effect using a dimensionless number (ς is `varsigma`)

$$\varsigma \equiv \frac{\sigma_s}{\sigma} - 1. \quad (7.9)$$

$\varsigma < 0$ indicates a decrease in entropy per particle, which is understood as cooling, and $\varsigma = -1$ means zero entropy for system particles. We note that if there were no offset, $\sigma_S = \sigma_R = \sigma$, and $\varsigma = 0$.

Finite size effect and other imperfections

The previous section worked with system sizes that approach the thermodynamical limit, and the energy orbitals are generated by fine-sampling the analytical DoS of an infinitely large kagome lattice. We know that in our experiments, the system sizes are much smaller, and it is fair to ask whether the conclusions that we have obtained in the thermodynamic limit still hold in a small system. To take finite system sizes into consideration, we work with a different model, where we explicitly construct and diagonalize the real-space tight-binding Hamiltonian. Diagonalizing the Hamiltonian gives a list of orbitals $\{|\psi_i\rangle\}$ and corresponding energy levels $\{E_{orbs}\}$, with which we can use Eqn. (7.7) to find N and S in the grand canonical treatment.

The downside of this approach is that it is less straightforward to define $\sigma_{S(R)}$ in the subregions. For example, consider a state that extends throughout the entire lattice, such as a typical Bloch-like state in a lattice without V_{offset} . Since this is a pure state, the von Neumann entropy as defined in Eqn. (7.2) is zero. However, by tracing out a subregion, the

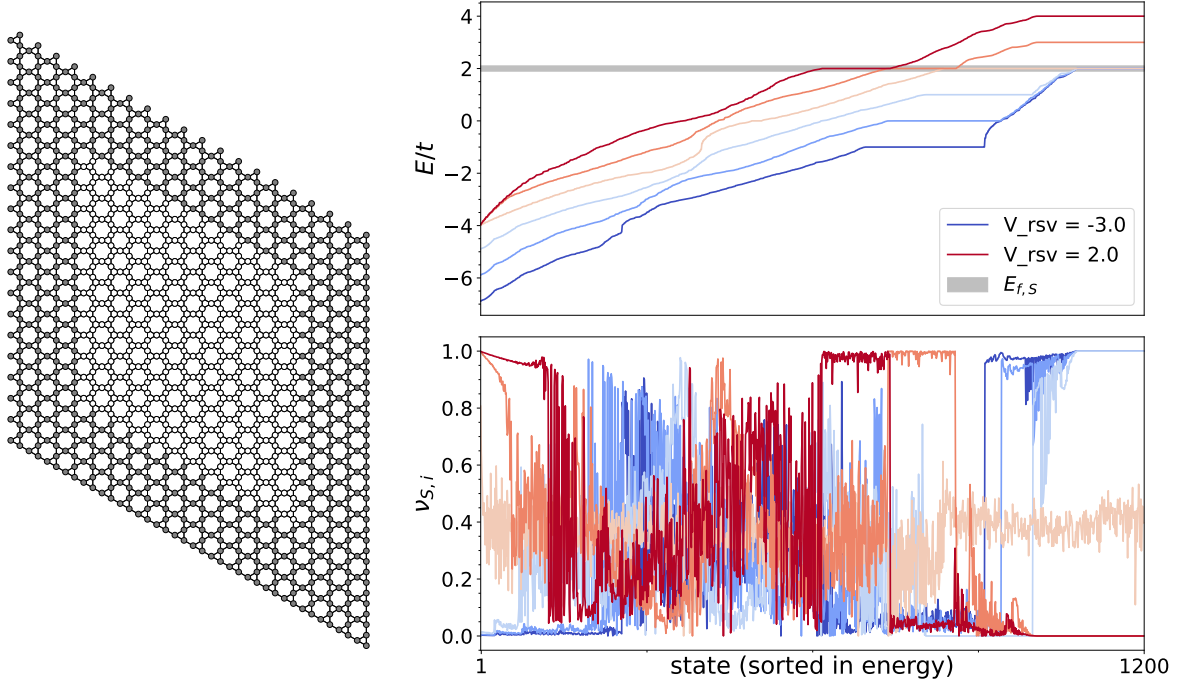


Figure 7.7: The finite kagome lattice. Left: visualization of the finite kagome lattice. The lattice sites in the reservoir region (gray sites) are at an offset V_{offset} . Right: $\{E_{\text{orbs}}\}$ and $\nu_{S,i}$ for different V_{offset} . The gray shaded region highlights the energy of flat band states in the system region, which is at $E_{f,S}/t = 2$ regardless of V_{offset} .

state is now represented by a density matrix with nonzero entropy. In this section, we only show the EoS of the whole system, and focus on how the finiteness of the lattice modifies the EoS compared to the thermodynamic limit.

The real space Hamiltonian with site-dependent offsets V_i can be written as

$$H = \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i, \quad (7.10)$$

where $V_i = V_{\text{offset}}$ for $i \in R$, and $V_i = 0$ for $i \in S$ in an ideal world. With $V_{\text{offset}} = 0$, we have the usual kagome tight binding model (with open boundary condition). By construction, the orbitals are not strictly separated into the system and reservoir region. We define the number of particles that each orbital contributes to the system region as the expectation value of the system projector:

$$\nu_{S,i} = \langle \psi_i | P_S | \psi_i \rangle = \sum_{j \in \mathcal{S}} \langle \psi_i | c_j^\dagger c_j | \psi_i \rangle. \quad (7.11)$$

From which we calculate the filling factor in the system region ν_S , or the average number of particles per site in $\mathcal{S}$:

$$\nu_S = \frac{\sum_i \nu_{S,i} f(E_i)}{L_S}. \quad (7.12)$$

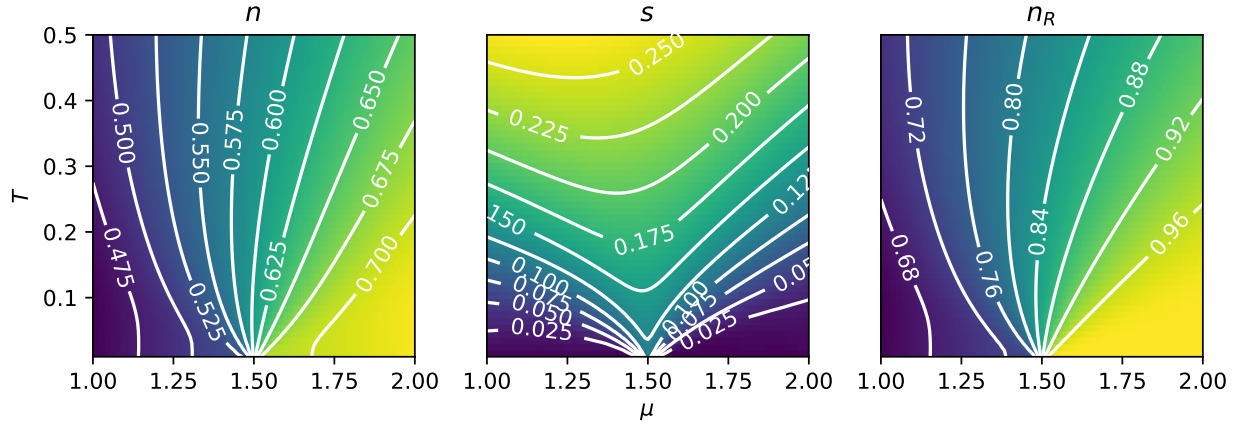


Figure 7.8: EoS of the finite size kagome lattice with $V_{offset} = -4.5$. The μ -axis is shifted by $4t$ for direct comparison to Fig. 7.5.

Fig. 7.7 shows an example of $\nu_{S,i}$ for kagome lattices with 20×20 unit cells, of which the middle 12×12 cells are the system region. We see that there are still states that are completely localized within the system ($\nu_S = 1$) or the reservoir ($\nu_S = 0$), which correspond to the CLS in the flat bands. The system CLS always form a plateau at $E/t = 2$, while the reservoir CLS form a plateau at $E/t = 2 + V_{offset}$.

We plot the resulting EoS from $V_{offset} = -4.5$, the same value used in the exact DoS calculation. From Fig. 7.8, we see that even though the system is much smaller than the thermodynamic limit system studied previously, the n and s plots look qualitatively identical. This provides us confidence that the findings from the exact DoS calculation can be reproduced in experimentally realistic system sizes.

Adding imperfections

By explicitly constructing the real space Hamiltonian, we can also account for imperfections that we expect in our system. We consider the following modifications:

- From plane wave expansion calculations, we know that the third band in our experimentally realized optical kagome lattice is not exactly flat, see Fig. 3.11 and the discussion therein. In the tight binding model, we account for the unflattening of the band by including second order hopping terms t' between next nearest neighbors. We do not attempt to introduce coupling to additional orbitals (such as the p -orbitals, or the s -orbitals in the excluded D sites) for simplicity.
- V_i should vary smoothly due to the finite spatial resolution of the imaging system. We can replace the step function potential by a Gaussian potential with a width w_{diff} set by the diffraction limit of our system.

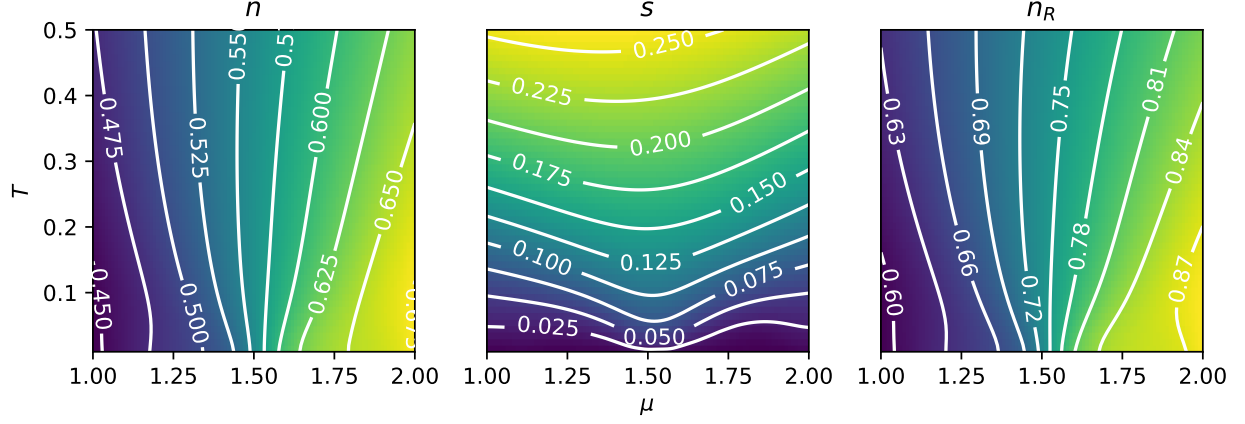


Figure 7.9: EoS of the finite size kagome lattice with $V_{offset} = -4.5$ and imperfections. The parameters used were $t' = 0.01t$, $w_{diff} = a_{kag}$, and $\delta V = 0.1t$, with their meaning described in the main text. Compare to Fig. 7.8.

- There can be some small random fluctuation on V_i due to speckles from the light that forms the optical potential required to create the offset. We can represent this by adding a random value sampled from some normal distribution with variance δV to each lattice site⁷.

The finite resolution is somewhat qualitatively different from the other two imperfections in two ways: the number of sites affected by this perturbation scales like $\sqrt{L_S}$ instead of L , and it doesn't affect the CLS deep inside the system or reservoir. But in general, we expect that the flat band will become slightly dispersive due to the imperfections, reducing the cooling effect.

In Fig. 7.9, we plot the resulting EoS obtained by including imperfections. Comparing to Fig. 7.8, we see that the temperature decrease as the chemical potential is tuned to the reservoir flat band is less significant, especially at lower temperatures. The higher constant entropy lines are less affected, which is understandable, since $k_B T \gtrsim$ (imperfections). This can be understood as a broadening of the flat band, and indeed, the constant occupation lines in the n_R plot no longer converges at the flat band energy.

In summary,

- The flat band cooling intuition developed with the toy model holds in the sense that the temperature decreases when the flat band is partially filled.
- When the cooling is measured in decrease of σ_S , a lower temperature does not necessarily imply cooling. In particular, σ of the joint system must be low enough, or the

⁷In principle the variance of the normal distribution should be proportional to the light intensity at each lattice site, and since we plan to use a blue detuned light to offset the system region, the random potential should be stronger in the system. Here we will use the same variance across the whole system for simplicity.

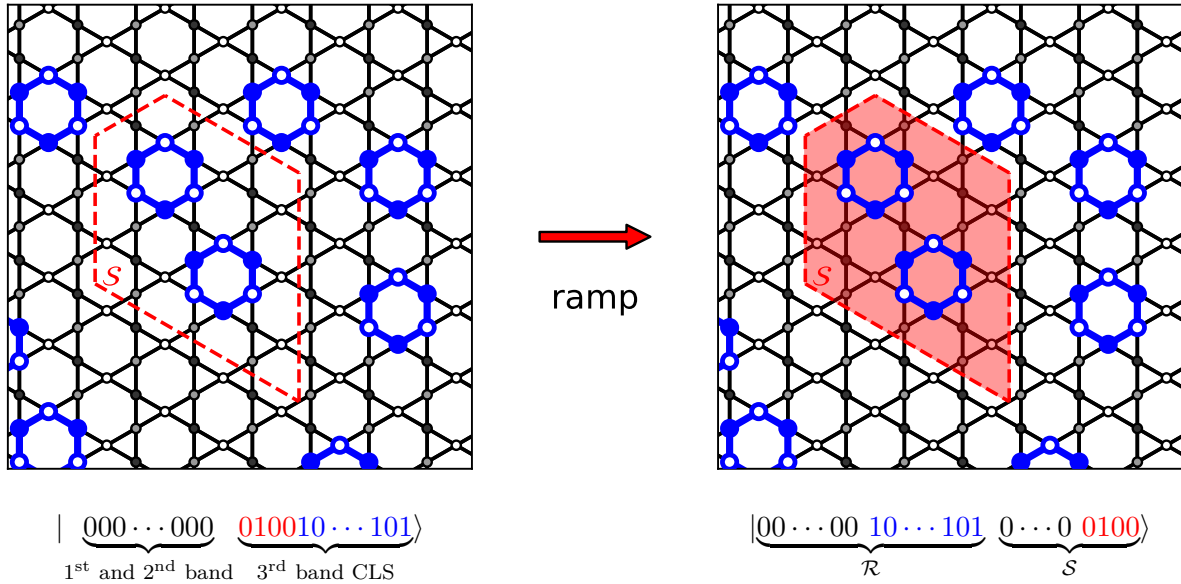


Figure 7.10: An example showing nonadiabaticity in the noninteracting case. The sparsely filled state shown in the figure is an eigenstate of the system throughout the ramp with or without interaction. At the end of the ramp, the potential offset is taken to be large enough that all the system states are higher energy than the reservoir states. The CLS in $\mathcal{S}$ will not scatter away by introducing more particles, unless there is interaction between particles. The orbitals in the ket are sorted in increasing energy.

excess entropy can reside in the system.

- The EoS of a finite size kagome lattice do not qualitatively differ from that of a large kagome lattice.
- Adding imperfections to the finite size lattice reduces the decrease in temperature, especially for systems with low entropy.

7.2.2 Role of interaction

So far, we have assumed that the system somehow remains at thermal equilibrium and at constant entropy, without questioning how it equilibrates. However, the fact that we are working with flat band systems allows us to find simple arguments that this is a nontrivial problem. Let us consider the extreme case shown in Fig. 7.10, where we start with a state with atoms sparsely occupying non-overlapping CLS. This state is clearly not in thermal equilibrium, since there are many orbitals with lower energies in the dispersive bands but left unoccupied. It is also easy to see that this state will never evolve in time, apart from a dynamical phase. Now consider uniformly increasing the potential offset in $\mathcal{S}$, the system region. The state remains an eigenstate all the time as long as all the CLS sees a uniform

potential locally. Therefore, the ramp will never be adiabatic even if it is infinitely slow, in the sense that if the state is labeled by the occupation number of each orbital in increasing energy, it can't remain the same⁸.

Now let's consider what happens in a more experimentally relevant setting, where the lower energy orbitals are appreciably occupied. If there is no interaction between particles, the CLS in the center remains there even if more particles are introduced, and the system will still never evolve adiabatically. It is unclear if by introducing interaction, the system can now evolve adiabatically to the final offset, but at least the CLS in the center can now scatter with other particles. This suggests that we need to include interaction if we want to cool the system with the reservoir flat band.

It is unclear if these states affect thermalization properties, as it is believed that most of the eigenstates of integrable systems (such as any noninteracting systems) “look” thermal⁹, and it is unlikely that we will prepare such a pure state experimentally. However, from the previous argument, it does seem to be related to the timescale over which thermalization can happen. Including interaction in our calculations is thus not only due to its experimental relevance, but an important part of the flat band cooling argument.

Exact numerical simulation of interacting systems is difficult because the Hilbert space grows exponentially with system size. While numerical techniques such as density matrix renormalization group exists, they work much better in one dimensional systems, as the computational cost grows linearly in one dimension and exponentially in the other [157]. To make the problem more tractable, we therefore look for a 1D system with a flat band, and then attempt to shift the flat band to be energetically in contact with the dispersive bands to reproduce the QBTP featured in a kagome lattice. This leads to the study of the sawtooth lattice described in the next section.

For simplicity, instead of considering on-site interaction U of a spin-1/2 system, we instead work with spinless fermions with nearest neighbor interaction V , and find the EoS at different temperatures and chemical potential, which can be done with high numerical precision. The tensor network calculations of interacting systems is done by Sajant Anand.

7.2.3 A one-dimensional flat band model: sawtooth lattice

The sawtooth lattice is shown in Fig. 7.11. It is a 1D lattice with two sublattice sites per unit cell, and we denote the annihilation operators of the sites in unit cell i as a_i and b_i . The

⁸One can also show that there are exponentially many such sparsely occupied states. Consider a choice of non-overlapping hexagons, for example, the ones that form the Wigner crystal-like state at $1/9$ filling in [1]. The number of hexagons is $N_{hex} = L/9$. Each of the hexagon can either be occupied or not, and the resulting many-body state will be an eigenstate of the Hubbard Hamiltonian, regardless of U . For $N \sim N_{hex}/2$, there are then $\binom{N_{hex}}{N_{hex}/2} = O(e^L/\sqrt{L})$ such eigenstates. For each of them, one can add in any number of particles in different orbitals, and without interaction, the CLS in $\mathcal{S}$ will behave in the same way.

⁹This refers to the weak eigenstate thermalization hypothesis, which states that besides from an exponentially small number of states, the expectation values of “a large class of” operators of the some eigenstate agrees exponentially well with the prediction of a microcanonical ensemble [156]. Local operators, such as operators that only look at a subsystem, are generally believed to fall within this class.

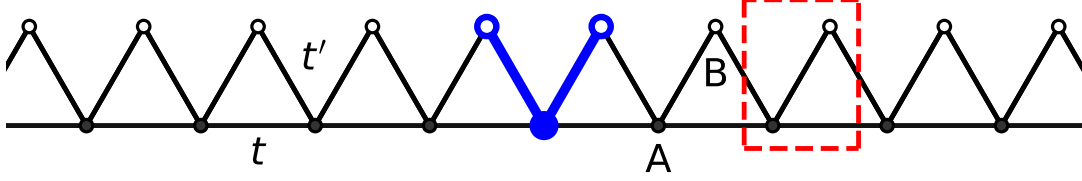


Figure 7.11: The (unmodified) sawtooth lattice with hoppings t and t' . The CLS that arises when $t' = \sqrt{2}$ is shown in blue. The red box contains one unit cell of the lattice.

noninteracting Hamiltonian is then given by

$$H_{ST} = - \sum_i t' \left(\hat{a}_i^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{a}_{i+1} + \text{h.c.} \right) + t \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.} \right). \quad (7.13)$$

where $t \equiv 1$ and t' are non-negative real hopping parameters. I will also set the lattice constant to be $a = 1$.

The dispersion relation is given by [1, 158]

$$\lambda_{\pm} = -t \cos(k) \pm \sqrt{t^2 \cos^2(k) + 2t'^2(1 + \cos(k))} \\ \xrightarrow{t'=\sqrt{2}t} \begin{cases} 2t \\ -2t(1 + \cos(k)) \end{cases}. \quad (7.14)$$

We will focus on the case $t' = \sqrt{2}$, where the upper band becomes dispersionless. We also note that the band gap between the two bands is 2. Since our argument for cooling is entirely based on the band structure of the system, we would like to mimic the band structure of kagome lattices more closely by moving the flat band downwards by $V_{shift} = -2$ so that it touches with the dispersive band at $k = \pi$. It can be shown [158] that this can be done by adding infinite range, but exponentially decreasing hopping terms (see B.1). This is purely a shift for the flat band only for $t' = \sqrt{2}$; for other cases, the dispersion also changes slightly.

We note that CLS will no longer be exactly compact. Since CLS arises from the destructive interference of hopping amplitude, the inclusion of infinite range hopping means that even lattice sites that are infinitely far away have non-zero amplitude when one attempts to construct a CLS, although the wave function amplitude is expected to drop exponentially.

7.2.4 Overview of the EoS matching algorithm

The input from tensor network calculations¹⁰ is a large dataset of EoS, which gives $n(\mu, \beta) \equiv N/L$ and $s(\mu, \beta) \equiv S/L$ on a grid of μ and β for a set of parameters $\{L, t', V, V_{shift}\}$. An example of the EoS is shown in Fig. 7.12. There are no on-site offsets in these calculations.

¹⁰A few details on the calculation: the calculation is done with the **TenPy** package [159], with bond dimension $\chi = 64$. The entropy S quoted in this section is the Rényi entropy, $S_2 \equiv -\text{Tr}[\rho^2]$, which is easier to calculate than the von Neumann entropy in Eqn. (7.2) and (7.7).

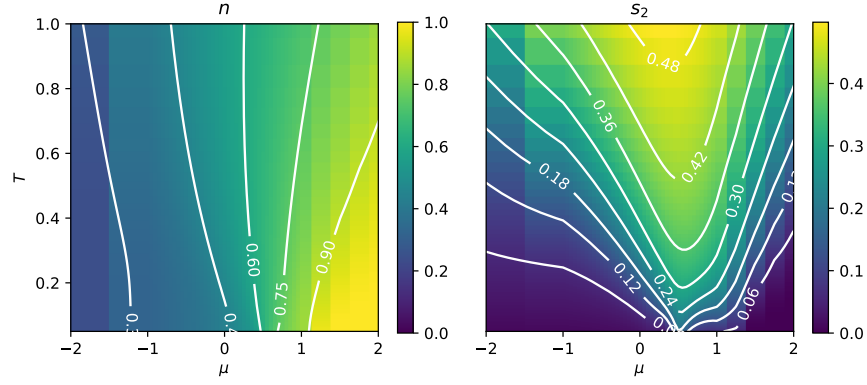


Figure 7.12: An example of the numerical EoS obtained from tensor network calculations. The parameters used are $\{L = 2 \cdot 50, t' = \sqrt{2}, V = 0.3, V_{shift} = -2\}$.

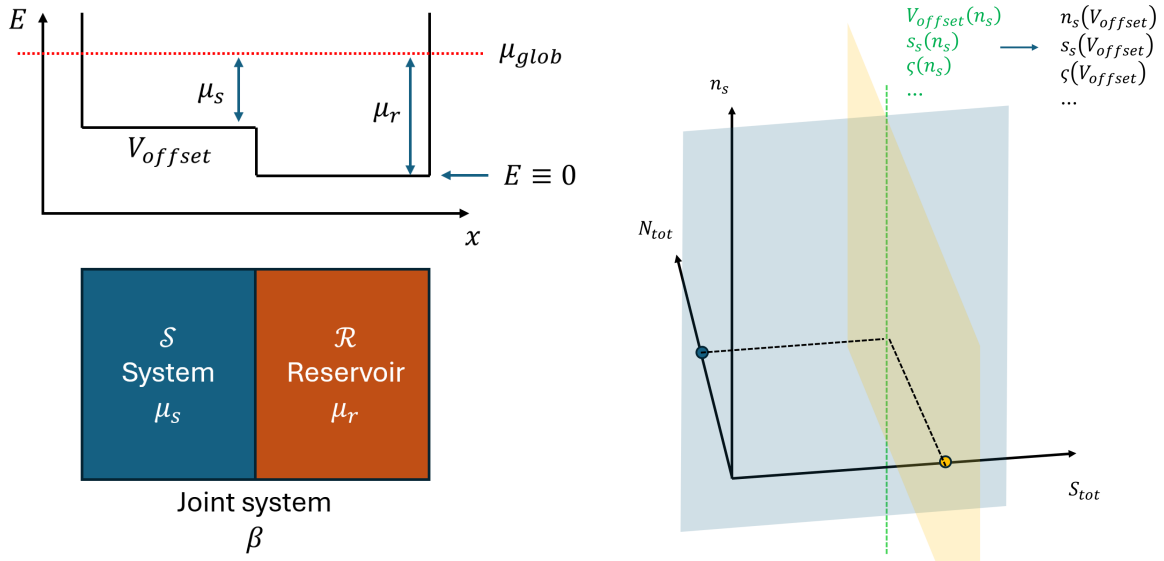


Figure 7.13: Left: Illustration of the situation considered in the EoS matching algorithm. Right: Illustration of the inversion between n_s and V_{offset} in the parameter space. The inversion between S and β is conceptually similar.

The situation we consider is shown pictorially in Fig. 7.13. We consider the system and reservoir regions both with size $L = 2L_u$ in thermal equilibrium, described by β and μ of the joint system. L_u is the number of unit cells in each subregion. The only difference between the two subregions is a uniform offset V_{offset} , which sets the local chemical potential μ_S and μ_R in the two subregions. We can then use the numerical EoS to find the number of particles $N_{S(R)}$ and total entropy $S_{S(R)}$ in the two regions. The value of β and μ is determined by requiring that $N = N_S + N_R$ and $S = S_S + S_R$. The physical idea behind this setting is that we usually consider having a quantum gas with a certain number of atoms and entropy before ramping on a predefined optical lattices and holographic potentials, so the properties of the system is eventually determined by N , S , and V_{offset} . Since we don't consider the dynamics of the system, the actual geometry of the joint system doesn't affect our results.

The algorithm is implemented as follows:

1. Start by picking some atom number N .
2. Specify the density in the system, $n_S \equiv N_S/L$. This also sets the density in the reservoir, $n_R \equiv N_R/L = (N - N_S)/L$.
 - The smallest change in n_S is $1/L$, i.e. only one more particle is in the system. I always take the smallest step possible.
3. Find $\mu_{S(R)} = \mu(\beta)|_{n(\mu,\beta)=n_{S(R)}}$ by inverting $n(\mu, \beta)$.
 - I can do this one $\beta = \beta_0$ at a time: assuming that $n_{\beta_0}(\mu) \equiv n(\mu, \beta_0)$ is a smoothly varying function in μ (true if $V \neq 0$ or $T > 0$), we can simply do a linear interpolation to find $\mu_0 = n_{\beta_0}^{-1}(n = n_{S(R)})$.
4. Find $S_{S(R)} = S(\mu_{S(R)}, \beta)$. As I vary β I should get a smooth change in $S = S_S + S_R$.
 - At this point I can find all the thermodynamical quantities of interest, given by $\mu \equiv \mu_R$, $V_{offset} = \mu_R - \mu_S$, $s = S/N$, and $\sigma_{S(R)} = s_{S(R)}/n_{S(R)}$.
5. Do this for different N_{tot} . Now I've done a scan in the (N, S) space, and the EoS can be written as $(n_S; N, \beta) \rightarrow (V_{offset}; \mu, S)$.
6. Invert the S, β conjugate to get $(n_S; N, S) \rightarrow (V_{offset}; \mu, \beta)$.
 - While we should in general accept $T < 0$ as possible solutions since we are working with a finite system, we will restrict ourselves to $T > 0$, within which we expect $S(\beta)|_{N=N_0}$ to be a monotonic function, and the inversion can be done.
7. Invert n_S and V_{offset} to get $(V_{offset}; N, S) \rightarrow (n_S; \mu, \beta)$.

7.2.5 Results

We first summarize the conclusions from the EoS matching algorithm. Overall, including a weak interaction mainly results in qualitative corrections to the noninteracting case.

- At high entropy, we don't find $\varsigma > 0$ when the reservoir flat band is half filled, in contrast to the argument in Sec. 7.2. However, we do find that the smallest value of ς is achieved at a different filling factor, and for smaller entropy a half-filled flat band becomes favorable.
- The flat band cooling effect is weakened but still exists in the presence of weak interactions. The offset required to optimize cooling effect is strongly modified by interaction.
- A system at flat band filling is hard to cool. While this is obvious from the large DoS of the system, we point this out specifically to contrast with the toy model, where the DoS of the system is always finite.
- The region described in Sec. 7.1.2 where no solution exists for a grand canonical ensemble shrinks under finite interaction strengths. For sufficiently low total entropy and weak interaction strengths, this region does not completely go away. This is suspicious, because the DoS should become finite for any nonzero interaction strengths. It is possible that with a larger system size, we will be able to resolve finer features in the EoS and find solutions for all the parameter space considered, but the computational overhead may be prohibitive.

The results are best understood by considering the entropy capacity of the flat bands in the noninteracting case. Let us define

$$S^\circ(n_S) \equiv S(n_S)|_{\beta=\infty} = L_u \sum_{x=S,R} [-(1 - n_{f,x}) \ln(1 - n_{f,x}) - n_{f,x} \ln n_{f,x}], \quad (7.15)$$

where $n_{f,x} = \max(2n_x - 1, 0)$ is the filling factor within the flat band, assuming zero temperature. Depending on the number of atoms in the system, the contribution from $\mathcal{S}$ and $\mathcal{R}$ can either overlap or not, and I will show examples for both situations.

Too much entropy

We first look at the case where $S > S^\circ(n_S)$ for all values of n_S . The values of S and $S^\circ(n_S)$ are plotted for two choices of n in the first row. The small n case (left column) is chosen such that the contributions to $S^\circ(n_S)$ from $\mathcal{S}$ and $\mathcal{R}$ do not overlap, in contrast to the large n case (right column).

In Sec. 7.2.1, we have argued that when the entropy per particle is above a threshold roughly given by Eqn. (7.6), there would be an increase in σ_S ($\varsigma > 0$) when the reservoir flat band is half filled. We would like to know if this still holds when the system is not described by a grand canonical ensemble, but a fixed N and S . Focusing on the noninteracting case

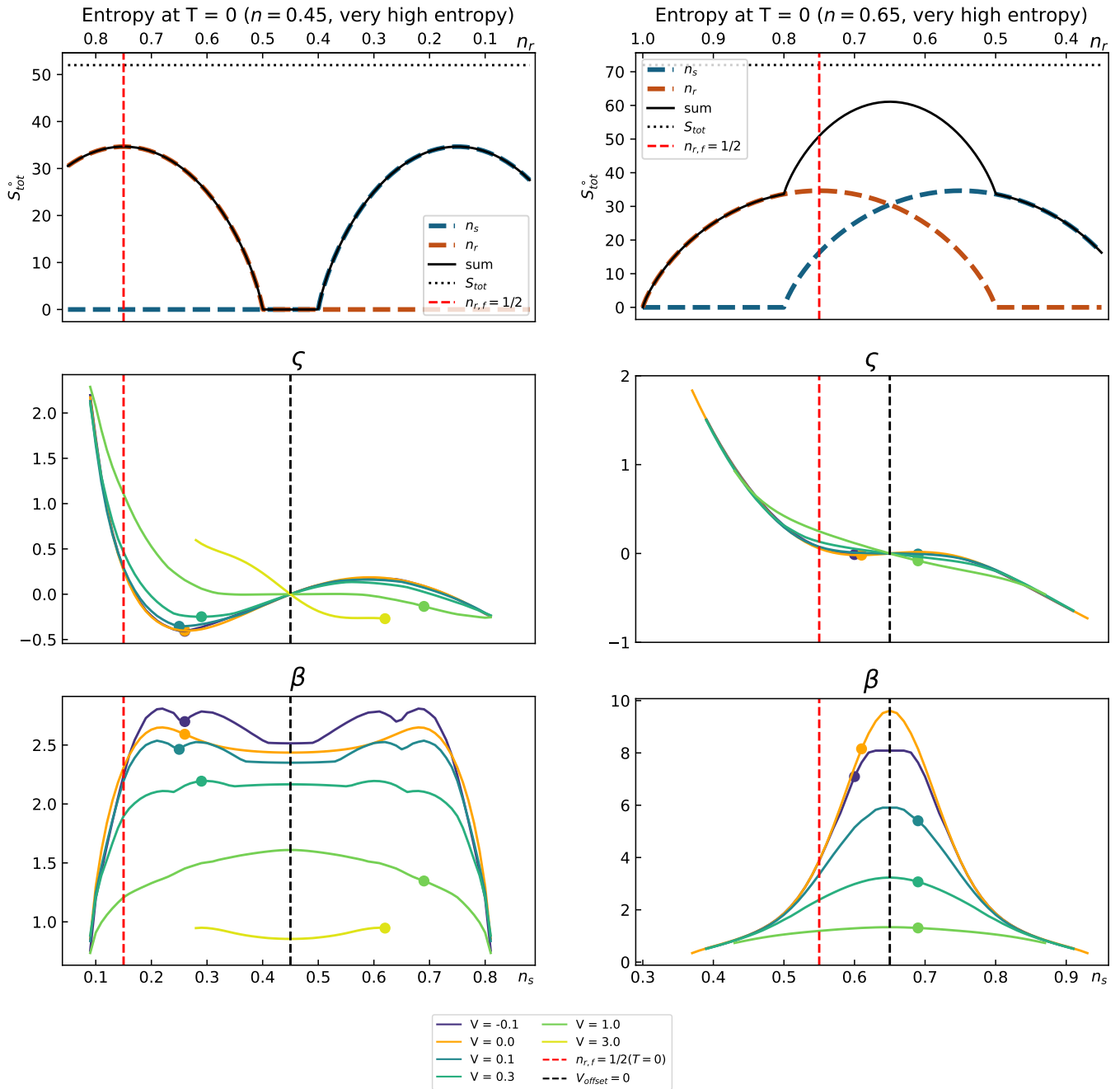


Figure 7.14: Values of the cooling parameter χ for selected examples. S is chosen to be much larger than $\max[S^o(n_S)]$. The marker labels where minimum χ is achieved.

(orange lines), we do not see $\varsigma > 0$ when the flat band is half filled (at largest β ; see Fig. B.1). However, ς is also not optimized at the lowest temperature, so we indeed see the effect of excess entropy.

We do not see a big change in temperature compared to the case of zero offset (vertical black dashed line) for the small entropy case, which indicates that the effect of flat band cooling is not yet significant. We will turn our attention to the more interesting cases, where the total entropy in the system is comparable to the entropy capacity of the flat bands.

Just too much entropy

Next, we lower the entropy such that S is only slightly larger than $\max[S^\circ(n_S)]$ just holds. The total entropy in the system (black dotted line) is still larger than the $T = 0$ entropy capacity (black solid line), so we do not expect the temperature to go to zero at any filling.

Let us first focus on the noninteracting results (orange curves). For the small density case, the entropy in flat band is maximized by filling one of the flat band to half filling. In contrast to the large entropy case, now the minimum ς is actually realized by a half-filled flat band. This indicates that ignoring the dispersive bands in the reservoir is an good approximation when the flat band can accommodate most of the entropy.

On the other hand, for the large density case, the entropy in flat band is maximized when neither the system flat band nor the reservoir flat band is half filled. In this case, the lowest ς is still achieved close to where the reservoir flat band is half-filled, but is much less pronounced than the small N case. This is because the partially filled system flat band always contribute a considerable amount of entropy, pushing up σ_S . In particular, ς is not minimized when the temperature of the joint system is the lowest, as a lot of entropy is in the system flat band. We only see low σ_S when the system is close to completely filled, which is a somewhat boring situation, as we know that band insulators have exactly zero entropy.

Now let us try to understand the effect of interactions. Starting from the low density case, we see that the lowest ς achievable is higher for increasing interaction strength, and the cooling effect has largely disappeared when V is as strong as the hopping. At this point, the flat band is broadened by an amount comparable to the bandwidth of the dispersive bands. We also see that ς is rather insensitive to V_{offset} , and the offset mainly changes n_S (see Fig. B.2). It is still possible to get $\varsigma < -0.5$ in the presence of weak interactions, although the offset at which this is realized is shifted. The high density case does not show strong signs of cooling in the system to begin with¹¹. Overall, the findings suggest that we should work with densities that are low enough so that the system flat band stays unoccupied, and interaction strengths small compared to the hopping strength.

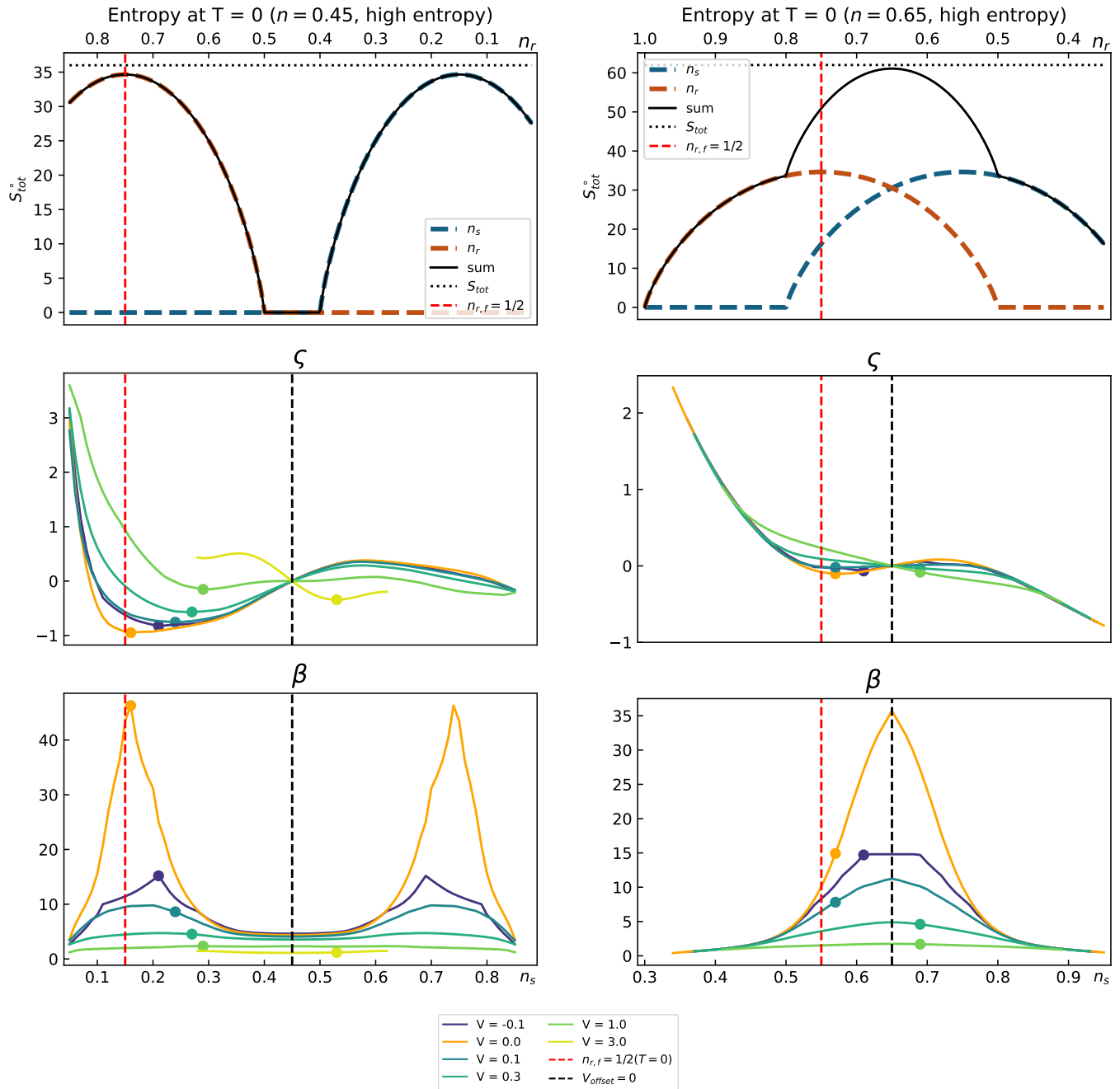


Figure 7.15: Values of the cooling parameter ζ for selected examples. S is chosen to be slightly larger than $\max[S^o(n_S)]$.

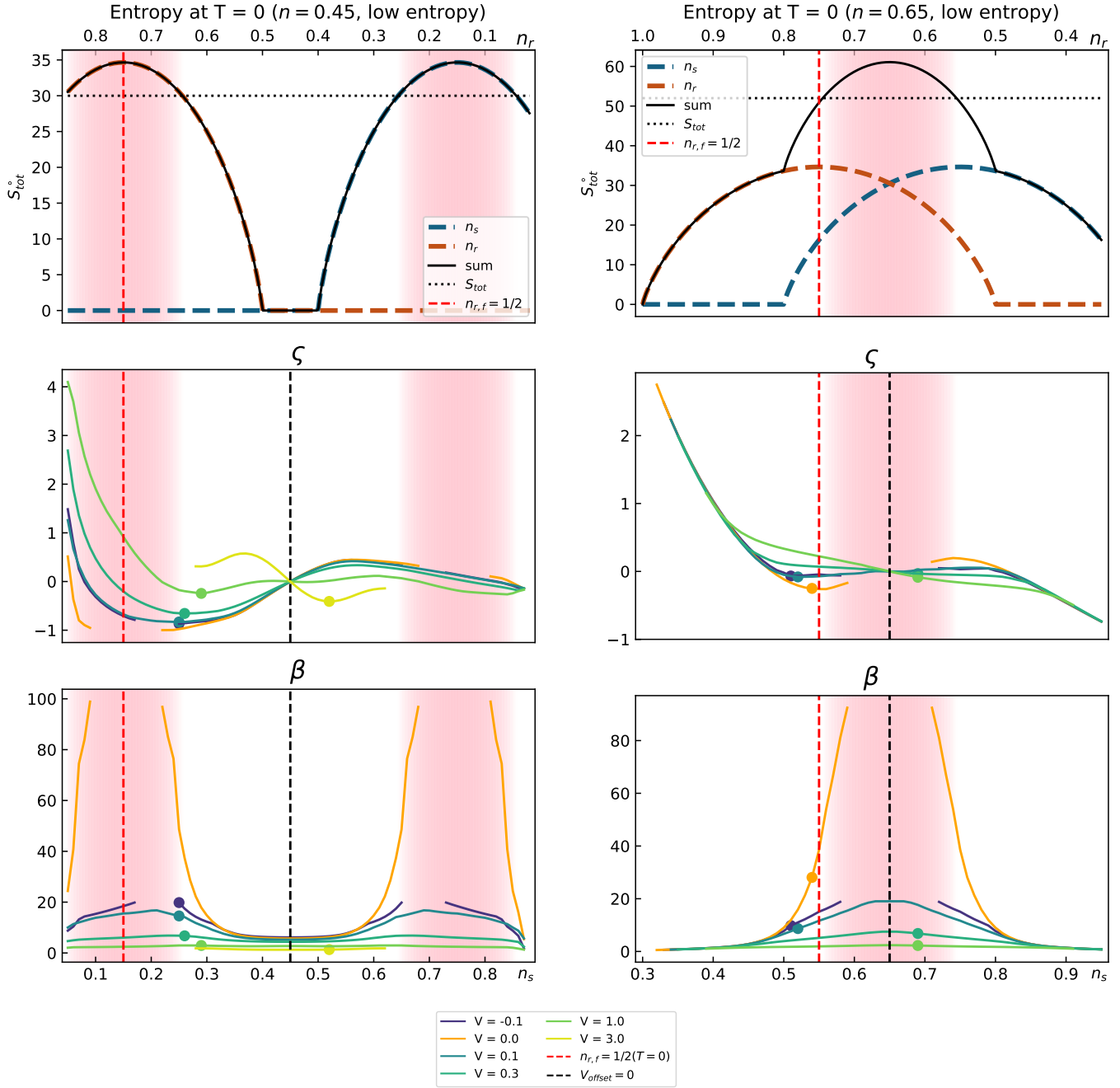


Figure 7.16: Values of the cooling parameter ζ for selected examples. S is chosen to be slightly less than $\max[S^o(n_S)]$. Regions where the joint system is not compatible to a global μ, T assignment in the noninteracting case are shaded in pink. Note that the orange line in the bottom right panel is disconnected at $V_{offset} = 0$.

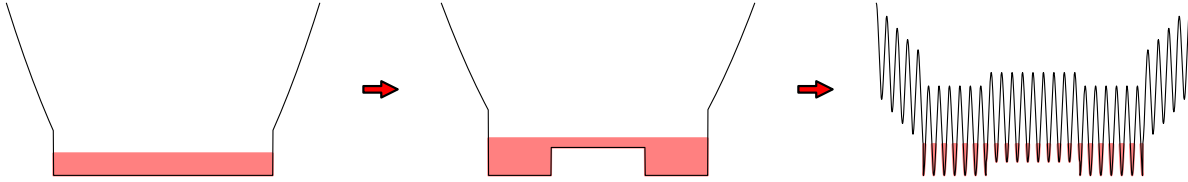


Figure 7.17: Illustration of the proposed experiment sequence.

Too little entropy

Now, we turn our attention to the case where $S < \max[S^\circ(n_S)]$. In the first row of Fig. 7.16, we highlight the region where the flat band entropy at $T = 0$ is larger than the total entropy in the joint system, with $S - S^\circ(n_S)$ plotted below. We would like to know whether the system is cooled to zero temperature where $S < S^\circ(n_S)$, or if there is a breakdown of the grand canonical treatment similar to what was seen in Sec. 7.1.2, in which case no solution would be found by the algorithm.

Let us again look at the noninteracting cases first. In the two densities shown, we find that when $S^\circ(n_S) - S$ is small (at the edges of the pink shades), it is still possible to find solutions at $T > 0$. This must mean that the entropy in flat bands is *lower* at a finite temperature compared to $T = 0$. A way to understand how this can happen is by noting that the entropy in flat bands is not a monotonic function of T , and furthermore is only determined by the filling factor within the flat band, n_f . In a closed system, it is not very straightforward to see whether n_f of the flat band at lower energy increase or decrease when T is increased. Eventually, it is no longer possible to find a solution with $T > 0$ when $S^\circ(n_S) - S$ becomes too large. It is possible that we can find solution with negative temperature in part of the red region, as shown in appendix B.2 for the noninteracting case. (At the time of writing, no numerical calculations were done at $T < 0$ for interacting cases.)

When interaction is turned on, we see that the region where no solution is found either shrinks ($V = -0.1$) or disappear altogether ($V > 0$), which can be roughly explained by a broadened flat band band width. The qualitative behavior of the traces otherwise look similar to Fig. 7.15.

7.3 Experiment proposal

From Sec. 7.2, we learned that even on a purely thermodynamical level, we need to start with very low entropy and a well-defined number of particles for flat band cooling to work. Both of these are inaccessible with conventional evaporation cooling techniques, but can be realized by preparing band insulators (BI) of known sizes, as demonstrated in [44] (or [146] for bosons, which starts with a Mott insulating state instead). Using the 1064 nm lattice to

¹¹No solution is found for $V = 3.0$ in the high density case, since the largest chemical potential ($\mu = 5$) at which we performed the numerical calculations only reaches a filling factor of 0.62.

prepare the BI is closer to the implementation in [44], but in our system, the 532 nm slices each 1064 nm lattice site into three, so the resulting density is not high enough to fill the flat band of the reservoir. Since σ does not increase appreciably during an adiabatic expansion in [44], one may hope that this will also be the case for compression. Alternatively, one may create a BI with the 532 nm lattice, and hope that the heating observed in [43] is reduced if the lattice depth is lowered during expansion. The most natural thermodynamic variable to specify in the system would likely be the total particle number N , and the entropy per particle σ : σ is determined by how well one can prepare a BI, and N is determined by the size of the BI.

Another important realization from experiments that reached record low entropies [44, 146, 43] is that particle transport in a deep optical lattice results in a lot of entropy increase, which is also studied numerically [160, 161]. This means that after preparing and splitting a low entropy BI, we will likely need to first ramp up the offset potential and allow atoms to redistribute in a shallow lattice, before ramping the lattice back up. This sequence is illustrated in Fig. 7.17. In our experiment, we plan to generate the offset potential using a digital micromirror device (DMD). Depending on how the atoms redistribute themselves throughout the lattice ramp up, it is possible that the DMD offset potential also needs to be adjusted during the sequence. One can imagine stopping at several intermediate lattice depths during the ramp up, taking *in situ* density distribution, and adjust DMD light intensity accordingly.

If the cooling scheme works, the high entropy reservoir region can be separated from the system with a potential projected using a DMD. Eventually, whether the system will remain cold if the interaction strength is further increased to be comparable to t is an open question. This will be a subject for future investigation, and will not be discussed here. We will instead focus on whether flat band cooling works when we consider the dynamics of the system.

7.3.1 Numerical simulation of the proposed sequence

It would be desirable to be informed by numerical simulations on the feasibility of the proposed scheme. The main goal would be to identify the time scale for thermalization, and if it is possible at all to evolve isentropically. However, a simulation of the density distribution-matched sequence is much more involved, requiring a discretized spatial grids much finer than the lattice spacing, and makes the sawtooth a lot more extended in the narrow direction [160, 161]. This is an ongoing effort with Sajant Anand that will be published in a future study.

7.3.2 Thermometry of the system

Eventually, we need to experimentally confirm that the entropy in the system region is decreased. Thermometry of fermions in optical lattices has been a subject of active research, but no matter what observables are probed experimentally, one needs to compare those to

theoretical results. This means that observables that are adapted to what theorists can calculate are more advantageous in some sense, and that when such calculations struggle, so does experimental thermometry.

Spin- and charge-correlations

While we have been exclusively performing momentum space measurements so far, I will discuss approaches that requires single-site resolution, since we plan to install a high numerical aperture objective in the future. In quantum gas microscope experiments, one can compare measured charge and spin correlations to numerical calculations, such as numerical linked cluster expansions (NLCE) [162, 163, 164] or quantum Monte Carlo (QMC) [44, 165, 164]. This method has also been adapted to frustrated lattices, such as triangular lattices [166], and there are ongoing efforts to perform QMC [167, 168] and NLCE¹² calculations for kagome lattices.

Round-trip measurements

Heating from optical lattices can be estimated by ramping up and down the optical lattice, and then measuring the temperature change of the gas [169, 19]. The lattice can be ramped off completely, followed by a usual time-of-flight measurement of a bulk gas. Fitting to the temperature of a Fermi gas is difficult on its own (see Sec. 3.2.3), but the fitting function is well-understood. Round-trip measurements have also been done in site-resolved experiments, where the entropy in the final system is measured by counting the density of singly-occupied sites in the band insulator phase [43].

This method measures the entropy increase in the system, and by designing the ramp sequence appropriately, it provides some information on which part of the sequence results in the most heating [43]. The momentum space measurement version of this method fails to capture the spatial dependence of entropy distribution, which may be resolved by first expelling all the atoms in the reservoir with a projected potential prior to measurements.

Double occupancy

Double occupancy is first proposed as a thermometry tool for noninteracting fermions in lattices [170], but is also a useful tool for interacting fermions if numerical results at different temperatures and interaction strengths are available. Many of the references quoted in the correlation section also calculates double occupancy.

Double occupancy has been measured by converting atoms in the doubly-occupied sites to molecules by sweeping through a Feshbach resonance [171]. The molecules are no longer resonant to the imaging pulse, so the fraction of atoms lost is a measure of double occupancy. Alternatively, one can tune the magnetic field close to a Feshbach resonance, which shift the energy of atoms on doubly-occupied sites by the binding energy of a molecular state. One

¹²For example, at the Khatami group (private conversations).

can then transfer atoms in one of the two internal states to a third state using a RF pulse which is only resonant to energy-shifted atoms [172]. In experiments that are both spin- and site-resolved, measuring double occupancy is very straightforward.

Fluctuation-dissipation theorem

The fluctuation-dissipation theorem relates the temperature T and the isothermal compressibility $\kappa \equiv \frac{\partial N}{\partial \mu}$ through $k_B T \kappa = \delta N^2$, where δN^2 is the atom number fluctuation. Under local density approximation, the compressibility can be measured using the relation $\frac{\partial N}{\partial \mu} = \frac{\partial N}{\partial x} \left(\frac{\partial \mu}{\partial x} \right)^{-1}$, allowing experimental determination of T . This has been measured for Fermi gases in harmonic potentials [173, 174], and proposed as a thermometry method for lattice systems shortly after [175]. Since then, this idea has been adapted in many experiments [176, 177, 178, 179].

Chapter 8

Conclusion and outlook

In this thesis, we described the construction and working principles of an apparatus capable of producing degenerate quantum gases of Rb and ^{40}K . The degenerate gases are then loaded into hexagonal superlattices with tunable geometries for quantum simulation. While a major goal of the optical kagome lattice experiment is to study many-body correlated phases in the presence of interactions, in this thesis we have focused on the characterization of quantum geometry of band structures using noninteracting particles. The measurement techniques presented in this thesis are transferrable not only to other optical lattice experiments, but potentially also to other spatially periodic systems as well, in particular solid state systems. We also theoretically investigated the thermodynamics of systems with flat bands, which is a potentially impactful direction for future experiments.

In the remaining sections, I would like to briefly discuss possible research directions that extend the findings presented in this thesis. I would also like to discuss the motivation for implementing a high resolution imaging system, which has not been installed at the time of writing. I will refer the reader to John Ciavarras's undergraduate thesis [180] for the characterization of the objective and the generation of arbitrary optical potential using a digital micromirror device. The task of installing the objective will be handed to the steady hands of the next generation of graduate students, Erin Moloney and Ke Lin.

8.1 Optical excitations

Chapter 6 established the fundamental relation between interband quantum geometry and optical excitations, and how this relation can be explored in optical lattice experiments. The flexibility of our lattice setup allows us to investigate how the geometrical structure of Bloch bands is modified by break different symmetries. For example, we can break the C_6 rotational symmetry of the kagome lattice by imbalancing one of the 532 nm lattice beam, which results in the Lieb-kagome lattice briefly discussed in Sec. 3.4.2. The QBTP between the flat band and the dispersive band is broken into two LBTP along the remaining mirror symmetry axis, and the orientations of the plane in which the fictitious field lies rotate

in different ways for the two LBTP [131]. It should be in principle possible to track the evolution in band geometry using the optical excitation technique.

We point out an interesting opportunity to study nonlinear optics in a quasimomentum-resolved way. Honeycomb lattice is inversion symmetric, which is why we measured a real Berry connection field (see Ref. [50]). Based on basic nonlinear optics arguments, we do not expect second order nonlinear optical responses [181]. However, given the quasimomentum resolution in our measurement scheme, we can consider what is the expected response of a Bloch state at a particular quasimomentum $\mathbf{q}$. For simplicity, we only consider three of the Bloch bands (say, $n = \{1, 2, 3\}$), so we are effectively studying a three-level system. We will denote the modulation frequencies that are near-resonant between band 1 and 2 (2 and 3) as f_{12} and f_{23} , and assume that they are only near-resonant between those bands.

Within this model, we argue that it must be possible to drive population transfer from band 1 to 3, as long as the magnitudes of $\mathbf{A}_{12}(\mathbf{q})$ and $\mathbf{A}_{23}(\mathbf{q})$ don't vanish. For example, we can align the polarizations ϵ_{12} and ϵ_{23} to the direction of the connection field, since we have individual control over the polarizations. The observation of population transfer to $n = 3$ represents a sum-frequency generation second order process. To reconcile this with the fact that there is no second order nonlinear optical responses in an inversion symmetric material, it must be the case that the contribution from the nonlinear excitation at $-\mathbf{q}$ cancels that of $\mathbf{q}$. We can contrast the measurement results to that of a lattice with broken inversion symmetry, where there is indeed an overall second order response after summing over contributions from all quasimomentum states.

8.2 High resolution imaging system

The ability to resolve observables on single lattice sites is a significant technical breakthrough in optical lattice experiments [182]. These devices, known as quantum gas microscopes, directly access observables such as the correlation functions between any lattice sites, which allows direct comparison with theoretical results. On the other hand, the ability to image with single-site resolution also implies the ability to address individual sites optically. This is done by projecting programmed optical intensity patterns using a spatial light modulator, such as digital micromirror devices.

The ability to generate arbitrary, high resolution potential is actually the main motivation for us to install a high numerical aperture (NA) objective. We have discussed in the introduction that different strongly correlated phases have been predicted for various filling factors in kagome lattices. It is then deeply problematic that the external trapping confinement prohibits us from fine-tuning the Fermi energy to a particular filling, especially to the narrow flat band. To work around this, we will need to be able to shape the optical potential such that the local Fermi energy is uniform throughout the system. This ability is also an enabling ingredient for the flat band thermodynamics experiment proposed in chapter 7.

Achieving such resolution requires a combination of well-engineered optical imaging system, and for imaging, a measurement scheme that collects enough information from trapped

atoms without degrading the sample during measurement (for example, due to heating during imaging). A large part of the engineering challenge is now handed to the industry, where companies such as Special Optics design and produce high-NA objectives customized to the needs of each experiment. Of course, there are still many difficult tasks for the experimentalists, including mounting and integration into the experiment, and adjusting the alignment using images of atoms. In this section, we briefly discuss the design considerations and performance goals of the objective.

Custom objective

The objective lens in our current setup is an achromatic doublet (Thorlabs, AC508-150-B) with a small NA of around 0.16. For the D2 line of potassium, this gives a diffraction limited resolution of $0.61\lambda/\text{NA} = 2.8\text{ }\mu\text{m}$ based on Rayleigh's criterion. The imaging resolution is further limited by the combination of the small magnification ($2.2\times$) and large pixel size ($8.3\text{ }\mu\text{m}$) to $3.7\text{ }\mu\text{m}$. This is much larger than the lattice spacing in kagome lattices, $a_{\text{kag}} = 355\text{ nm}$.

In principle, a larger NA would both increase the collection efficiency of photons, and lower the diffraction limit. In our system, there are a few mechanical constraints on the design of the objective:

- Assuming that the atoms are trapped at the center of the glass cell, the distance from the atoms to the exterior surface of the glass cell is (10.2 mm vacuum) + (4 mm fused silica), which places a lower bound on the working distance of the objective. This can in principle be adjusted slightly using a top-down bias field to shift the trap center of the magnetic trap, but displacements of more than one or two mm would require a new vertical transport scheme.
- The Feshbach coil limits the radius of the objective housing to 22.5 mm, and the extended magnetic transport coil mount further restricts the radius to be 20 mm at 60 mm away from the atoms.

Aiming for a diffraction limit that matches the lattice spacing is impractical, since it would require an NA of around 1.32. This is not a necessary condition for single-site resolution; in fact, in most of the existing quantum gas microscope experiments, the ratio between the diffraction limited resolution and the lattice spacing is larger than 1.5. It has also been demonstrated that the lattice site occupancy can be reconstructed with high fidelity when this ratio is as large as 2.2 using machine learning [183]. Therefore, we simply aim for the largest NA achievable with the physical constraints, with the following requirements:

- The objective should achieve diffraction limited performance within wavelengths ranging from 767 to 780 nm (imaging wavelengths of ^{40}K and Rb), and at 638 nm (DMD potential).

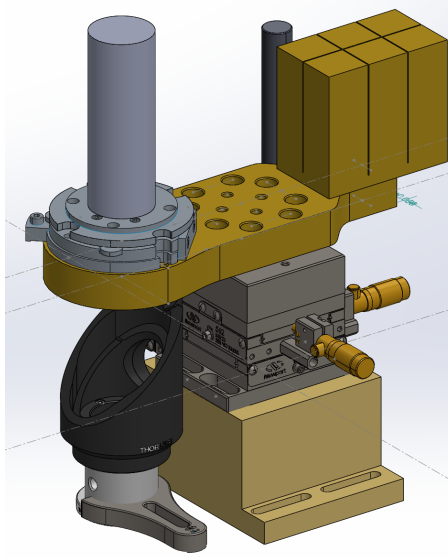


Figure 8.1: CAD rendering of the mechanical mounting design for the objective (represented by the gray cylinder). The brass block on the opposite end of the mount represents a counterweight. Translation stage: Newport 562-XYZ-LH. Tip-tilt stage: Newport TTN80. DC servo actuator (only for the vertical axis): TRB12CC.

- The front surface of the objective should be coated for high reflection at the wavelength 1064 nm for the vertical lattice, and the coating must withstand continuous illumination of a > 3 W 1064 nm Gaussian beam with a waist of 100 μm .
- The field of view should be at least comparable to the beam waist of our trapping beams, which is around 100 μm .

Given the above specification, Special Optics was able to design and manufacture an objective with an NA of 0.6. The resulting diffraction limited resolution on ^{40}K D2 line is 780 nm, or $2.2a_{\text{hc}}$, which gives us hope that with a proper cooling scheme and image postprocessing, we would be able to reach single-site resolution. This objective will be mounted on a custom-built mount shown in Fig. 8.1.

Appendix A

Derivation of the optical lattice potential

We will make use of the spherical basis vectors, given by

$$\begin{aligned}\boldsymbol{\sigma}^+ &= -(\mathbf{x} + i\mathbf{y})/\sqrt{2} \\ \boldsymbol{\pi} &= \mathbf{z} \\ \boldsymbol{\sigma}^- &= (\mathbf{x} - i\mathbf{y})/\sqrt{2}\end{aligned}, \quad (\text{A.1})$$

where the notation is suggestive of taking the polarization axis to be $\mathbf{z}$. The radial unit vector $\boldsymbol{\rho}(\theta)$ can be decomposed in the spherical basis as follows:

$$\boldsymbol{\rho}(\theta) \equiv \cos \theta \mathbf{x} + \sin \theta \mathbf{y} = \frac{-e^{-i\theta}\boldsymbol{\sigma}^+ + e^{i\theta}\boldsymbol{\sigma}^-}{\sqrt{2}}, \quad (\text{A.2})$$

so the polarization vectors are

$$\boldsymbol{\epsilon}_1 = \boldsymbol{\rho}(-\frac{2}{3}\pi), \quad \boldsymbol{\epsilon}_2 = \boldsymbol{\rho}(0), \quad \boldsymbol{\epsilon}_3 = \boldsymbol{\rho}(\frac{2}{3}\pi). \quad (\text{A.3})$$

Now, we copy the expression for optical intensity, Eqn. (A.4):

$$I(\mathbf{r}) = I_0 |r_1 e^{i(\mathbf{k}_1 \cdot \mathbf{r} + \phi_1)} \boldsymbol{\epsilon}_1 + e^{i\mathbf{k}_2 \cdot \mathbf{r}} \boldsymbol{\epsilon}_2 + r_3 e^{i(\mathbf{k}_3 \cdot \mathbf{r} + \phi_3)} \boldsymbol{\epsilon}_3|^2, \quad (\text{A.4})$$

This can be simplified by decomposing each polarization vector in the spherical basis vectors. Using Eqn. (A.2) and $\boldsymbol{\sigma}^+ \cdot \boldsymbol{\sigma}^- = 0$, we can rewrite Eqn. (A.4) as

$$\begin{aligned}I(\mathbf{r}) &= I_0 \left| - (r_1 e^{i(\mathbf{k}_1 \cdot \mathbf{r} + \phi_1 + \frac{2}{3}\pi)} + e^{i\mathbf{k}_2 \cdot \mathbf{r}} + r_3 e^{i(\mathbf{k}_3 \cdot \mathbf{r} + \phi_3) - \frac{2}{3}\pi}) \boldsymbol{\sigma}^+ \right. \\ &\quad \left. + (r_1 e^{i(\mathbf{k}_1 \cdot \mathbf{r} + \phi_1 - \frac{2}{3}\pi)} + e^{i\mathbf{k}_2 \cdot \mathbf{r}} + r_3 e^{i(\mathbf{k}_3 \cdot \mathbf{r} + \phi_3) + \frac{2}{3}\pi}) \boldsymbol{\sigma}^- \right|^2 / 2 \\ &= I_0 \ell_+(\mathbf{r}) + I_0 \ell_-(\mathbf{r}),\end{aligned}$$

where

$$\ell_{\pm}(\mathbf{r}) = \frac{1}{2} \left| r_1 e^{i(\mathbf{k}_1 \cdot \mathbf{r} + \phi_1 \pm \frac{2}{3}\pi)} + e^{i\mathbf{k}_2 \cdot \mathbf{r}} + r_3 e^{i(\mathbf{k}_3 \cdot \mathbf{r} + \phi_3 \mp \frac{2}{3}\pi)} \right|^2 \quad (\text{A.5})$$

for σ^+ and σ^- polarizations, respectively.

Using

$$\begin{aligned} & |Ae^{\alpha i} + Be^{\beta i} + Ce^{\gamma i}|^2 \\ &= A^2 + B^2 + C^2 + 2AB \cos(\alpha - \beta) + 2BC \cos(\beta - \gamma) + 2AC \cos(\gamma - \alpha), \end{aligned} \quad (\text{A.6})$$

we can simplify Eq. (A.5) to find

$$\begin{aligned} \ell_{\pm}(\mathbf{r}) &= \frac{c_0}{2} + r_1 \cos(\mathbf{g}_3 \cdot \mathbf{r} + \phi_1 \pm \frac{2}{3}\pi) \\ &\quad + r_3 \cos(\mathbf{g}_1 \cdot \mathbf{r} - \phi_3 \pm \frac{2}{3}\pi) \\ &\quad + r_1 r_3 \cos(\mathbf{g}_2 \cdot \mathbf{r} + \phi_3 - \phi_1 \pm \frac{2}{3}\pi) \end{aligned} \quad (\text{A.7})$$

where $c_0 = r_1^2 + 1 + r_3^2$.

When only the scalar polarizability is considered, we can directly sum the contribution from ℓ_+ and ℓ_- . Using $\cos(A + 2\pi/3) + \cos(A - 2\pi/3) = -\cos A$, we finally arrive at

$$I_S(\mathbf{r}) = I_0 [c_0 - r_1 \cos(\mathbf{g}_3 \cdot \mathbf{r} + \phi_1) - r_3 \cos(\mathbf{g}_1 \cdot \mathbf{r} - \phi_3) - r_1 r_3 \cos(\mathbf{g}_2 \cdot \mathbf{r} + \phi_3 - \phi_1)]. \quad (\text{A.8})$$

One realizes that this is the sum of three 1-D lattices, which can be understood by observing that the 1-D lattice formed by beams i and j only has contribution from the polarization component in the direction of propagation of beam k (i.e. $\mathbf{G}_k \parallel \epsilon_k$), so beam k doesn't interfere with the beam- ij 1-D lattice.

On the other hand, the polarization dependence in Eqn. (3.5) means that atoms also see a m_F -dependent potential given by

$$\begin{aligned} I_A &\propto I_0(\ell_+(\mathbf{r}) - \ell_-(\mathbf{r})) \\ &= -a_{m_F} I_0 [r_1 \sin(\mathbf{g}_3 \cdot \mathbf{r} + \phi_1) + r_3 \sin(\mathbf{g}_1 \cdot \mathbf{r} - \phi_3) + r_1 r_3 \sin(\mathbf{g}_2 \cdot \mathbf{r} + \phi_3 - \phi_1)] \end{aligned} \quad (\text{A.9})$$

using $\cos(A + 2\pi/3) - \cos(A - 2\pi/3) = -\sqrt{3} \sin A$. Here, $a_{m_F} = \frac{\sqrt{3}\pi c^2}{\omega_0^3} \frac{\Gamma \Delta'_{\text{FS}}}{\Delta^2} g_F m_F$.

Appendix B

Supplemental information for chapter 7

B.1 Exact form of the band shifting Hamiltonian

In its full glory, we have

$$\begin{aligned}
H' &= H'_{AA} + H'_{BB} + H'_{AB} \\
H'_{AA} &= \frac{V_{shift}}{2\pi\sqrt{3}} \sum_x \left[\hat{a}_x^\dagger \hat{a}_x + \sum_{y>0} z_+^y \hat{a}_x^\dagger \hat{a}_{x+y} + \text{h.c.} \right] \\
H'_{BB} &= \frac{V_{shift}}{2\pi} \sum_x \left[\left(1 - \frac{1}{\sqrt{3}}\right) \hat{b}_x^\dagger \hat{b}_x - \frac{1}{\sqrt{3}} \sum_{y>0} z_+^y \hat{b}_x^\dagger \hat{b}_{x+y} + \text{h.c.} \right] \\
H'_{AB} \left(\frac{t'}{t} = \pm\sqrt{2} \right) &= \mp \frac{V_{shift}}{2\pi\sqrt{6}} \sum_x \left[(1 + z_+) \hat{a}_x^\dagger \hat{b}_x + \text{h.c.} \right] \\
&\quad \mp \frac{V_{shift}}{2\pi\sqrt{6}} \sum_x \sum_{y>0} \left[z_+^y (1 + z_+) \hat{a}_x^\dagger \hat{b}_{x+y} + \text{h.c.} \right] \\
&\quad \pm \frac{V_{shift}}{2\pi\sqrt{6}} \sum_x \sum_{y>0} \left[z_+^y (1 + z_+^{-1}) \hat{b}_x \hat{a}_{x+y}^\dagger + \text{h.c.} \right] \\
z_+ &= -2 + \sqrt{3}.
\end{aligned} \tag{B.1}$$

B.2 Extended plots for results in Sec. 7.2.5

In the plots below, the “filling factor in reservoir flat band” is given by the Fermi-Dirac distribution, $n_{f,R} = f(E = 0; \mu)$. There is a flat band at $E = 0$ only in the noninteracting case (orange lines).

$n = 0.45$, very high entropy ($N_{tot} = 90$, $S_{tot} = 52$)

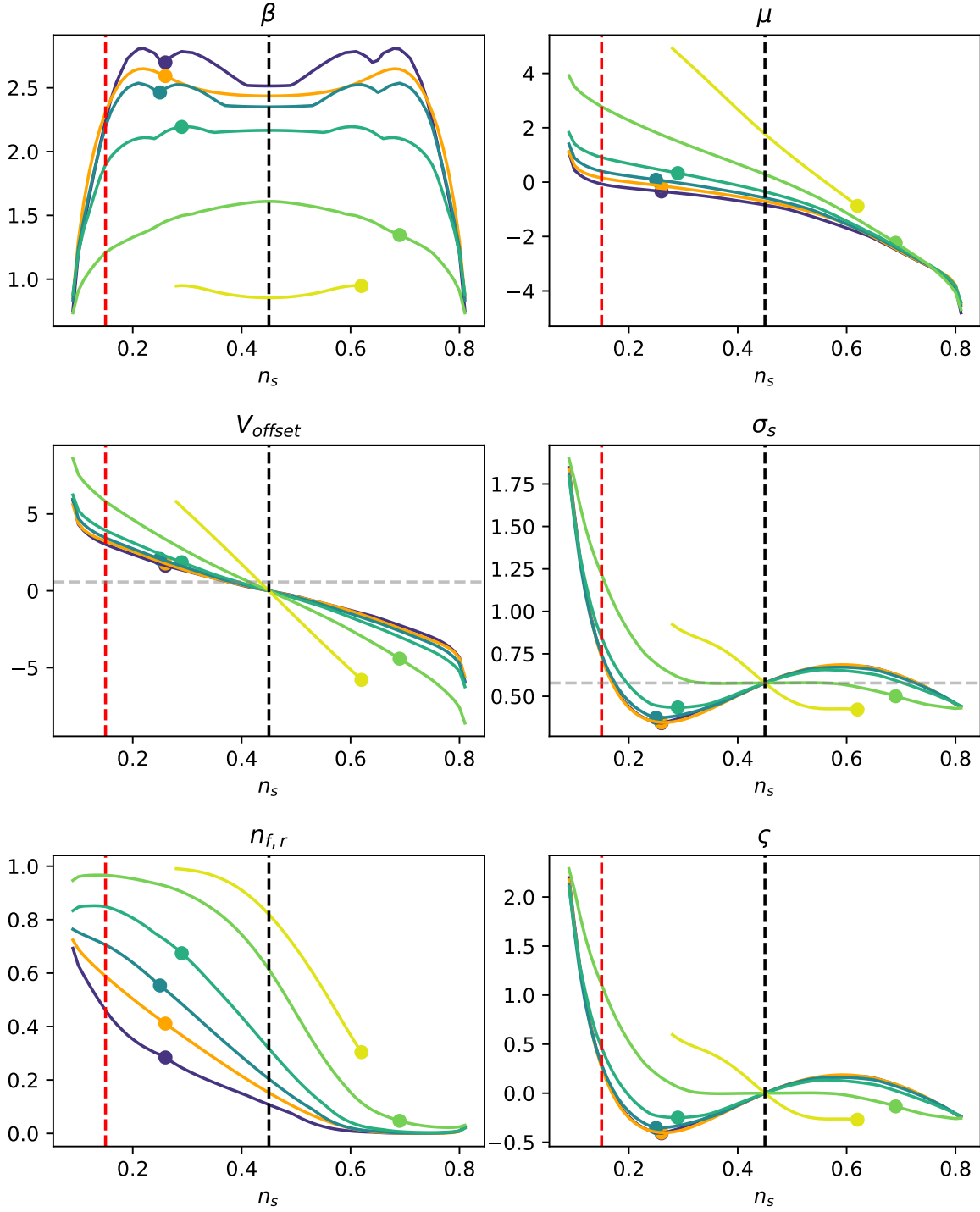


Figure B.1: Small density ($n = 0.45$), too much entropy.

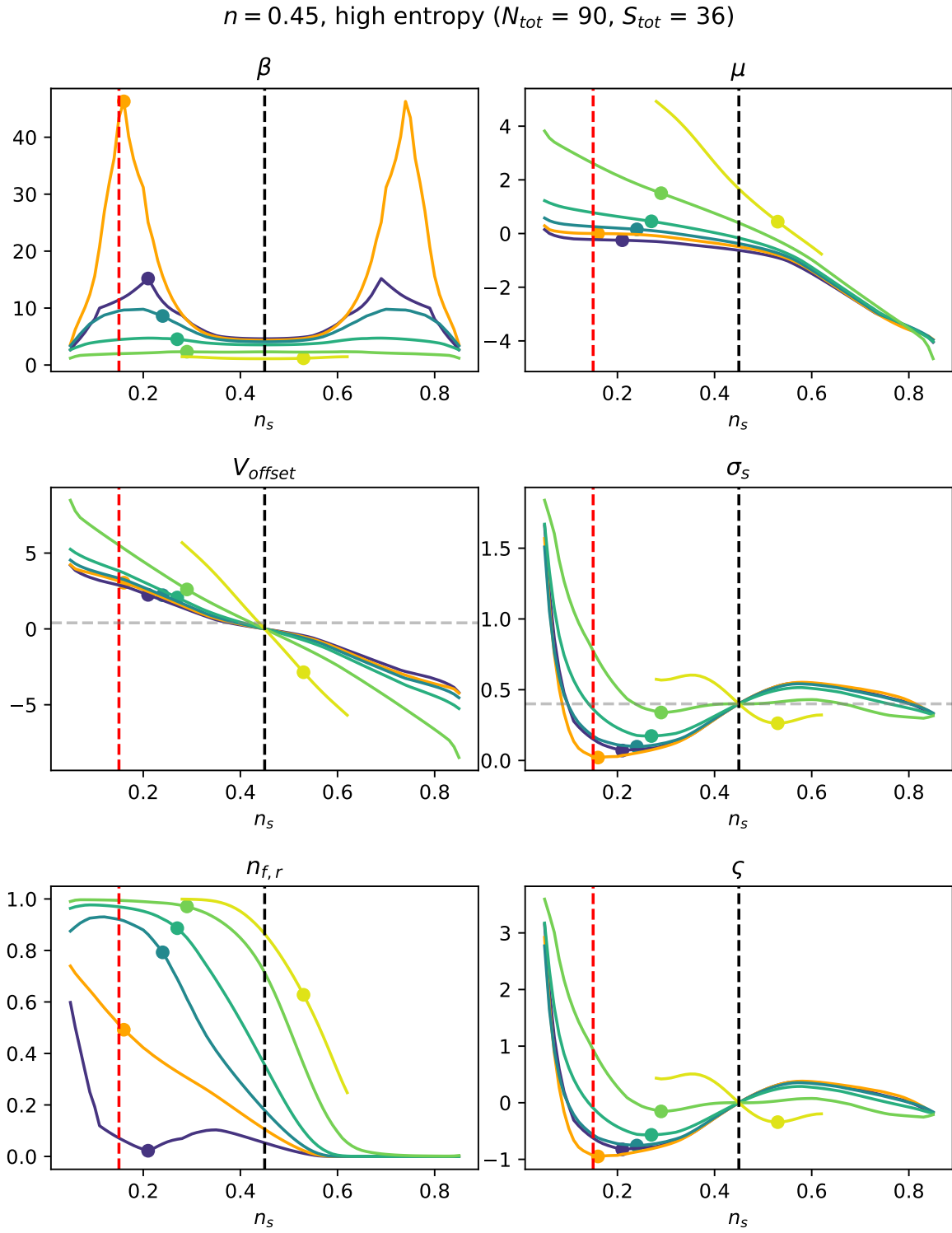


Figure B.2: Small density ($n = 0.45$), just too much entropy.

$n = 0.45$, low entropy ($N_{tot} = 90$, $S_{tot} = 30$)

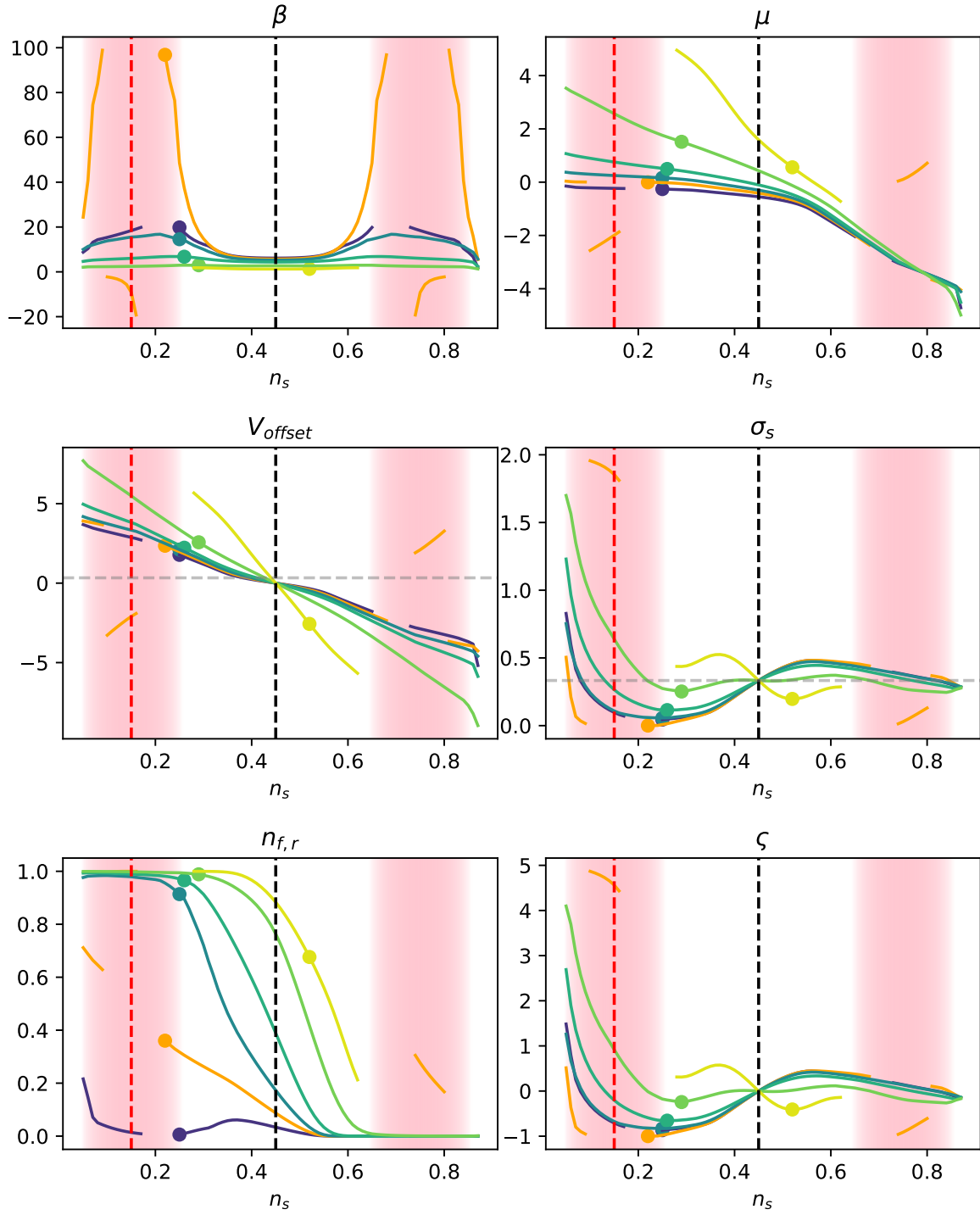


Figure B.3: Small density ($n = 0.45$), too little entropy.

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