Probing Long Range Antiferromagnetism and Dynamics in the Fermi-Hubbard Model

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Probing Long Range Antiferromagnetism and Dynamics in the Fermi-Hubbard Model

A dissertation presented
by
Anton Mazurenko
to
the Department of Physics
in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the subject of
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Probing Long Range Antiferromagnetism and Dynamics in the Fermi-Hubbard Model

Abstract

Exotic phenomena in strongly correlated electron systems emerge from the interplay between spin and motional degrees of freedom. For example, doping an antiferromagnet is expected to give rise to pseudogap states and high-temperature superconductors. Quantum simulation with ultracold fermions in optical lattices offers the potential to answer open questions about the doped Hubbard Hamiltonian, and has recently been advanced by quantum gas microscopy. In order to take advantage of these possibilities, a stable, high-power, 2D square lattice system was developed and coupled with an image plane based spatial light modulator. The ability to finely tune the atomic potential has made it possible to realize an antiferromagnet in a repulsively interacting Fermi gas on a 2D square lattice. At our lowest temperatures of $T/t = 0.25(2)$, antiferromagnetic long-range order (LRO) manifests through the divergence of the correlation length that reaches the size of the system, the development of a peak in the spin structure factor and a value of the staggered magnetization approaching the ground state value. Similarly, by carefully shaping the confinement, we have produced ultra-low entropy band insulators, which promise to be a perfect starting point for more advanced cooling schemes. In addition to the production of new states, Fermi gas microscopy is superbly well suited to studies of many-body dynamics. To this end I report on preliminary measurements of the propagation of holes in a Mott insulator. These results demonstrate that Fermi gas microscopy can address open questions on the low-temperature Hubbard model.
## Contents

Abstract ..................................................... iii  
List of Tables ................................................ vii  
List of Figures ............................................... viii  
Acknowledgements .............................................. xv  
Dedication ....................................................... xviii  

0 Introduction .................................................. 1  
0.1 Code availability .......................................... 3  
0.2 Copyright acknowledgements ................................ 3  
0.3 Bibliography ................................................ 4  

1 Introduction to the Fermi-Hubbard model with cold atoms .... 5  
1.1 Introduction ................................................ 6  
1.2 Atomic physics .............................................. 8  
1.2.1 Atomic structure of $^6$Li ................................ 8  
1.2.2 Feshbach resonances ...................................... 10  
1.3 Optical lattice fundamentals ................................ 10  
1.4 Band structure ............................................. 13  
1.4.1 Solving the Mathieu equation ............................. 13  
1.4.2 Band structure and quasimomentum ....................... 15  
1.4.3 Wannier functions and the tight binding model ......... 18  
1.5 The Fermi-Hubbard model .................................... 18  
1.6 Phase diagram .............................................. 20  
1.7 Analytic techniques ......................................... 22  
1.7.1 High temperature series expansion (HTSE) ............... 22  
1.7.2 Non-interacting fermions ................................ 23  
1.7.3 Heisenberg model ....................................... 27  
1.7.4 Characterizing antiferromagnetic order ................... 30  
1.7.5 Dimensionality and spin systems ......................... 31  
1.8 Numerical analysis using exact diagonalization .............. 36  
1.8.1 Magnetism in small systems ............................. 38  
1.9 Bibliography ............................................... 45  

2 A history of quantum gas microscopy .......................... 52  
2.1 Introduction ................................................ 53  
2.2 Fermi gas microscopy ....................................... 55
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Conclusion</td>
<td>2.3</td>
<td>58</td>
</tr>
<tr>
<td>2</td>
<td>Bibliography</td>
<td>2.4</td>
<td>59</td>
</tr>
<tr>
<td>3</td>
<td>A high power, low noise optical lattice</td>
<td>3.1 Introduction</td>
<td>66</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.2 Relative intensity noise (RIN)</td>
<td>65</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.2.1 Parametric heating</td>
<td>67</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.3 Low noise seed laser</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4 High power laser system</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4.1 Fiber amplifier system</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4.2 Mode and beam shaping</td>
<td>71</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4.3 High power feedback</td>
<td>74</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4.4 Low power feedback</td>
<td>77</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.4.5 Heating rates</td>
<td>89</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.5 Beam monitoring and alignment</td>
<td>89</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.6 Long-term stability of the lattice structure</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.7 Affine transformations</td>
<td>96</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.8 Bibliography</td>
<td>98</td>
</tr>
<tr>
<td>4</td>
<td>Imaging a spatial light modulator</td>
<td>4.1 Introduction</td>
<td>101</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.2 Digital micro-mirror device fundamentals</td>
<td>102</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.2.1 DMD in the image plane</td>
<td>102</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.2.2 DMD’s in the Fourier plane, an aside</td>
<td>105</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.3 Experimental assembly</td>
<td>106</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.3.1 Light source</td>
<td>106</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.3.2 Digital micro-mirror device optical assembly</td>
<td>107</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.3.3 Why two DMD’s?</td>
<td>111</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.4 DMD Imaging</td>
<td>112</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.4.1 Light coherence</td>
<td>112</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.4.2 Error diffusion</td>
<td>113</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.4.3 The DMD, the camera and the lattice</td>
<td>118</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.5 Using a DMD in a cold-atom experiment</td>
<td>119</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.5.1 DMD communications via USB an HDMI</td>
<td>119</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.5.2 Suppressing switching noise</td>
<td>121</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.6 Manipulating single atoms</td>
<td>124</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.7 Conclusion</td>
<td>124</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.8 Bibliography</td>
<td>125</td>
</tr>
<tr>
<td>5</td>
<td>Antiferromagnetism in the Hubbard Model</td>
<td>5.0 Chapter origin</td>
<td>129</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.1 Introduction</td>
<td>129</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.2 Detecting antiferromagnetism</td>
<td>130</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.3 Cooling via entropy redistribution</td>
<td>132</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.3.1 State preparation</td>
<td>134</td>
</tr>
</tbody>
</table>
List of Tables

3.1 Conversions of common decibel measurements to the most widely used dBm/Hz, $R_{\text{source}}$ is the impedance of the signal source (typically 50Ω) and $R_{\text{sink}}$ is the resistance of the measurement device (typically either (typically 50Ω or $\infty$)) ......................... 67
List of Figures

1.1 Examples of cellular automata showing both ordered and chaotic emergent behavior [93]. .................................................. 6
1.2 Level structure of the $^{2}\text{Li}_{1/2}$ ground state of $^{6}\text{Li}$ as a function of magnetic field [23]. ........................................... 8
1.3 Feshbach resonances of the lowest three hyperfine states of fermionic lithium [91]. ............................................................. 9
1.4 Depth distribution of a typical 1D optical lattice. The focus is chosen to be a few wavelengths, to illustrate divergence due to the underlying Gaussian beam. ........................................... 12
1.5 Spectrum of the sinusoidal optical lattice. Characteristic solutions to the Mathieu equation, known as $a, b$ are plotted for a variety of lattice depths. .................................................. 14
1.6 Dispersion relations for sinusoidal lattices at different lattice depths. 17
1.7 A cartoon view of the phase diagram of the half filled Hubbard model at low temperature. Reproduced from [62] ....................... 22
1.8 HTSE model predictions at different interactions $U/t = .1$ (top row), $U/t = 1$ (middle row), $U/t = 10$ (bottom row). ......................... 24
1.9 Non-interacting fermion model compared with the high-temperature series expansion. .................................................. 28
1.10 Anderson tower of states computed for a 4 × 3 system. .......... 30
1.11 Dimension of the Hilbert space in the Hubbard model with $S$ = 1/2 particles. ............................................................. 38
1.12 Diagonalization of $2 \times 1$ sites at half filling, filled with an even spin mixture. .................................................. 40
1.13 Diagonalization of $2 \times 2$ sites at half filling, filled with an even spin mixture. .................................................. 41
1.14 Diagonalization of $3 \times 3$ sites at half filling, filled with a 5 : 4 spin mixture. .................................................. 42

2.1 Initial demonstration of single site imaging. Reproduced from [28]. 56
2.2 Fermionic metal-Mott insulator transition. (A) experimental images of the atoms in a lattice at varying $U$. (B) Density profiles for the experimental parameters in (A), showing Mott-insulators, band-insulators, and metals. (C) Radial profiles of occupation and variance fit, with an HTSE model. Reproduced from [11]. ....................... 57
3.1 **High level overview** showing the major components of the lattice laser feedback system. ............................................. 65

3.2 **Laser noise of the lattice system.** (a) Shows the laser noise of unmodified Nufern fiber amplifiers and the Mephisto seed. (b) Shows the open (OL) and closed (CL) loop behavior of the high power feedback loop. (c) Shows open loop behavior of the low power feedback loop after making the modifications. (d) Closed loop behavior of the loop system without additional filtering, measured on the same setup as (c). .................................................. 72

3.3 **Optical layout of the optical lattice system for beam shaping and modulation.** ................................................................. 73

3.4 **Berek compensator** performance as a function of the Berek tilt angle $\phi$ and waveplate tilt angles. .................................... 76

3.5 **Berek compensator based feedback loop** performance showing the impulse response (a) at relatively low powers and the corresponding Bode plots (b-c). .................................................. 77

3.6 **Feedback circuits.** (a) The reverse-biased photodiode. (b) Externally referenced phase-locked loop. (c) Nonlinear loop filter. (d) RF power modulation using a mixer. ........................................... 78

3.7 **PLL performance** (a) The spectrum of the PLL, exhibiting phase noise of better than $-90$ dBc 100 kHz away from the carrier. (b) The RIN of the local oscillator based on the PLL. The noise level is seen to be at or below the noise floor of the measurement device. .... 81

3.8 **Photodiode photo** showing that the “can” of the photodiode has been cut, to prevent etalon-like behavior. ................................. 82

3.9 **Relative intensity noise of the digital to analog converter** at a fixed output voltage and while changing values. To measure the transient RIN, a 20 ms, triangle wave with a DC offset and modulation depth of 15% of the DC offset was produced by the device. The triangle wave accounts for the series of spurs at low frequencies that fall with increasing frequencies. At frequencies above approximately 4 kHz, the spectrum is dominated by noise due to transient “glitches” that emerge when the device changes its output state. ............... 83

3.10 **Loop bandwidth dependence on the set-point.** (a) shows the 3 dB and $\pi$ phase shift points for the X lattice (also known internally as the “northeast” lattice. (b) shows the same for the Y lattice, known as the “northwest”. ........................................... 85

3.11 **Laser noise of the lattice system with and without additional low pass filters** (a) Closed loop laser made a fiber amplifier (different than the one in figure 3.2. (b) Noise on the same system as (a), but with extra filters. ................................................................. 88

3.12 **Heating Rates for various lattice depths.** Reproduced from [4]. .... 89
3.13 **Averaged images of Mott insulators.** A series of Mott insulators was created over the course of approximately one hour, and the average image is shown\[7\]. If the lattice fluctuated across more than a small fraction of a lattice site, the modulation contrast would be quickly washed out. The absence of this effect means that the phase of the optical lattice is very stable.  

3.14 **Short term positional stability.** (a) A histogram of shot-to-shot step sizes along the transverse and longitudinal directions, with a Gaussian fit. (b) Correlations between the step size of subsequent shots. (c) Calibration data for the “affine fit” of the conversion from camera pixels to lattice dimensions. (d) Predicted location versus measured location along the transverse and longitudinal directions. (e,f) The measured position and predicted position of the atomic cloud.  

3.15 **Long term positional stability over approximately nine months.**  

4.1 **Satisfying the blazing condition.** (a) Depicts the DMD architecture of pivoting mirrors, in the orientation used in the experiment. (b) Multiple diffraction orders are shown emerging from the mirror for an incoming beam at a given incidence due to grating structure. (c) The grey and black lines show diffractive order angles for a given incidence angle. The red line shows the specular reflection. The blazing condition is satisfied at the only unique solution corresponding to angles $(\theta_i, \theta_m) = (-41.2^\circ, 17.2^\circ)$, since the other solution is the same up to a negative sign.  

4.2 **DMD illumination light source.** (a) The layout of the optics on the laser preparation tables. (b) The spectral power density of the source (solid) and a Gaussian fit (dashed).  

4.3 **DMD mechanical assembly** optics layout used for illumination of the DMD and projection into the imaging system.  

4.4 **Texas Instruments LC6500 DMD** mounted on custom supports and a monolithic, stable flexure mount.  

4.5 **Advantages of using two DMD’s** in the image plane (a) increased coverage of the image plane (b) schematic drawing of the ramp sequence yielding adiabatic transformation of potentials.  

4.6 **Fourier optics treatment of imaging a DMD.** (a-d) Show the initial and final light fields after passing through a diffraction limited imaging system. The energy distribution, as well as the filter (white circle), are shown in the last row.  

4.7 **Intensity at the center of the light fields shown in figure4.6.** The coherent nature of the light results in ringing behavior which can locally increase the local light intensity.
4.8 A demonstration of different types of image binarization. (a) Original demo image, “camera” from [28]. The range is fixed from 0 (black) to 1 (white). (b) Threshold at 0.5 applied to the original image. (c) Threshold applied at 0.5 + δ, where δ is drawn from a 0 mean normal distribution with standard deviation σ = 0.3. (d) Randomized threshold as in (b), but with σ = 0.5. (e) Non-randomized Floyd-Steinberg error diffusion. (f) Randomized error diffusion with σ = 0.1. (g) Randomized error diffusion with σ = 0.3. (h) Randomized error diffusion with σ = 0.5.

4.9 Observation of DMD switching noise: (a) a simple experiment to measure the switching noise. (b) reflected power as a function of time, clearly showing the periodic switching behavior and its suppression.

4.10 Effects of DMD switching noise on atoms (a) atomic cloud prepared with the DMD without suppressing switching noise. (b) atomic cloud prepared while suppressing DMD switching noise.

4.11 Preparing atoms in specified configurations. Averaged images showing the selective reduction of occupation on specified lattice sites. (a) Atomic symbol of lithium. (b) A cartoon face (perhaps that of a tired graduate student?).

4.12 Preparing a line of holes. An averaged image of Mott insulators with a line of pairs of holes cut out. The probability of finding a hole on a given site of the cut-line is > 95%.

5.1 Detecting antiferromagnetism with a quantum gas microscope. Reproduced from [49].

5.2 Probing antiferromagnetism in the Hubbard model with a quantum gas microscope. a, Schematic view of the 2D Hubbard phase diagram, including predicted phases. This chapter explores the trajectories traced by the red arrows for a U/t = 7.2(2) Hubbard model. The strongest antiferromagnetic order is observed at the starred point. b, Experimental setup. We trap 6Li atoms in a 2D square optical lattice. We use the combined potential of the optical lattice and a DMD to trap the atoms in a central sample Ω of homogeneous density, surrounded by a dilute reservoir. c, Exemplary raw and processed images of the atomic distribution of single experimental realizations, with both spin components present (upper) and one spin component removed (lower). The observed checkerboard pattern in the spin-removed images indicates the presence of an antiferromagnet.

5.3 Raw images of the AFM states. a, an image of the antiferromagnet with no spin removal, clearly showing Ω, the region of interest, and the surrounding sparse reservoir. b, an image of the antiferromagnet with only the |↑⟩ remaining, showing the characteristic checkerboard pattern.
5.4 Amplitude of light fields applied to atoms a, The computed light field generated by the DMD, applied to the atoms for half-filled samples. A gradient compensates residual gradients in the lattice. The rim of the reservoir provides sharp walls for the inner subsystem. A broad, shallow paraboloid in the center flattens the potential when combined with the optical lattice. The cartoon shows a schematic view of a radial cut of the potential, including the contribution of the lattice. b, The amplitude of the light field with an offset in the center of the trap, used to dope the system with a finite population of holes.

5.5 Average density profile in the system. a, The average singles density map for a sample at half-filling shows a central region of uniform density, surrounded by a ring of low density. The dotted white circle indicates our system size, excluding edge effects. b, The azimuthal average of the singles density shown in a, for the system as well as the inner edge of the donut where the density drops off to the reservoir density. The vertical dotted lines denote the boundary of the system. c, Azimuthal average of singles densities for three values of the hole doping used in the experiment, indicating uniformity of atom number across our system to within 4%. The horizontal lines are at the system-wide average densities.

5.6 Observing antiferromagnetic long-range order. a, The spin correlator $C_d$ is plotted for different displacements $d$ ranging across the entire sample for five temperatures $T/t$. We record $>200$ images for each temperature. Correlations extend across the entire sample for the coldest temperatures, whereas for the hottest temperature only nearest-neighbor correlations remain. b, The sign-corrected correlation function $(-1)^d C_d$ is obtained through an azimuthal average. The exponential fits to the data ($d > 2$) are shown in blue, from which we determine the correlation length $\xi$, and the fit of the coldest sample is plotted in grey for comparison. c, The measured spin structure factor obtained from averaged Fourier transformations of single images. A peak at momentum $q_{\text{AFM}} = (\pi/a, \pi/a)$ signals the presence of an antiferromagnet. d, The measured correlation length $\xi$, fitted to equation (1.36), diverges exponentially as a function of temperature, and is comparable to the system size for the lowest temperature. The inset is a semi-logarithmic plot of the same quantity versus inverse temperature. e, The measured staggered magnetization $m_z$ increases drastically below temperatures $T/t \approx 0.4$. We find good agreement with quantum Monte Carlo calculations of the Hubbard model, shown in grey.
5.7 Comparison of staggered magnetizations obtained directly through single-spin images and from spin correlations. We calculate the staggered magnetization from images with one spin state removed. The staggered magnetization can also be calculated from the spin correlator, where the two are exactly equal in the limit of no noise and exactly one particle per site. Plotting these two quantities against each other, we find very good agreement with the line $y = x$ (dotted line), indicating that any error due to deviation from one particle per site is small.

5.8 Full-counting statistics of the staggered magnetization operator $\hat{m}_z$. a, Selected images with one spin component removed (checkerboard overlaid to guide the eye) show a large variation in ordering strength at the coldest temperature. This variation is a consequence of the SU(2) symmetry of the underlying Hamiltonian, which leads to different orientations of the staggered ordering vector relative to the measurement axis $z$, as shown schematically by the spin-vectors. b, Measured distributions of $\hat{m}_z$ are plotted at different temperatures. We find excellent agreement with quantum Monte Carlo simulations of the Heisenberg model with no free fitting parameters.

5.9 Alternative basis measurement. We optionally apply a $\pi/2$ or $\pi$ RF pulse prior to the spin removal pulse and correlation measurement. The sign-corrected spin correlation functions show an insensitivity to the presence and duration of this RF pulse, consistent with an SU(2) symmetry of the state.

5.10 Doping the antiferromagnet. a, We move horizontally in the phase diagram by doping the system with holes (inset), where $0.0 \lesssim \delta \lesssim 0.25$. The staggered magnetization $m^z_c$ settles at $\delta_c \approx 0.15$. b, The magnitude of the sign-corrected nearest-neighbor correlator decreases less rapidly with hole doping than correlators at larger distances. For large doping, only the nearest-neighbor correlator is appreciable, so this correlation is predominantly responsible for the non-zero staggered magnetization away from the antiferromagnetic phase. c, We show the spin structure factor, as in Fig. 2c, for each doping value.
5.11 Staggered magnetization obtained from spin correlations, with and without nearest-neighbor contribution included. To investigate the contributions to the staggered magnetization at high dopings, we consider the staggered magnetization calculated from the spin correlator. For all points shown, we omit the longest-range correlations, which have the greatest level of noise due to the low number of pairs of sites extending across the cloud. The red points shown also omit the nearest-neighbor correlations, essentially the only non-zero correlator outside of the AFM phase. In the high-doping regime, we see that the greatest contribution to the staggered magnetization is the nearest-neighbor correlation, followed by the noisy longest-range correlations. The value of the staggered magnetization without either of these contributions is plotted in red.

6.1 (a) Propagation of a particle performing a classical random walk. (b) Propagation of a particle performing a quantum random walk.

6.2 Simulating the propagation of a single hole on a 1D lattice. (a) Hole positions immediately upon release. (b) Hole positions approximately 3 tunneling times later. Note that the data is post-selected on having exactly one hole in each row.

6.3 Time resolved lattice filling, showing the propagation of a single hole. (a) Quantum walk on a shallow lattice. (b) Quantum walk on a deep lattice. The behavior is observed to be essentially identical, but on very different timescales.

6.4 Propagation of a pair of holes on a 1D lattice. (a) Hole positions immediately upon release. (b) Hole positions approximately 3 tunneling times later.

6.5 Joint probability distribution for finding the holes at some pair of locations, showing distinct anti-bunching.

6.6 Propagation of a single hole on a 2D lattice. (a) Hole position immediately upon release. (b) Hole positions approximately two tunneling times later.

6.7 Time resolved lattice filling, showing the propagation of a single hole in 2D. Note that this data is preliminary.

6.8 Band insulator cooled with entropy redistribution. Much like in the AFM case, a BI can be cooled using entropy redistribution. (a) A typical image of a single BI that lies within the central region of a redistribution potential, in exact analogy to chapter 5. (b) Averaging many lattice occupations allows the determination of the spatially resolved single particle occupation, shown here.

A.1 Deconvolved image, reproduced from [1]

B.1 Water cooling layout

B.2 Water cooling room
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1“T’ve just gotta stay one lesson ahead of the student.” - Marge Simpson, on teaching kids piano.
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Outside of lab, I would like to thank my friends for their help and support - (in no particular order), Matthew Rispoli & Melis Tekant, Sam Markson, Ivan Kozyryev, Juan Porras, Sebastian & Irina Blatt, Ahmed Omran, Geoffrey Ji, Robert Schittko, Daniel Greif and Florian Huber. I would also like to acknowledge my cat, Chloe - she may be “just a cat”, but in times of stress, she brought me a lot of joy. The greatest thanks, of course, goes to my family - Victor & Elena Mazurenko, Alexander Mazurenko, and my lovely girlfriend, Caitlin Millett. I am deeply grate-
ful for the support of these individuals, is the main thing that got me through the harder times in the lab.
Chapter 0

Introduction

“Begin at the beginning,” the King said gravely,
“and go on till you come to the end: then stop.”

- Lewis Carroll, Alice’s Adventures in Wonderland
The goal of this work is threefold:

1. To bring a non-specialist experimental physicist up to speed on the current state of the art regarding Fermi gas microscopy, both regarding the experiment and the basics of the relevant theory.

2. To describe useful technical aspects of the experiment that I hope will be useful to those doing related work.

3. To describe our experiments studying antiferromagnetic order in the Hubbard model and our preliminary experiments observing time dependent dynamics.

To this end, the work is organized in the following way.

- **Chapter 1:** Brief introduction to the relevant theory. I will describe the relevant theoretical techniques used throughout the paper, and hopefully give the reader some intuition for the work.

- **Chapter 2:** Survey of recent relevant experimental results. In the last few years there has been a self-reinforcing swarm of activity in this field. The goal of this chapter is to summarize the relevant results, and put them in the proper context.

- **Chapter 3:** Description of the high power lattice laser setup. Low temperatures require correspondingly low heating rates, and thus a quiet, high power laser is essential to the physics under consideration. This chapter enumerates some of the challenges and their solutions.

- **Chapter 4:** Description of the digital spatial light modulator used for precision engineering of optical potentials.
• **Chapter 5:** Experimental realization of an ordered antiferromagnet in the Hubbard model.

• **Chapter 6:** I consider the future of Fermi gas microscopy to be bright, and here I detail my arguments, based 50% on optimism and 50% on preliminary experiments.

### 0.1 Code availability

After all embargoes on the data contained in this thesis have been lifted, I will post this thesunder my GitHub page (username: mazurenko) as the repository “AntonMazurenkoPhDThesis”. This repository will contain:

1. \LaTeX{} code to generate the thesis.

2. Python code to generate most figures.

3. Python code to perform some of the self-contained theoretical analysis, particularly from chapter one.

### 0.2 Copyright acknowledgements

Parts of this thesis are heavily based on (including some verbatim passages in chapter 5) papers that I have been an author on. I have cited these instances in every case, but am taking this opportunity to especially warn the reader about chapters two [2, 5, 6], three [1], four [3] and five [4, 5].

Further, I would like to thank Mary Wahl, who very kindly provided the template for the thesis and Mark Senn, the maintainer of this template at Purdue University.
0.3 Bibliography


Chapter 1

Introduction to the Fermi-Hubbard model with cold atoms

“Don’t panic.”

- Douglas Adams, The Hitchhiker’s Guide to the Galaxy
Figure 1.1: **Examples of cellular automata** showing both ordered and chaotic emergent behavior [93].

### 1.1 Introduction

The modern physics community has a solid grasp of microscopic laws in a wide array of conditions, barring well known extremes [92]. Despite this knowledge, collective systems of many particles can still exhibit behavior that defies simple explanation - or, according to Anderson, “More is different” [2]. Predicting emergent phenomena from underlying causes is complicated for two reasons - the underlying physics can be insufficiently well known, and exceedingly complex behavior can come from even the simplest laws, such as in the case of 1D cellular automata (shown in figure 1.1) [93], fractal geometries [60], among many others [43, 44].

As such, making sense of observations in condensed matter systems turns out to be a difficult task indeed:
1. The governing Hamiltonian contains many terms interacting over a variety of ranges [11].

2. Interesting phenomena, such as high temperature superconductivity [20, 52, 94], incommensurate ordering [79], colossal magneto-resistance [20] and others [3, 24, 50, 53, 74, 77], can emerge from the interplay of many parts of the Hamiltonian, and with experimental signatures that are not always obvious.

3. Despite rapid progress [1, 5, 18, 53], condensed matter systems still limit the experimentalist to those materials that can be produced in the lab - one cannot set fundamental lattice parameters or interactions to see what might happen.

Two of these challenges are especially relevant for the present work - the condensed matter Hamiltonian and the experimental limitations of condensed matter systems. Loosely speaking, a system of electrons ($e^-$) in a crystalline lattice is subject to many interactions, such as Coulomb $e^- - e^-$ interactions, phonon-$e^-$ interactions and $e^-$-lattice interactions (e.g. disorder) [11]. Which of these interactions are important, and which are not, for a given phenomenon of interest? Further, the length- ($\text{"Å} \text{"}$) and time-scales (fs) relevant to solid state systems make them more difficult to probe directly.

Happily, cold atom systems can directly address these concerns [9, 10, 46, 47], making them ideal complements to traditional condensed matter experiments. Specifically, cold-atom systems utilizing fermionic species trapped in an optical lattice can be used to analyze a simplified lattice model of condensed matter, the Hubbard model [22, 37]. “How is this done?”, “What do these experiments tell us?” and “What is the way forward?” are questions that the rest of this work seeks to answer.
Figure 1.2: **Level structure of the $2^2\text{Li}_{1/2}$ ground state of $^6\text{Li}$** as a function of magnetic field [23].

### 1.2 Atomic physics

Experimental cold-atom techniques rely on exploiting the quantum properties of individual atoms and their interactions with quantized electromagnetic fields [16, 17] to cleanly prepare quantum states of interest. Common laser cooling and control techniques are used to prepare the ultracold gas used in this experiment. As these techniques are well known [15, 30, 64, 73], and have been discussed in previous thesis works [38, 70, 81], this section will only briefly review several key features.

#### 1.2.1 Atomic structure of $^6\text{Li}$

The element of choice for this work was $^6\text{Li}$, primarily for two reasons:

1. It is an alkali atom, meaning that laser cooling it is relatively straightforward.
Figure 1.3: **Feshbach resonances** of the lowest three hyperfine states of fermionic lithium [91].

2. The broad Feshbach resonance makes it convenient to tune interactions between atoms, essential for simulating interesting Hamiltonians.

3. The small mass ensures that all timescales in the system are relatively fast, as will be seen in the analysis of the Hubbard model.

Li is a commonly used species in cold atom experiments, and a detailed enumeration of its properties can be found in the appendix to [23]. The ground state manifold of lithium contains six states, typically indexed $|1\rangle \rightarrow |6\rangle$, based on their energy at a finite magnetic field [23], as seen in figure 1.2. Our experiments typically use the lowest two states, although $|3\rangle$ is also commonly used [69]. Further, most experiments carried out in this work take place firmly in the Paschen-Back regime ($B \geq 100$ G).
1.2.2 Feshbach resonances

A particularly useful tool in cold-atom systems is the Feshbach resonance [15], which enables tuning the inter-atomic scattering length by varying an external magnetic field. First, it is important to note that the exact inter-atomic potential does not need to be computed, and at low energies can be well approximated by a delta function potential \( V(r) = V_0 \delta(r) \), directly related to the “scattering length”, \( a \), of this potential \( V_0 = \frac{4\pi \hbar a}{m} \) [47]. Depending on the internal structure of the atom, \( a \) can be tuned almost arbitrarily by varying a magnetic field [15]. For \(^6\text{Li}\), the requisite fields are easily accessible experimentally (< 1000 G, for \(^6\text{Li}\)).

\(^6\text{Li}\) turns out to be an excellent choice in regards to the Feshbach resonances available. Figure 1.3 shows the scattering lengths that can be achieved between the lowest three hyperfine states. The resonances are located at less than 1000 G, and are hundreds of Gauss wide, placing only loose constraints on the magnetic field coil engineering and magnetic field stability.

An important feature of the \(|1\rangle - |2\rangle \) resonance structure is that in addition to the broad resonance used for the experiments there is a narrow resonance at 543 G. This feature must be accounted for in experiments taking place above this field, and has been detailed in a previous work [70].

1.3 Optical lattice fundamentals

Most traditional cooling techniques, such as magneto-optical trapping, utilize dissipative interactions between atoms and photons to carry away entropy via spontaneous emission [73]. Optical dipole traps, however, produce conservative potentials [29, 30] by driving the system far off resonance. Consider the dipole moment of an atom is given by \( \mathbf{p} = \alpha \mathbf{E} \), where \( \mathbf{E} \) is the electric field amplitude and \( \alpha \) is the
complex polarizability. In steady state, the interaction energy $U_{\text{dip}}$ will be [30]

$$U_{\text{dip}} = -\frac{1}{2}\langle pE \rangle = -\frac{1}{2\varepsilon_0 c} \text{Re}(\alpha) I,$$  \hspace{1cm} (1.1)

where $I$ is the incident intensity. The system can be modeled classically by assuming that the electron is trapped in a dissipative, driven harmonic oscillator

$$\ddot{x} + \Gamma \dot{x} + \omega_0^2 x = -\frac{e}{m} |E_0| \cos \omega t,$$  \hspace{1cm} (1.2)

where $\Gamma$ is the dissipation term, $\omega_0$ and $\omega$ are the natural and drive frequencies, respectively, and $E_0$ is the amplitude of the incident wave. $\alpha$ can then be derived analytically to be

$$\alpha = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega \Gamma}. \hspace{1cm} (1.3)$$

This equation, although not entirely correct, provides valuable intuition. Specifically, the phase shift, $\delta$, approaches 0 for $\omega \ll \omega_0$ and $\pi$ for $\omega \gg \omega_0$, which producing an attractive (repulsive) potential for a red-detuned (blue-detuned) incident light field [30].

Optical lattices are a subset of optical dipole traps [30], created by interfering laser beams [29], which results in potentials that exhibit high spatial frequencies.

The canonical one dimensional optical lattice potential, shown in figure 1.4, is produced by a retro-reflection a Gaussian beam [67], producing a standing wave. Superpositions of multiple mutually-noninterfering 1D lattices can be used to produce a separable potential that is periodic along one, two or three dimensions [29]. Introducing mutual interference between lattices along multiple directions can be used to produce more exotic potentials, such as hexagonal, dimerized lattices and others [26, 28].
Figure 1.4: **Depth distribution of a typical 1D optical lattice.** The focus is chosen to be a few wavelengths, to illustrate divergence due to the underlying Gaussian beam.

Mathematically, the potential generated by a simple 1D optical lattice can be written [8]:

\[ U(z, r) = -U_0 \cos^2(kz) \exp(-2r^2/w_0^2), \]  

(1.4)

where \( k \) is the wavevector of the light, \( U_0 \) is the lattice depth, \( w_0 \) is the beam waist, and \( r, z \) are the radial and axial coordinates, illustrated in figure 1.4. Expanding the series to second order in \( r \) and \( z \) yields that

\[ U \approx U_0 \left( -1 + k^2 z^2 + 2r^2 / w_0^2 \right). \]  

(1.5)

By construction, this equation follows the form of the quantum harmonic oscillator.
Here it is convenient to define the recoil energy and frequency \( E_R \) and \( v_R \), which sets a natural scale to the system:

\[
E_R = h v_R = \frac{(\hbar k)^2}{2m}, \tag{1.6}
\]

where \( h \) is the Planck constant. Rearranging (1.5) to extract the harmonic oscillator trap frequencies along the \( z \) and \( r \) directions, \( v_z \) and \( v_r \):

\[
v_z^2 = 4 v_R \frac{U_0}{\hbar} \tag{1.7}
\]

\[
v_r^2 = \frac{U_0}{2\pi^2 \omega_0^2 m^2}. \tag{1.8}
\]

1.4 Band structure

1.4.1 Solving the Mathieu equation

A convenient way of understanding the band structure in a simple lattice is via the Mathieu equation. This is particularly convenient for a square lattice, since it is separable along the \( x, y \) directions, such that each can be analyzed independently. The 1D Schrodinger equation for an optical lattice is:

\[
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_0 \cos^2(kx) \right] \psi = E \psi \tag{1.9}
\]

By a change of variables, \( E / E_R \rightarrow E', U_0 / E_R \rightarrow U_0' \) and \( kx \rightarrow s \):

\[
\left[ \frac{d^2}{ds^2} - U_0' / 2 + E' - U_0' / 2 \cos(2s) \right] \psi = 0. \tag{1.10}
\]
Figure 1.5: **Spectrum of the sinusoidal optical lattice.** Characteristic solutions to the Mathieu equation, known as $a, b$ are plotted for a variety of lattice depths.

A further change of variables, $q = U_0'/4, a = E' - 2q$, reduces this to the Mathieu equation:

$$\frac{d^2\psi}{ds^2} + (a - 2q \cos 2s)\psi = 0. \quad (1.11)$$

Happily, this is a well known ordinary differential equation (ODE), with well developed\(^1\) numerical and analytic tools \([8, 19]\). Relying on existing numerical solutions, the spectrum of a lattice can then be calculated, as shown in figure 1.5.

The behavior of the spectrum is extremely intuitive - there are two regimes to consider, energies above the depth $U_0$, and below. Above the depth, the system exhibits a continuum of states, mathematically represented by many continuous bands. Below the depth, however, these bands split apart, and band gaps develop. In the limit of $E \ll U$, the spectrum resembles that of a harmonic oscillator.

\(^1\)Caution: users of the scipy Python library should watch out - there is a bug where the mathieu_a, mathieu_b commands frequently return incorrect values. Mathematica computes them correctly, however.
1.4.2 Band structure and quasimomentum

The fundamental properties of band structure can be derived in an alternate way from a general periodic potential [42, 48]. First, consider again the 1D Schrödinger equation in real space with a general periodic potential $V(x)$,

$$
\hat{H}\psi = \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi = E\psi. \quad (1.12)
$$

A fundamental consequence of translational symmetry, known as the Bloch theorem, states that solutions to this problem take the form

$$
\psi_{q}^{(n)}(x) = \exp(iqx)u_{q}^{(n)}(x), \quad (1.13)
$$

where $u_{q}^{(n)}(x)$ is a periodic function of the same period as $V(x)$, and $q$ is called the “wavenumber”, with the quantity $hq$ known as the “quasimomentum”. $n$ is the band index. The periodic structure can be further exploited by a change of basis, where

$$
V(x) = \sum_{l \in \mathbb{Z}} V_{r} \exp(i2rkx) \quad (1.14)
$$

$$
u_{q}^{(n)}(x) = \sum_{l \in \mathbb{Z}} c_{l}^{(n,q)} \exp(i2lkx), \quad (1.15)
$$

where $k = 2\pi/a$ and $a$ is the lattice spacing\(^3\). Under this basis, the entire problem can be simplified to a simple eigenvalue equation,

$$
\sum_{p} \hat{H}_{l',l}^{(n,q)} c_{p}^{(n,q)} = E_{q}^{(n)} c_{l}^{(n,q)}. \quad (1.16)
$$

---

\(^{2}\)This section heavily follows [29]

\(^{3}\)a being commonly used as the lattice constant and the scattering length is one of the unfortunate degeneracies of physics. The usage is typically obvious from context, but be careful
This equation takes on a particularly simple, tri-diagonal form when a sinusoidal lattice is assumed. Solutions of numerical diagonalization of this equation are shown in figure 1.6. In the limit of an infinitely shallow lattice, the dispersion relation resembles a “folded” parabola, consistent with a free particle dispersion relation. As the lattice depth is increased, energy splittings are introduced and distinct bands form. Finally, in the limit of a deep lattice (the tight binding model [48]), the bands are nearly flat and well approximated by cosines.

Although this technique yields results that are consistent with the Mathieu equation, it introduces several important concepts. First, unlike the Mathieu solutions, this technique can be generalized to any periodic potential. Second, utilizing this technique indexes the states by a new “quantum number” \( q \), which provides a lattice-based analogue to the free particle momentum.

Figure 1.6 also provides a valuable intuition about a particularly useful lattice characterization technique - band mapping [34, 90]. By adiabatically turning off the lattice in time \( T_{\text{ramp}} \), compared to the bandgap \( \omega_{\text{gap}} \), the quasimomentum can be mapped directly onto the real momentum. However, this ramp cannot be so slow as to become comparable to the frequency associated with the harmonic frequency of any external confinement \( \omega_{\text{HO}} \):

\[
\hbar \omega_{\text{HO}} \ll \hbar T_{\text{ramp}}^{-1} \ll \hbar \omega_{\text{gap}}. \tag{1.17}
\]

In practice, these constraints are not difficult to satisfy, and allow a high fidelity mapping of quasi-momentum to real momentum to be performed, as will be discussed in 3.
Figure 1.6: Dispersion relations for sinusoidal lattices at different lattice depths.
1.4.3 Wannier functions and the tight binding model

As seen in section 1.4.2, Bloch states are the analogues of plane waves in the context of a lattice - what then, are the analogues to spatially localized states? To answer is found by exact analogy to the free particle case where a particle localized at \( x_0 \) is

\[
\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp ik(x - x_0). \tag{1.18}
\]

For a lattice system, this analogy yields the basis of Wannier functions \([29, 89]\)

\[
w_n(x - x_0) \propto \sum_q \exp(-iqx_0/\hbar) \psi_q^{(n)}(x). \tag{1.19}
\]

Spatially resolved measurements in an optical lattice project the quantum state onto this basis, making them essential to quantum gas microscopy. Further, one definition of the tight binding limit \([48]\) (the regime where most of this work is performed), is that there is a nonzero coupling only between adjacent sites, making this a convenient basis to work with. The tight binding model also makes it convenient to write down the dispersion relation of the ground band

\[
E(q) = -2t \cos qa, \tag{1.20}
\]

where \( t \) is known as the tunneling energy, which will be an important energy scale in section 1.5.

1.5 The Fermi-Hubbard model

The remainder of this thesis will be concerned primarily with a single Hamiltonian describing particles trapped by an optical lattice under several assumptions worth stating explicitly \([37, 48]\):
1. The constituent particles are fermions.

2. The system is in a tight binding regime - coupling between sites that are not adjacent approaches zero.

3. The interactions are of a contact form - only atoms occupying the same site interact.

4. The system is well described by a single band - populations of higher bands are negligible.

If these assumptions are satisfied, the Hubbard [22, 37] model can be written as

\[ \hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.C.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{i,\sigma} (\mu - V_i) n_{i,\sigma}, \] (1.21)

where \( c_{i,\sigma}(c_{i,\sigma}^\dagger) \) are the fermionic annihilation (creation) operators of Wannier states on site \( i \) and spin \( \sigma \), and the \( \langle \cdots \rangle \) denotes a summation over nearest neighboring sites. The terms \( t \) and \( U \) are the free parameters of the Hamiltonian, respectively describing the mobility of the constituents tunneling and the interaction strength.

Typical lattice experiments with cold atoms involve loading a fixed number, \( N \), of ultracold atoms into a lattice with slowly varying envelope potential \( V \). However, it is more convenient to work in the grand canonical ensemble and use the local density approximation (LDA) [25]. Thus, is is possible to treat the last term not as a spatially varying potential, but as a spatially varying chemical potential \( \mu \).

The importance of this Hamiltonian is difficult to overstate, since it almost exactly\(^4\) describes our experimental system. This is a surprisingly powerful statement, and one of the reasons cold atoms are an excellent tool - a complicated system of atoms interacting with a magnetic field and numerous optical fields has been reduced to a one-line Hamiltonian.

\(^4\)Strictly speaking, the next nearest tunneling is present, but it is < 1% of the nearest neighbor tunneling, and can be neglected for all experimentally relevant situations.
Naturally, the next question to ask is, how do $t$ and $U$ relate to “real-world” parameters? These terms can be estimated from the underlying physics using [41],

$$ t = \int d^3 x w^*_0(x) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] w_1(x) $$

$$ U = 4\pi a h^2 \int d^3 x |w(x)|^4. $$

The value of $t$ can also be read off from the bandwidth, as seen in equation (1.20), $t = \text{bandwidth}/4$, where bandwidth is the width of the band at a given lattice depth. This can be heuristically veriﬁed in ﬁgure 1.5, where increased lattice depth leads to ever-narrower bands, as expected. It is also worth noting here, that since the system is separable, tunnelings in a 2D system can differ from each other [12, 41].

Calculating $U$ is much harder - equation 1.23 treats the interaction as a ﬁrst order perturbation and calculates the appropriate energy shift using overlap integrals of Wannier functions$^5$ [12, 41], although Mathieu functions can also be used [8].

### 1.6 Phase diagram

A full discussion of the phase diagram of the Hubbard model is beyond the scope of this work [52], but it is worth discussing several states that will play a role in this thesis. Broadly speaking, the community typically divides the phase diagram into two components, one concerned with temperatures on the scales of $t$ and $U$ (commonly called the charge sector), and one concerned with temperatures on the scales of $J = 4t^2/U$ (commonly called the spin sector). The charge sector is primar-

---

$^5$in practice, the lattice depth is usually $\approx 100\text{kHz}$ and the interaction is $\approx 10\text{kHz}$. 

20
ily concerned with motional degrees of freedom, while the spin sector is concerned with spin degrees of freedom.

In the charge sector, there are three states that must be addressed: metals, band insulators and Mott insulators. The metallic and band insulating states can be understood simply from a non-interacting band structure picture - a state with an incompletely filled band is termed a metal, while one with a filled band is a Band insulator [27]. In real space, metals tend to manifest as states with a large occupation variance, while Band insulators have close to the maximum of 2 particles per site (assuming a single-band, $S = 1/2$ system, which is the case throughout this work). A Mott insulator will be seen to emerge when strong repulsive interactions are present in the system near half filling. These interactions place a severe energy cost to pairs of atoms occupying the same site, and thus make an insulating state qualitatively similar to the Band insulator, but with only one particle per site. Although qualitatively similar, the Mott insulator and band insulator have a major difference - the spin degree of freedom. The band insulator has a $|\uparrow\downarrow\rangle$ on every site, leaving no degrees of freedom. The Mott insulator, however, can have either a $|\uparrow\rangle$ or a $|\downarrow\rangle$ on a given site, making it possible for spin structures to emerge.

Near half filling, at temperatures $k_B T \approx J = 4t^2/U$, motional degrees of freedom are largely “frozen out”, and antiferromagnetic spin ordering begins to emerge$^7$. This regime is extremely interesting because high temperature superconducting states [94], have been experimentally found to emerge by doping an antiferromagnetically ordered Mott insulator [52]. Numerical studies of the Hubbard model have produced a phase diagram resembling figure 1.7 [51, 52, 57, 58, 59, 77, 84]. The phase diagram is found to contain several states of interest, includ-

$^6$This can be argued from dimensionality, and will be discussed in more depth later

$^7$Interestingly, for a given temperature and at half filling, the degree of spin correlation is maximized for $U \approx 8t = \text{Bandwidth}$ - for $U > 8t$, $J$ becomes small, and for $U < 8t$ thermal holes begin to degrade the correlations.
In the attractive regime, several other phases emerge, which can be mapped to the repulsive in several regimes [22]. I will not discuss the attractive regime because no experiments in this work were performed there.

1.7 Analytic techniques

1.7.1 High temperature series expansion (HTSE)

Among the simplest and most powerful techniques of analyzing the Hubbard model is the high temperature series expansion (HTSE) [68]. Although it is most valid in regimes that are also the easiest to calculate numerically (high temperatures and high interactions), it can provide a great deal of intuition and is one of the relatively few analytic results available.
The main intuition behind the HTSE is treating the tunneling term as a perturbation, in the regime where \( U \gg \beta^{-1} \gg t \), and expanding to second order in \( \beta t \), where \( \beta = (k_B T)^{-1} \). In the case of the 2D Hubbard model [26, 27, 68], the grand potential \( \Omega \) can be found to be

\[
\beta \Omega = \log z_0 + \frac{\beta^2}{z_0^2} (t_x^2 + t_y^2) \left( 2 \xi (1 + \xi^2 w) + \frac{4 \xi^2}{\beta U} (1 - w) \right),
\]

where \( z_0 = 1 + 2 \xi + \xi^2 w \), the single particle partition function, \( \xi = \exp \beta \mu \) and \( w = \exp \beta U \). With the help of standard thermodynamic relations [43], useful observables can be calculated, such as the local entropy density \( s \) and particle density \( n \), plotted in figure 1.8.

The results of the HTSE make intuitive sense on a number of levels:

1. At low temperatures, the assumptions of the model break down, and non-physical oscillations manifest themselves.

2. At low interactions, the chemical potential smoothly tunes the average occupation, \( n \) from 0 to 2 particles per site.

3. At large repulsive interactions, an energy cost must be paid for two particles to occupy the same site, which stretches the region of single particle occupation, known as a Mott insulator [27].

### 1.7.2 Non-interacting fermions

The high temperature series expansion is phenomenally useful in the high-interaction regime, but fails near low interactions since its underlying assumptions are violated. Regardless, one might ask, down to what temperatures can the high temperature expansion be trusted? What is the exact failure mode?
Figure 1.8: **HTSE model predictions** at different interactions $U/t = .1$ (top row), $U/t = 1$ (middle row), $U/t = 10$ (bottom row).
To answer these questions, let us consider one of the few exactly solvable regimes in the Hubbard model - the non-interacting regime. Although the physics is not dramatic, having a theoretical grasp of the non-interacting regime can help understand the band insulator state, which is a critical ingredient in several cutting edge cooling techniques [7, 56].

Consider a system in macrostate $q$ containing $N_q$ particles, total energy $E_q$,

$$N_q = \sum_i n_i$$  \hspace{1cm}  \text{(1.25)}

$$E_q = \sum_i \epsilon_i n_i$$  \hspace{1cm}  \text{(1.26)}

where the particles are distributed among microstates indexed by $i$, where the microstate having energy $\epsilon_i$ has occupation $n_i \in \{0, 1\}$ [33]. The partition function is given by:

$$Z = \sum_q \exp\left( -\beta (E_q - \mu N_q) \right) = \sum_{n_q=0}^{1} \cdots \sum_{n_{\text{max}}=0}^{1} \prod_i \exp\left( -\beta n_{qi}(\epsilon_i - \mu) \right)$$ \hspace{1cm}  \text{(1.27)}

$$= \prod_i \left( \exp\left( -\beta (\epsilon_i - \mu) \right) \right)$$ \hspace{1cm}  \text{(1.28)}

This is a well known result that assumes nothing about the particles save that they are non-interacting fermions. Now a further few approximations have to be made. Specifically, let us assume a large system where we are interested in intrinsic variables only, $n$ (the particle density) and $s$ the entropy density. These quantities can be derived from the grand potential density $\phi = -\frac{1}{\beta V} \log Z$. In the continuum limit with a density of states $D(E)$, the potential density can be approximated as:

$$\phi \approx -\frac{1}{\beta} \int_{-\infty}^{\infty} D(E) \log \left( \exp\left[ -\beta (E - \mu) \right] + 1 \right) dE$$ \hspace{1cm}  \text{(1.29)}
Thermodynamic relations relate derivatives of this quantity to \( n, s \) as follows:

\[
\begin{align*}
    n &= \int_{-\infty}^{\infty} \frac{D(E)dE}{1 + \exp(\beta(E - \mu))} \\
    s &= k_B \beta \int_{-\infty}^{\infty} D(E) \left[ \frac{E - \mu}{1 + \exp(\beta(E - \mu))} + \frac{1}{\beta} \log [1 + \exp(\beta(E - \mu))] \right].
\end{align*}
\] (1.30) (1.31)

These are still general formulas that do not account for the lattice potential that holds the fermions in our system. We can do this, however, by choosing an appropriate density of states (DOS). Conveniently, the DOS for the rectangular lattice assuming the dispersion relation (1.20) has been derived [72]. The isotropic lattice will be considered from this point on, but a generalization to the anisotropic lattice is also known. For an isotropic lattice, the density of states is:

\[
D(E) \propto \mathcal{K} \left( \sqrt{1 - \epsilon'^2/16} \right) \] (1.32)

where \( \epsilon' = E/t \) and \( \mathcal{K} \) is the complete elliptic integral of the first kind. The proportionality symbol is used because the normalization must account for the volume of interest and number of spin states. The normalization chosen for this case ensures that there are two available spin states per lattice site.

With this choice of DOS, the \( n \) and \( s \) can be evaluated directly, and the results, as well as the comparison to the HTSE with low interactions, can be seen in figure 1.98. The results are relatively intuitive, when \( \beta^{-1} \gg |\mu| \) the dependence on chemical potential is negligible. When \( |\mu| \approx \beta^{-1} \), it can set the filling to be anywhere from no particles per site at low chemical potential to two particles per site at high chemical potential (a band insulator). By construction, no more than two particles can occupy a single site.

The entropy per site similarly exhibits relatively predictable behavior. At high temperatures, there are four available site occupations \( |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle \),

\[8\text{The code to generate this figure is available on the GitHub}\]

26
leading to \( s = k_B \log 4 \). The local entropy is saturated at zero in regimes where the system is nearly certain to be at filling of zero or two particles per site. Most interestingly, in the regime were the filling is 1 particle per site at temperature comparable to \( t, s \approx k_B \log 2 \), for the two available spin states.

Predictably, the high temperature series expansion fails dramatically at low temperatures and low interactions, as seen by the difference plots between the non-interacting theory and the HTSE predictions. Surprisingly, the HTSE predictions at weak interactions agree reasonably well, especially given that the HTSE expansion has terms of the form do better than might be expected because the expansion contains terms of the form \( (\beta U)^{-1} \).

### 1.7.3 Heisenberg model

As we have shown in the preceding sections, the motional degrees of freedom in the Hubbard model can be “frozen out” at sufficiently low temperatures or sufficiently strong interactions in the band insulating and Mott insulating regimes [52]. Specifically, in the large and repulsive \( U \) limit (which produces a Mott insulator), there is a prohibitively high energy cost to any site that does not contain a doublon (BI) or a single particle (MI). In this case, every site can be a superposition of the \(|\uparrow\rangle\) and \(|\downarrow\rangle\) states.

Mathematically, this corresponds to the limit of \( \lim_{U/t \to \infty, t \to 1} \), where the sole contribution to the Hamiltonian comes from virtual tunneling processes [71]. Specifically, every particle can virtually tunnel to the neighboring site if the neighbor is occupied by a particle of opposite spin. The particles can virtually interact and then return - implying that perturbation theory would place an energy cost of \( \approx 4t^2/U \) on sites of parallel alignment.
Figure 1.9: Non-interacting fermion model compared with the high-temperature series expansion.
This heuristic argument can be sharpened into a famous model in physics, known as the Heisenberg model

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j,$$  \hspace{1cm} (1.33)

where $\langle i,j \rangle$ denotes adjacent sites, as before. A more rigorous derivation [71], finds that the energy scale $J = 4t^2/U$.

The Heisenberg model is notably simpler than the Hubbard model and permits a more thorough analytic treatment. Specifically, the ground state is exactly known, as stated by Marshall’s Theorem [3, 86]

**Theorem 1.7.1** Marshall’s theorem\(^9\): for the Heisenberg model on a bipartite lattice with lattice of equal size, and all couplings $J > 0$, the ground state $|\psi_0\rangle$ is non-degenerate and is a singlet of total spin

$$\hat{S}|\psi_0\rangle = 0,$$  \hspace{1cm} (1.34)

where $\hat{S} = \sum_i \hat{S}_i$, where $i$ are the lattice site indices.

This theorem is surprisingly intuitive, despite the mathematical formulation. At first glance, the ground state of (1.33) appears to be a Néel ordered state ($|\uparrow_{1} \cdots \uparrow_{n}\rangle$, like in the Ising model [4, 32, 36]), contrary to Marshall’s theorem. This is not the case, however, because where the Ising model depends only on the $z$ projections of the spins, while the Heisenberg model depends on projections along all axes. What is not surprising, however, is that due to the singlet-like nature of the state, a tendency toward antiferromagnetic order will occur [31].

In an experiment, we will never produce the ground state deterministically. Thus, it is reasonable to ask if this “singlet-like” nature of the ground state is robust with respect to excitations. Happily, it turns out that the spectrum of the excited

\(^9\)Reproduced nearly verbatim from [86]
states of the Heisenberg model follows a predictable structure, known as the Anderson tower of states [65], seen in figure 1.10\textsuperscript{10}. This structure shows that the excitations do affect the spin, as expected, but the maximum “available” spin of the system grows linearly with the temperature. A full description of this structure and its implication is beyond the scope of this text [66] and requires spin-wave theory [49].

\subsection*{1.7.4 Characterizing antiferromagnetic order}

To understand antiferromagnetism in the Hubbard and Heisenberg models, it is important to consider the relevant order parameter\textsuperscript{11}. This order parameter of the antiferromagnet on a bipartite lattice is quantified by the staggered magnetization $m = |m|$. The component along the $z$ spin direction is

$$m_z = \sqrt{\langle (\hat{m}_z)^2 \rangle} = \sqrt{\langle \left( \frac{1}{N} \sum_i (-1)^i \hat{S}_i^z \right)^2 \rangle},$$

\textsuperscript{10}this numerical calculation was done with the help of the “qutip” package for python, which I strongly recommend.

\textsuperscript{11}This section closely follows [62]
with $m^2 = (m^x)^2 + (m^y)^2 + (m^z)^2 = 3(m^z)^2$ for SU(2) symmetry [61]. Here $\hat{S}_i^z$ is a spin-$S$ operator on lattice site $i$, $N$ denotes the number of lattice sites, and $(-1)^i$ is 1(-1) on the A(B) sub-lattice. The ground state of the classical Heisenberg model on a square lattice is a perfectly ordered Néel state with $m = 1$. However, in the quantum case superposition states such as local singlet pairs can reduce the energy of the many-body state. These quantum corrections decrease the staggered magnetization in the ground state and in the thermodynamic limit to $m = 0.61$ (i.e. $m^z = 0.35$) for the $S = 1/2$ Heisenberg model [76]. In 2D, LRO disappears ($m = 0$) in the thermodynamic limit for finite temperatures, as stated by the Mermin-Wagner-Hohenberg theorem.

The Heisenberg model can also be treated using the nonlinear sigma model (NLSM), a field-theoretic generalization of the Heisenberg Model [3, 14, 44]. There the spin correlations decay exponentially over a correlation length $\xi$, which grows exponentially with inverse temperature ($k_B = 1$)

$$\xi(T) = C_\xi \exp \left(\frac{2\pi \rho_s}{T}\right),$$ \hspace{1cm} (1.36)

where $\rho_s$ is the spin stiffness and $C_\xi$ is a constant [61]. However, for the finite-size system investigated in this work, a crossover to antiferromagnetic long-range order occurs at a non-zero temperature, where $\xi$ becomes comparable to the system size and $m^z$ becomes of order unity.

### 1.7.5 Dimensionality and spin systems

Dimensionality of the system under consideration plays a major role in determining the behavior of a spin system. In order to demonstrate this, I will discuss a basic example of renormalization, and discuss the Mermin-Wagner-Hohenberg theorem and its implications.
Prior to that, let us qualitatively consider systems of spins in $d$ dimensions. In the limit of $d \to \infty$, every spin will have many $(2^d)$ neighbors, and so its behavior will be strongly driven by the environment, since “going against the grain” will have a prohibitive energy cost. For this reason, in this limit, so-called mean field techniques become increasingly accurate [11]. Although the success of these techniques is very much a victory, systems described by a mean field model tend to not be very interesting, since the only two ingredients in the model are a single spin and the “background” field. Surprisingly, the artificial $d \to \infty$ limit is not at all a bad approximation down to as low as 3D. In the opposite limit $d = 1$, mean field techniques fail, but powerful analytic and numerical techniques (DMRG in particular [78]) become very successful. In particular, 1D systems have relatively few neighbors, so fluctuations tend to dominate [24]. Further, many 1D systems obey the notion of “integrability”, which strongly constrains the trajectories taken by a system, and has deep consequences for dynamics and thermalization [13, 21] While undeniably interesting, 1D systems also lack key features, for example, strongly repulsive particles can never “get past” each other in a 1D space. Studying 2D is interesting because it turns out to be an interesting intermediate case, sharing qualitative features with both 1D and $d \geq 3$ and the challenges inherent to both [77, 85]. Further, 2D systems can be found in a diverse array of natural phenomena [52]. With that in mind let us discuss some toy models in depth.

The simplest interesting spin model is the Ising model without a bias field [6],

$$\hat{H} = J \sum_{\langle i, j \rangle} \hat{S}_i^z \hat{S}_j^z. \quad (1.37)$$

Although the model has been written as a quantum mechanical Hamiltonian for consistency with the rest of the chapter, to build intuition, let us consider the clas-
classical Ising model,

\[ E = J \sum_{\langle i,j \rangle} S_i S_j, \]  

(1.38)

where \( S = \pm 1 \) is a classical spin. The partition function for a system with \( N \) spins is

\[ Z = \sum_{S_0 = -1,1} \cdots \sum_{S_{2N} = -1,1} \prod_{i \in N} \exp(K S_i S_{i+1}), \]  

(1.39)

where \( K \) will be the relevant scale parameter \( K = \beta J \).

The key idea of renormalization, and what makes it such a powerful technique for statistical physics in both the classical regimes is that interesting features can be observed by looking over a range of length scales [44, 45, 88]. Mathematically, this means that we make an ansatz that our “system“ is composed of only some subset of the spins - we will take the ones carrying the even index, that interact via the remaining portion of the system. Can a well behaved effective model be written down? It is possible to separate the equipartition function by changing the order of summation and multiplication, to get the following:

\[ Z = \sum_{S_0 = -1,1} \cdots \sum_{S_{2N} = -1,1} \prod_{i \in N} \exp(K S_i S_{i+1}) \]

(1.40)

\[ = \sum_{S_0} \sum_{S_2} \cdots \prod_{i = 0,2,\ldots} 2 \cosh K (s_{i-1} + s_{i+1}) \]  

(1.41)

The summation now does not “concern itself“ with spins that were on odd sites! Ideally, however, we would rewrite the partition function as [88]:

\[ Z = [z(K)]^{N/2} \sum_{S_0} \sum_{S_2} \cdots \prod_{i = 0,2,\ldots} \exp K'(K) S_i S_{i+2}. \]  

(1.42)

This is great because it recasts the “renormalized“ partition function into the same form as the original model, just with a new coupling constant \( K' \), and an overall multiplicative factor \( z \). It turns out that for the 1D Ising model, these parameters
are [88]:

\[ z(K) = \sqrt{4 \cosh 2K} \tag{1.43} \]
\[ K'(K) = \frac{1}{2} \log \cosh 2K. \tag{1.44} \]

The powerful fact about recasting the model in the same form (also known as decimation) is, of course, that the procedure can be applied multiple times, which will tell us interesting information about the system. \( K' \) can be either smaller, equal to, or larger than \( K \), and each of these cases corresponds to differing physical pictures. If \( K'(K) < K \), as in equation (1.44), no ordering is present, since two “adjacent” spins, considered after some number of renormalization decimations, can have arbitrarily low coupling. If \( K'(K) > K \), the system appears colder with each decimation and the coupling only grows, causing spins to be correlated across arbitrary distances. The fixed point \( K' = K \) is special, but frequently unstable. It means that the coupling is constant across all length scales, resulting in a fractal like behavior [88].

The work in this thesis is primarily concerned with systems in the regime of \( K' < K \), so it is worth analyzing in more depth. Global correlations do not exist, but over what range do they disappear? Renormalization can help solve this as well. Consider a characteristic length for correlations in the system, \( \xi \). By construction, to keep \( \xi \) in consistent units, the relation [45],

\[ \xi(K'(K)) = \frac{\xi(K)}{2}. \tag{1.45} \]

In the limit of \( \lim_{K \to \infty} K'(K) = K - \frac{1}{2} \log 2 \), leading to the relation

\[ \xi(K - n/2 \log 2) = \frac{\xi(K)}{2^n}, \tag{1.46} \]
after \( n \) decimations. Thus, we find that \( \xi = O(\exp K) \) in the 1D Ising model.

The same technique can largely be applied to the 2D Ising model on a square lattice, with surprising results [88]. Predictably, the decimation is facilitated by the bipartite nature of the lattice. The two partitions, termed the \( A \) and \( B \) sub-lattices, can be split apart as in the decimated summation in the 1D case. However, the problem quickly emerges that the new effective model after renormalization no longer only couples nearest neighbors. To see this, consider a site on the \( A \) sub-lattice, which we will call \((0,0)\) for convenience. Performing the decimation over the \((1,0), (0,1), (-1,0), (0,-1)\) sites necessarily couples the \((0,0)\) site to \((2,0), (0,2), (-2,0), (0,-2), (1,1), (1,-1), (-1,1), (-1,-1)\). Naturally, this problem gets exacerbated with every decimation, so careful approximations need to be made in order to keep the problem tractable [88]. Performing the calculation in 2D while accounting for these interactions yields an interesting result - for sufficiently high \( K, K' > K \), leading to the development of order. The coupling in the 1D and 2D Ising model is identical - the cause for this extension of correlations and the emergence of order is simply the dimensionality of the system.

This is a basic picture of renormalization, applicable to a variety of models, including the Heisenberg model [82], but this treatment has ignored a major feature of the experiment. The key missing point is that the Ising model has discrete symmetry, while the Heisenberg model has a continuous one. In the Ising model, the smallest possible excitation is an energetically unfavorable spin flip, which cannot cost less than a fixed bound. In a continuous model, such as the Heisenberg model, excitations can manifest as slow “windings” of the spin, meaning that an excitation can cost arbitrarily little energy, and this fact can prevent ordering. Formally, this gives rise to the Mermin-Wagner-Hohenberg theorem:
Theorem 1.7.2  Mermin-Wagner-Hohenberg Theorem [35, 63]: there can be no spontaneous magnetization or sub-lattice magnetization in an isotropic Heisenberg model with finite-range interactions\textsuperscript{12}.

Effectively, this theorem says that, in the thermodynamic limit, the system will not exhibit global magnetic order. The question is, however, “What really constitutes the thermodynamic limit?” or, alternatively “At what system size for a given temperature do MWH effects prevent ordering?”. The excitations of ever-lower energies occur over ever-longer length scales. Since the maximum spatial extent of the system scales as $O(N)$, and the only relevant parameter is $\beta J$, it can be shown [39, 54] that the condition for an effective long range order transition occurs when

$$\beta T \geq \log N.$$  \hfill (1.47)

Coincidentally, this is consistent with the exponential scaling of the correlation length in the Ising model and Heisenberg model. Physically, this corresponds to the situation where the correlation length of the system reaches the side of the system, all physically meaningful excitations have been “frozen out”, and the MWH theorem does not hold. In realistic systems (including macroscopic ones), the size of the system required for the MWH theorem to “kick in” can be quite large indeed [54].

1.8  Numerical analysis using exact diagonalization

Although this work is primarily experimental, it is nevertheless interesting to consider the state of the art in terms of theoretical understanding and numerical complexity - is it worth doing these experiments at all? I will argue that, yes, it is. There\textsuperscript{12}  Amusingly, the MWH theorem was derived first in the quantum case, and later in the classical, as opposed to the other way around.
is a slew of analytic and numerical techniques, and it is beyond the scope of this work to discuss all in depth, but a cursory overview follows.

The conceptually simplest technique for understanding the Hubbard model is simply through exact diagonalization (ED) of finite-size systems [40, 83, 95]. This is done by simply writing down the Hamiltonian and taking the eigenvector decomposition in a convenient basis. The strength of this approach is obvious - no approximations are made and the system is understood down to the lowest level. Strictly speaking, this approach will never reveal anything about the thermodynamic limit, but this may not be a problem if “sufficiently large” systems can be analyzed, such that quantities of interest show a clear convergence as the system size is increased.

The problem with this approach, of course, is that for a system of \( N \) sites, populated by spin \( S \) particles (\( S = 1/2 \) throughout this work), the Hilbert space \( \mathcal{H} \) has dimension

\[
\dim \mathcal{H} = 2^{N(2S+1)}.
\]

This problem can be ameliorated by approximately an order of magnitude by noting that the Hubbard Hamiltonian is block diagonal for particular numbers of particles, i.e. it does not convert, create or destroy constituents of a particular spin state. Thus, all analysis can be carried out for just the “block” of interest, corresponding to some particular combination of spin state populations. If the Hilbert space is thus restricted to a subspace \( \mathcal{H}' \),

\[
\dim \mathcal{H}' = \prod_{i=1}^{2S+1} \binom{N}{n_i},
\]

where \( n_i \) are the numbers of particles of each spin state. Figure 1.11 shows these numbers for small lattice plaquettes up to \( 4 \times 4 \) sites. Since a dense matrix has \( O(\dim \mathcal{H})^2 \) entries, and even a sparse matrix has \( O(\dim \mathcal{H}) \) entries, these high
Figure 1.11: **Dimension of the Hilbert space** in the Hubbard model with $S = \frac{1}{2}$ particles.

dimensionalities clearly prevent approaching the thermodynamic limit using exact diagonalization. Further reductions of the Hilbert space can be accomplished by exploiting symmetries [55], but the improvements are limited.

As a practical matter, systems up to 9 sites can be diagonalized straightforwardly on a personal computer. Systems up to 16 sites can be solved with more advanced hardware, such as GPU’s or other parallel techniques, but rather challenging [83]. The obvious problem is that a single state vector of 32 bit integers in a 16 site system takes up approximately 17GB of memory. These systems are not large enough to approximate the thermodynamic limit, since edge effects are still dominant.

### 1.8.1 Magnetism in small systems

Despite the limitations of the technique, some intuition can still be gained from exactly analyzing small systems. Specifically, can we support the notion that the repulsive Hubbard model exhibits antiferromagnetic properties?

Figure 1.12 shows the results of the diagonalization of a $2 \times 1$ system populated by 1 spin up atom and 1 spin down atom. In the deeply repulsive regime,
the ground state is \(1/\sqrt{2}|\uparrow, \downarrow - \downarrow, \uparrow]\), which clearly exhibits antiferromagnetic behavior. To quantify how antiferromagnetic a given state is, we look at the projection of the diagonalized ground state \(|\psi_{gs}\rangle\) onto every possible ground state \(|n\rangle\), given by \(|\langle n|\psi_{gs}\rangle|^2\) and find that the largest projection is onto the Néel state. This evidence is not convincing, however, because the system has, by construction, two anti-aligned spins on two sites - making some degree of antiferromagnetism all but assured. However, the \(2 \times 1\) system can also be easily analyzed using the Heisenberg model, which quickly reveals the ground state to be a spin singlet.

A stronger piece of evidence is the diagonalization of the \(2 \times 2\) system, where the ground state is dominated by the two antiferromagnetic states, as seen in figure 1.13. The largest system that could be analyzed on my personal computer in a reasonable amount of time (a few seconds per set of parameters), was \(3 \times 3\). Full diagonalization of the system containing a \(5:4\) balance of particles showed that the dominant overlap of the ground state was with the perfectly ordered state, as seen in figure 1.14. The ground states are not precisely Néel states because boundary conditions inducing finite size effects and quantum fluctuations further degrade the ordering.

Although limiting, ED has unambiguously implied that heuristic arguments that favor AFM order may hold in larger systems, and made clear some of the computational difficulties in analyzing the Hubbard model.

**Exact diagonalization algorithm**

As an aside, I found it instructive to analyze some simple numerical techniques for working with the Hubbard Hamiltonian. This section goes into detail regarding setting up the ED problem in a “computer-friendly” fashion and working with the Hubbard model in matrix form. It can be skipped without any loss of physics.
Figure 1.12: **Diagonalization of $2 \times 1$ sites at half filling**, filled with an even spin mixture.
Figure 1.13: **Diagonalization of $2 \times 2$ sites at half filling**, filled with an even spin mixture.
Figure 1.14: **Diagonalization of $3 \times 3$ sites at half filling**, filled with a $5 : 4$ spin mixture.
To set up the ED problem in a systematic way, one must overcome two challenges:

1. How do you index the states?

2. How do you populate the Hamiltonian, taking care of the fermionic creation and annihilation operators?

As it turns out there is an elegant approach to both of these problems. A general state can be written in second quantization [11] as

$$\prod_{i,\sigma \in Q} c_{i,\sigma}^\dagger |0\rangle,$$

where $Q$ is a set of pairs enumerating site and spin, representing occupied states, and $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the fermionic creation (annihilation) operator. An obvious difficulty arises due to the anti-commutation relations for fermions [11]:

$$\{c_{i,\sigma}^\dagger, c_{j,\sigma}^\dagger\} = 0$$

$$\{c_{i,\sigma}, c_{j,\sigma}\} = 0$$

$$\{c_{i,\sigma}, c_{j,\sigma}^\dagger\} = \delta_{i,j}.$$  

Unlike bosonic operators, which commute, this implies that swapping the order that creation and annihilation operators are applied to the vacuum changes the state (albeit only by a negative sign). Using fermionic operators can also be simpler since, by inspection, $(c_{i}^\dagger)^2 = (c_{i})^2 = 0$, also known as the Pauli exclusion principle.

Given these constraints, a system that permits $N$ distinct creation operators has $2^N$ basis states, since every operator can be applied to the vacuum zero or one times. Thus, each basis state can be mapped to an $N$-bit binary number, each bit corresponding to presence (1) or absence (0) of a particular creation operator, unambiguously mapping the state index to it’s real occupations. As an example,
consider the two by two plaquette, populated by a spin polarized population (such that we only have four operators to deal with). For to be clear, let us index the four sites as:

\[
\begin{bmatrix}
0 & 1 \\
2 & 3
\end{bmatrix}.
\] (1.54)

The state \(c_3^{\dagger}c_1^{\dagger}|0\rangle = |1010\rangle = |10\rangle\) and corresponds to the top right and bottom right sites being occupied.

Eq. (1.53) implies that writing down the Hubbard Hamiltonian in matrix form may be a challenge in book-keeping, because every time two operators are commuted, a negative sign is produced. This is complicated by the fact that the Hamiltonian contains many off diagonal tunneling matrix elements connecting various states, but the signs of these states must be found by carefully anti-commuting every creation operator to the correct location. In general, these off diagonal elements will take the form

\[
H_{k,l} = -\langle 0| \left( \prod_{i_k} c_{i_k}\right) t \sum_{\langle u,v \rangle} c_{i_u}^{\dagger}c_{i_v} \left( \prod_{j_l} c_{j_l}^{\dagger} \right) |0\rangle,
\] (1.55)

where \(k, l\) are the occupation states, and the \(i_k, j_l\) are the indices of the creation operators required to produce these states, and \(c_{u}^{\dagger}, c_{v}\) are terms in the Hamiltonian, where \(u, v\) are nearest neighbors. At most one term in the inner sum will connect the two states, but it’s sign is ambiguous. To simplify the equation to a single number for each matrix element requires commuting the operators from the Hamiltonian into the state, such that the left side of equation (1.55) equals the right side, each commutation yielding a negative sign. Fortunately, the binary representation of these states makes it possible to easily calculate the number of operators that one needs to commute past to place a creation operator at a particular location,
it is simply a sum of the binary representation of the target state preceding the bit index of the operator being commuted.

Based on these arguments, a relatively simple program can be used to unambiguously analyze small Fermi Hubbard systems. The GitHub page containing this thesis contains the source code used to compute these diagonalizations and also perform time-dependent calculations. I invite the interested readers to experiment!

1.9 Bibliography


Chapter 2

A history of quantum gas microscopy

“Arthur Dent: What happens if I press this button?

Ford Prefect: I wouldn’t-

Arthur Dent: Oh.

Ford Prefect: What happened?

Arthur Dent: A sign lit up, saying ‘Please do not press this button again.’”

- Douglas Adams, The Hitchhiker’s Guide to the Galaxy
2.1 Introduction

Quantum gas microscopy is a relatively new, exciting technique within the field of experimental cold atom research that has enabled unbelievably fine detection and control over pristine quantum systems. The fundamental idea is simple - placing a 2D array of atoms under an optical objective that can resolve the shortest relevant length scale in the system, typically the spacing of the optical lattice, and measure the site occupation \textit{in situ} using fluorescence imaging. Traditional cold atom experiments relied on relatively low resolution imaging systems ($NA \leq 0.5$) [19, 20] to study the systems of interest, due to several reasons:

1. The observable of choice was the momentum distribution, obtained by “time of flight” techniques [19, 20], requires a large field of view, which is easier to achieve with low resolution.

2. Imaging with high resolution through a vacuum window poses an engineering challenge, albeit a solvable one [1, 2]. Away from the paraxial limit (and high $NA$ objectives are very far away indeed), a vacuum window of finite thickness will apply an angle-dependent shift to every ray (an observer receiving the rays will then “see” every ray coming from a different location). This causes the system to have substantial spherical aberration that needs to be corrected for.

3. Imaging individual particles requires each atom to scatter many photons, which causes heating. This required the development of novel cooling techniques, such as polarization gradient cooling [6, 30], Raman sideband cooling [18] and electromagnetically induced transparency cooling [22].

These barriers, however, were only temporary, since the spatial distribution of atoms contains interesting information and experimental signatures, which are well worth the trouble of engineering proper imaging and cooling techniques.
Unlike many novel cold-atom experiments, which are prototyped using the workhorse of rubidium-87, the first experiment that imaged atoms in an optical lattice at the site resolved level used cesium [23]. The goal of these experiments was to treat individual atoms as qubits that could be addressed with high fidelity, with the aim of making a neutral-atom quantum computer [36]. Compared to these experiments, the work detailed in this thesis does not seek to make a universal computer, but to study a single Hamiltonian, with much stronger interactions and many more particles, and I will henceforth focus on our approach.

The original microscopes (as I will call these experiments for the remainder of the work) were developed using bosonic rubidium [1, 2, 34, 37]. These experiments used polarization gradient cooling to scatter $O(10^4)$ photons per Rb atom from a sample trapped in an optical lattice at the focus of a high $NA$ objective compensated to deal with the problem of imaging through a window. In addition to the objective, the Harvard group also used an in-vacuum hemispheric lens to enhance the $NA$ of the objective [2] and provide a convenient reference surface only microns from the atoms, a technique that is also used in our apparatus [14].

Naturally, this particular class of experiments proceeded to study the Bose-Hubbard model, which is identical to the Hubbard \(^1\) [13] model, save that the constituents are bosons. This difference leads to qualitatively different behavior, such as the absence of band insulators (Pauli exclusion does not apply to bosons, after all), or the occurrence of Mott insulators with more than one particle per site [1, 2, 34].

Due to the fact that imaging is a reversible process, single-site imaging also guarantees the ability to perform single-site addressing. In practical terms, this means that engineered light fields can be applied to the atomic system with res-

\(^1\)The original Hubbard model was derived for the purpose of studying fermions, so the terms “Fermi-Hubbard model” and “Hubbard model” are interchangeable. Typically “Fermi-Hubbard” is used to disambiguate the situation where required.
olution restricted only by the NA of the optical system. Not surprisingly, the bosonic microscopes (and now the fermionic ones, as we will see in chapter 4), quickly exploited this ability. The Munich group used a tightly focused laser beam and a microwave field to selectively spin flip individual atoms within their lattice [37, 38], while the Harvard group used a digital micro-mirror device to project a hologram of a desired potential in order to locally reshape the trap [40]. This degree of control has made a variety of new experiments possible, including studies of quantum walks [29], measurements of entanglement entropy [15] and studies of quantum thermalization [17], among others [32, 35].

With such an impressive record, it is not surprising that the community was excited about applying the same techniques to as many systems as possible. Predictably, the next frontier was to studying fermions with single-site resolution, an essential part of this work.

2.2 Fermi gas microscopy

After the initial success of imaging bosonic species, imaging fermions presented new challenges. Laser cooling techniques favor hydrogen-like atoms [21] - automatically restricting the choices to $^6\text{Li}$ and $^4\text{He}$. This decision is quite important, and while both have advantages and both have been studied by Fermi gas microscopes, we chose lithium, based on the analysis outlined in section 1.2 [14, 27, 33].

Despite initial problems, several years after the demonstration of the first bosonic microscopes, a host of machines demonstrating single-site resolution of fermions became operational [3, 5, 8, 12, 25, 28]. The initial images taken in our lab are shown in figure 2.1. The major challenge of the cited groups turned out to be that the same technique used to image rubidium could not be applied to the fermionic species. In lithium, this was due to the unresolved excited state hyper-
Figure 2.1: **Initial demonstration of single site imaging.** Reproduced from [28].

fine structure [10]. To solve this issue, a slew of well known techniques were applied in relatively novel ways. In our experiment [28] and the MIT experiment [5], Raman sideband cooling [18] was used, a powerful modification of sideband cooling [39]. Others [8, 12] have used EIT cooling [22] or a combination of EIT and Raman cooling.

As with the bosonic experiments, a wide variety of imaging techniques was implemented. The machines used at Harvard [28] and MIT [5] used hemispheric lenses coupled with commercial objectives to achieve \( NA \approx 0.85 \). Other experiments imaged through vacuum windows with compensated objectives [3, 8, 12, 25].

Once the technical challenges of imaging were overcome, the community quickly succeeded in measuring interesting physical states, first a spin-polarized band insulator in Munich [25], and then two-state Mott insulators and band insulators at Harvard [11] and MIT [4]. The Mott insulators and band insulators realized
Figure 2.2: **Fermionic metal-Mott insulator transition.** (A) experimental images of the atoms in a lattice at varying $U$. (B) Density profiles for the experimental parameters in (A), showing Mott-insulators, band-insulators, and metals. (C) Radial profiles of occupation and variance fit, with an HTSE model. Reproduced from [11].
in our experiment can be seen in figure 2.2, where the interaction was varied over a wide range to produce a set of diverse states.

As an aside, I find it important to point out that these experiments marked the first instance where the fermionic statistics made a difference as compared to the bosonic experiments, since cooling below degeneracy is required for any differences could manifest\(^2\). The factors limiting the temperatures of the initial results were largely technical in nature - in our case, a highly inefficient evaporation scheme, where a new evaporation coil had to be added to achieve sufficiently low temperatures [26].

No one doubted that a Mott insulator would exist in the Hubbard model, since it had already been observed [7, 9, 16, 31], and the theoretical understanding was solid [24]. However, in the context of quantum gas microscopy, Mott insulators\(^3\) have special significance, since the dramatically reduced occupation variance can be exploited to prepare specific states of interest [15, 17, 29, 35].

\section{2.3 Conclusion}

These results have largely characterized the regions of the Hubbard phase diagram governed by the motional degrees of freedom, also known as the “charge sector” in condensed matter physics. This brings us to the heart of the work involved in this thesis - the exploration of the region governed by spin degrees of freedom (also known as the “spin-sector”), which emerges if the system is cooled below the tunneling, \(t\) energy scale, to the scale of the super-exchange \(J = 4t^2/U\), which will be discussed largely in chapter 5. Before then, however, I will discuss two impor-

\(^2\)In the context of the Hubbard model, the temperature energy scale \(k_B T\) had to approach the interaction energy scale \(U\) and tunneling scale \(t\).

\(^3\)for fermionic systems, the same arguments hold for band insulators.
tant technical aspects of the experiment, which were critical for the realization of the interesting magnetic states.

2.4 Bibliography


Chapter 3

A high power, low noise optical lattice

“That’s no moon... It’s a space station!”

- Star Wars Episode IV: A New Hope
3.1 Introduction

As we have seen, ultracold atoms in optical lattices have become a powerful platform for experiments ranging from investigations of strongly correlated systems, quantum state engineering, quantum computing architectures, and precision metrology. Further, the recent advent of quantum gas microscopy has enabled studies that exhibit unprecedented control over few atom systems at extremely low energy scales. However, this rapid progress places ever more stringent technical constraints on the lasers used to trap and manipulate the atomic systems. For example, heating due to the intensity noise of any laser cannot be allowed to approach the longest thermalization timescales, lest the system fail to thermalize [15]. Since thermalization timescales generally grow with falling temperature, this complicates attaining low temperatures. Similarly, experiments that rely on a small number of atoms held by multiple traps places stringent requirements on the relative positional stability of the traps, to ensure that the operations performed by the traps have adequate fidelity.

In this chapter, I will discuss a high power optical lattice system that exhibits levels of intensity noise below -120 dBc between 1 kHz and 3 MHz. It also exhibits positional stability of the lattice phase at the < 0.5\mu m level and of the harmonic confinement at the few site level, both over the course of hours.

The architecture of the system is based on a single low-power, low-noise seed laser that supplies light to an array of four high-power fiber amplifiers (one for a transport beam [9], and one each for the X, Y, Z lattices). These amplifiers generate enough light to perform site resolved imaging [11], but also substantially increase the level of noise and degrade the mode shape. The fiber amplifier output is controlled by two feedback loops, which stabilize the light in the low power and high power regimes. After stabilization, the laser is mode-shaped to produce a desired
waist when focused in the atom plane. Just before the beam is launched toward the atoms, a small sample of it is imaged by a camera to monitor the pointing.

### 3.2 Relative intensity noise (RIN)

A commonly used metric of performance of low noise laser systems is relative intensity noise (RIN), which turns out to be critical to the design of our system. Several misconceptions exist about the measurement and comparison of RIN, and its expression in decibel (dB) units. The goal of this section is to provide an explicit description with no “shortcuts”.

Figure 3.1: **High level overview** showing the major components of the lattice laser feedback system.
Logarithmic units tend to take the form of dBx, where x is some reference amplitude or power. The definition of dB units is [8]

\[
dB_{x \text{ref}} = \begin{cases} 
10 \log_{10} \frac{x}{x_{\text{ref}}} & \text{if } x \text{ power} \\
20 \log_{10} \frac{x}{x_{\text{ref}}} & \text{if } x \text{ amplitude} 
\end{cases} \tag{3.1}
\]

To be clear, if the reference \(x_{\text{ref}}\) is a power, such as acoustic, optical or electric power of a signal, typically measured in W or mW, the first line is used, but if it is a voltage, pressure or some other amplitude, the second case is used. I stress this because it is a very commonly made error - essentially all decibel units are relative to a “power”, but sometimes, that “reference power” is defined in terms of an amplitude, as seen from the factors of 10 vs 20.

When decibels are expressed in terms of voltage, a load is implicitly assumed. Unless otherwise stated, that load is 50Ω. This can be confusing when the measurement device is high impedance, and strictly speaking the impedance of the measurement is very high (and can be well approximated as infinite). In this case, if a true comparison to power units is to be made, the voltage has to be divided to simulate the signal seen by a 50Ω load.

The next complication is that the decibel units are frequently encountered as a frequency density, such as dBm/Hz or dBV/√Hz. This occurs because in many practical applications\(^1\), the PSD of a signal is concentrated in a narrow-band, with components outside that band, all on top of a general noise floor, and decibel units are convenient to see both features simultaneously. Since PSD is a frequency density, decibel units of power now become dB/Hz, or similar. The complication is that the “/Hz”, or “√Hz” is an abuse of the notation, since the numerator is log-

\(^1\)I recommend playing around with some numerical FFT’s to see this, if you are not convinced.
Table 3.1: **Conversions of common decibel measurements** to the most widely used dBm/Hz, $R_{\text{source}}$ is the impedance of the signal source (typically 50Ω) and $R_{\text{sink}}$ is the resistance of the measurement device (typically either (typically 50Ω or $\infty$)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Reference</th>
<th>Conversion to dBm/Hz</th>
</tr>
</thead>
<tbody>
<tr>
<td>dBm</td>
<td>1 mW</td>
<td>$-10 \log_{10} \text{RBW}$</td>
</tr>
<tr>
<td>dBW</td>
<td>1 W</td>
<td>$-10 \log_{10} \text{RBW} + 30$</td>
</tr>
<tr>
<td>dBV$_{\text{RMS}}$</td>
<td>1 V, $R=\infty$</td>
<td>$-10 \log_{10} \text{RBW} + 10 \log_{10} \left( \frac{R_{\text{sink}}}{R_{\text{source}}+R_{\text{sink}}} \right)^2 - 10 \log_{10} \frac{(1V)^2}{R_{\text{sink}}} - 30$</td>
</tr>
</tbody>
</table>

In practice, spectrum analyzer tools frequently report decibel units, not densities, when reporting a PSD, which initially appears nonsensical. This behavior is due to the fact that each power reported is the power received by a particular frequency bin of width known as the resolution bandwidth (RBW). To convert the powers reported by a tool to dB/Hz, one has to subtract $10 \log_{10} \text{RBW}$.

The most commonly used decibel units, particularly in the context of this work, are shown in table 3.1.

### 3.2.1 Parametric heating

One of the major sources of heating due to laser noise is known as parametric heating [15]. To understand the mechanism, consider a simple, classical harmonic oscillator

$$\ddot{x} + \Gamma \dot{x} + \omega^2 x = F(t),$$

(3.2)

where $x$ is the spatial position, $\Gamma$ is a dissipative term, $\omega$ is the natural frequency and $F(t)$ is the forcing term. A typical driven oscillator has a constant $\omega$, but a periodic $F(t)$. However, the system can also be driven without the use of $F(t)$, but
through periodic driving of the natural frequency at $\omega_0$,

$$\omega(t) = \delta \omega \cos(\omega_0 t).$$

(3.3)

In a pendulum, for example, this can be done by dynamically changing the length of the rope. An interesting resonance occurs when $\omega_0 = 2\omega$, because energy can be continuously added to the system. To convince yourself that this is the case, note that in a single cycle, the oscillator passes through $x = \pm x_0$, where $x_0$ is the amplitude. Energy is added to the system by making the harmonic oscillator tighter at these times (e.g. by shortening the rope in the pendulum example), and energy is not taken away by making the harmonic oscillator weaker when $x = 0$ (since all of the energy of the particle is kinetic, changes to the potential do not affect the system), leading to a net influx of energy. This is known as “parametric drive”.

On a purely mathematical note, by coincidence the classical parametric oscillator can be solved using the Mathieu equation and its related special functions [17]. This mechanism is easily generalized to the quantum case using perturbation theory [15].

The situation is slightly more complicated in a lattice, where parametric drive promotes atoms from one band of the lattice to the next [4], but the physics is fundamentally the same. Intraband transitions also play a role in optical lattice experiments[13], but in the domain of the experimental work performed in this thesis, they are not dominant. The conclusion is simple - to prevent unwanted heating, noise at twice the trap frequency needs to me kept at a minimum, and since the depth of the lattice is varied over a wide range, resulting in trap frequencies from kHz to MHz, laser noise needs to be minimized over the same range.
3.3 Low noise seed laser

The lattice laser system is seeded by an Innolight Mephisto laser, which provides approximately 2 W of 1064 nm light. This commercial laser utilizes a non-planar ring oscillator (NPRO) design that ensures superb phase and intensity stability. This source is split into four fibers (Thorlabs PM980-XP) using polarizing beam splitters (PBS). To avoid interference of the lattice beams, two of the beam paths pass through acousto-optic modulators (AOM), which detunes the lattice frequencies from each other. Figure 3.2 shows the noise performance of only this subsystem.

3.4 High power laser system

3.4.1 Fiber amplifier system

Quantum gas microscopy of $^6$Li requires single site trap frequencies of approximately 1 MHz [12] in order to be in the Lamb-Dicke regime, which is necessary to perform Raman sideband cooling. Such trap frequencies may only be attained using tightly focused high power beams, which requires that the seed power be amplified to approximately 30 W per lattice axis, which is done using Nufern Fiber amplifiers (NuAmp SUB1174-34). These amplifiers can amplify 150 mW of seed light to up to approximately 45 W. They use a length of doped fiber pumped with 808 nm light from fiber coupled diode sources to amplify 1064 nm light. The amplification is performed using a two stage amplifier design, where the stages are controlled using separate power supplies and electronics. The high optical powers supplied by the fiber amplifiers raise two engineering difficulties:
1. The fiber amplification process is susceptible to many technical noise sources, such as acoustic coupling of the fiber to the environment and electrical design of the amplifier,

2. Stimulates Brillouin scattering (SBS) places a hard lower bound on the noise floor [1].

The NuAmp suffers from several problems: it is controlled via a USB interface, which is suspected to cause ground loops which add noise and interference to the analog systems, as seen in figure 3.2. We solve this problem by replacing the USB control board with a custom-designed, Ethernet based solution that is compatible with our custom control system and that carefully avoids ground loops. There are two power supplies in the fiber amplifier - a general purpose supply for the control electronics and first amplification stage and a high power current supply for the second stage. Despite the presence of a water-cooled cold-plate to cool the optical fiber and pump diodes, the high power supply is air cooled using a fan approximately 20 cm away from the gain fiber. This fan is suspected to lead to increased noise at acoustic frequencies. In order to reduce acoustic coupling and reduce switching power supply noise, both power supplies were removed from the fiber amplifier chassis, and the low power supply was replaced by a linear PSU (Acopian A24MT350M). Further, a high current line filter (MPE DS26387) was added to the high-power PSU (Lumina LDD-600-60-10-5VP/M). Combined, these changes serve to suppress many of the noise spurs measured in the RIN of the fiber amplifier, as seen in figure 3.2. The measurements in parts (a)-(d) were carried out on a single fiber amplifier, prior to and after the modifications. The initial and final noise spectra were verified to be consistent between amplifiers coming from the same manufacturing batch. The figure is based on fiber amplifiers from a relatively new batch, which, even in its unmodified configuration does not exhibit
a large switching supply spur. This is not the case for certain older batches, where the spur is approximately 30 dB higher than the background.

The operation of the Nufern fiber amplifiers can be further optimized by finely controlling the cooling water required, which by tunes the wavelength of the light supplied by the diodes that optically pump the gain fiber. Optimizing the temperature is advantageous because (1) the maximum output power of the fiber amplifier is increased due to the improved efficiency of the pump light and (2) the lifetime of the device is increased because less stray pump light needs to be absorbed when the pump light is separated from the desired light, reducing the thermal load on the system.

This is possible because the pump diodes are fixed directly to the water-cooling plate without additional temperature regulation. Adding a Peltier TEC and regulating to the optimal wavelength is possible, but is technically difficult as it requires large cooling power of $\approx 100$ W per each of the three pump diodes and carries the associated complexity of three feedback loops. We use a single, dedicated heat exchanger (TermoTek P21518970) to supply cooling water to an array of four fiber amplifiers and tune the temperature such that the average power supplied by the amplifiers supplying the $X$ and $Y$ lattices is optimized, while simultaneously keeping the temperature of the amplifier well within a safe range. Experimentally, we have found that more power can be gained by running the amplifiers at hotter temperature, but we have avoided doing this in an effort to increase the lifetime. We have experimentally found that there is variation in the sensitivity to the cooling water temperature between fiber amplifiers.

### 3.4.2 Mode and beam shaping

The free-space propagation of the fiber amplifier output presents several technical challenges:
Figure 3.2: **Laser noise of the lattice system.** (a) Shows the laser noise of unmodified Nufern fiber amplifiers and the Mephisto seed. (b) Shows the open (OL) and closed (CL) loop behavior of the high power feedback loop. (c) Shows open loop behavior of the low power feedback loop after making the modifications. (d) Closed loop behavior of the loop system without additional filtering, measured on the same setup as (c).
1. The high optical power poses a significant danger to users and equipment.

2. The high optical power is sufficient to induce substantial thermal lensing in some optics.

3. The positional fluctuations of the waist at the atoms cannot be allowed to exceed a few microns from shot to shot.

4. By construction, the beam is retro-reflected, threatening the lifetime of the amplifier unless sufficient isolation is used.

5. Approximately 1 W of power leaks into the undesired cladding modes of the fiber.

In order to address these challenges, we carefully engineered an optical system, shown in figure 3.3, that cleans up the beam, controls its intensity between $10 \mu W$ and 20 W, and ensures good pointing stability. Due to the high laser power, fused silica glass is used wherever possible. For the same reason, IBS coatings are used wherever possible, due to the higher damage thresholds. Further, even small reflections pose both a danger to the users and risk damaging cables or starting a fire, so to alleviate this danger, all undesired beams above 100 mW are directed to

Figure 3.3: Optical layout of the optical lattice system for beam shaping and modulation.
water cooled beam-dumps, which are placed as far as possible from critical beam paths. Weaker beams are dumped on uncooled diffusive beam catchers.

The large-diameter fiber tip at the output of the fiber amplifier is mounted in a monolithic mount made from oxygen-depleted copper. The beam is collimated using an $f = 20$ mm fused-silica, air-spaced triplet collimator (Opto-Sigma HFTLSQ-15-20PF1). Then, the polarization is cleaned up using an IBS coated thin-film plate polarizer (Precision photonics PO1056-FY), which has the added benefit of rejecting the undesired cladding modes. The fact that the lattice is retro-reflected, combined with the observation that optical isolation falls with applied optical power [19] means that two stages of optical isolators must be used. The optical isolators are based on 5 mm diameter isolators from Thorlabs (IO-5-1064-VHP), with the default cube polarizers replaced by IBS coated thin-film plate polarizers. Since the isolators are located approximately 1 m away from the ultracold atomic system, undesired stray fields can have a dramatic effect. To overcome this problem the isolators are enclosed in mu-metal shielding.

### 3.4.3 High power feedback

After the beam has been cleaned up and isolated, it is important to consider two aspects of the desired experiment:

1. The lattice power must be continuously tunable from around 10 $\mu$W to around 20 W.

2. The location of the minimum Gaussian beam waist must be accurately positioned to overlap the other lattices and dipole traps present in the experiment, and must remain there for the duration of the collection process (hours to days).
To satisfy the first of these requirements, a two-stage feedback system is implemented. The reason for the two stages is simple: the experiment typically operates in one of two regimes, which we will term detection and interaction. In the interaction phase of the experiment, the lattice is relatively shallow (≈ 100 – 200mW, corresponding to depths of ≈ 10E_R, where E_R is the geometric recoil of the lattice), allowing atoms to tunnel and interact with other atoms. In this regime, fine and potentially fast control is required. In the detection phase, the depth of the lattice is dramatically raised (≈ 2000E_R), isolating atoms in their individual wells so that Raman sideband imaging can be performed [12]. In the detection regime, the control need not be fast, and the passive stability of the Mephisto laser ensures that noise is low at relevant frequency scales (≈ 2 MHz). Thus, two loops are utilized, a fast loop that uses an acousto-optic modulator to actuate the laser power at low powers, and a slow loop which uses a Berek compensator, to actuate in the high power mode.

After the isolation stage, we use the sequence of optical elements shown in figure 3.3, consisting of a polarizer, half-wave plate (HWP), Berek compensator mounted on a precision galvo (Thorlabs GVS002, or Camtech 8320K, depending on beam path) half-wave plate, and polarizer. The Berek compensator is a simple z-cut quartz plate coated to be anti-reflecting at 1064 nm. By tilting the plate about its vertical axis, the extraordinary axis is mixed into the propagation of the beam, leading to a tilt-dependent bi-refringence that can be tuned from a zero-wave plate past a half-wave plate. Combined with the subsequent polarization optics, rotation of the Berek compensator changes the transmitted power with perfect contrast and transmitted power as a function of the tilt angle is shown in figure 3.4. Full modulation contrast is achieved when the fast axes of the waveplates around the Berek compensator θ are at 22.5° to the rotation axis of the Berek compensator. In that case, if the Berek compensator does not change the polarization, the light is
fully transmitted. If it functions as a half-wave plate, the light is fully rejected, with a smooth crossover between the two cases as the Berek angle, $\phi$, is adjusted. This contrast can be reduced by varying $\theta$, to the limiting case where $\theta = 0$, where the rotation of the Berek compensator does nothing, since the polarization of the light is parallel to the rotation axis of the quartz.

A key point is that, as seen in figure 3.4, if the two waveplates are rotated together, the maximum transmitted power is fixed, while the minimum can be raised. The waveplates are detuned such that the maximum power needed in interaction mode is the minimum power transmitted by the Berek compensator system, strongly suppressing fluctuations due to angle positioning noise of the Berek compensator. Naturally, rotation of a parallel plate in the beam path induces a shift of the beam, but this is acceptable because the Berek compensator is only active during the imaging phase of the experiment, when the position of the underlying harmonic trap is largely irrelevant. Fortunately, the spatial phase of the optical lattice is set by the retro-reflector mirror, which does not move, and is not affected by the rotation of the Berek compensator. This system functions as the actuator arm of a feedback loop, where the power of the beam is measured using a low noise photodiode. This feedback loop regulates the lattice between 1 W of optical power.

Figure 3.4: Berek compensator performance as a function of the Berek tilt angle $\phi$ and waveplate tilt angles.
and its maximum value (which depends on the amplifier, but is \( \approx 20 \) W). The step response and corresponding Bode plots [3] are shown in figure 3.5. A polarization rotation by \( 2\pi \) is produced by approximately \( 3^\circ \) of axial rotation of the quartz plate. Since we never need to rotate the plate outside this range, the position is constrained to this window in software.

### 3.4.4 Low power feedback

The high power feedback used in the imaging phase of the experiment is exceedingly robust because the heating rate from scattered resonant imaging light far exceeds any technical heating from the loop. Even if the loop was designed by your
worst enemy\textsuperscript{2}, the heating would be entirely compensated by the simultaneous Raman cooling [12].

In contrast, the low power loop that controls the lattice laser during the interaction phase of the experiment is critically important:

1. Its RIN is one of the factors limiting the system temperature.
2. It cannot affect the pointing.
3. It must have closed loop bandwidths of $\geq 1$ kHz, and open loop modulation bandwidths $\geq 100$ kHz.

To this end, we use actuate the optical power using a TeO\textsubscript{2} AOM (Gooch & Housego AOMO 3080-198), where the power of the RF supplied to the AOM is used to actuate the fast, low power feedback loop. The AOM was chosen for its low thermal lensing and easily-accessible RF powers. It is mounted on a custom-built, monolithic, water-cooled flexure mount that allows optimization of the AOM efficiency, that has been found to remain stable over years of operation.

\textsuperscript{2}I have received a number of comments about this particular statement. Yes, it was a hyperbole, and I concur - most likely readers of this thesis could design a system that would result in a heating rate exceeding the cooling, but you would definitely have to be malicious to do so.
The feedback circuit is shown in figure 3.6a. A pair of low noise photodiodes measures the optical power of the beam sampled with a weakly reflective optic (Thorlabs BSF10-C). The beam sampler is wedged in such a way that the two reflections diverge from one another, allowing us to illuminate both photodiodes. One of the sampled beams is attenuated by a factor of 20× by reflection off of an uncoated fused silica glass plate, such that the dynamic range of its photodiode covers 0 – 20 W of the beam directed at the atoms, and controls the Berek compensator based, high-power, feedback loop. The other beam is not attenuated, save by the beam sampler, and its dynamic range covers 0 – 1 W. To prevent damage to this photodiode when the system is at its highest powers, a shutter (Stanford Research Systems SR475) blocks the light when the high power loop is active. The low power photodiode passes its signal $V_{pd}$ to a loop filter circuit, which compares it to the control system’s set-point, generated by digital to analog converter. The loop filter’s output controls the IF port of a microwave mixer (Minicircuits ZFM-2-S+), effectively modulating the RF power supplied by a low noise phase-locked loop (PLL). The resulting RF signal is then amplified and sent to the AOM. Let us now consider every part of this signal chain individually.

**Phase-locked loop (PLL)**

The local oscillator (LO) RF source is a custom-built printed circuit board (PCB) implementing a phase locked loop (PLL) based on the ADF4002 IC and Crystek’s CVCO55CL-0060-0110 voltage controlled oscillator (VCO), preamplified with a low noise amplifier (Minicircuits PSA4-5043+3). To ensure frequency stability (which translates directly into beam pointing of the laser), the PLL is locked to the 10 MHz clock distributed around the lab. In addition to PLL functionality, the

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3This part has a plastic case which melts slightly if placed in a reflow oven, but still works as specified.
board also contains two, digitally-controllable, high-isolation RF switches, giving a total isolation exceeding 90 dB.

The spectrum and relative intensity noise of the PLL can be found in figure 3.7. Vitally, the spectrum of the PLL exhibits phase noise comparable to that of typical VCO\(^4\), without the slow frequency drift characteristic to these devices. Elimination of the carrier drift is worth the added phase noise because any drift of the frequency affects the steering of the laser beam passing through the AOM, which is entirely unacceptable since it would misalign the optical lattice.

**Photodiode**

Fast, low-noise photodiodes are required both to provide the monitoring arm of the feedback loop and to characterize the RIN of the system. An ideal device would have a bandwidth up to approximately 3 MHz\(^5\), with a noise floor below approximately -150 dBc over that range. To approach these specifications, we use a custom designed PCB that implements a simple trans-impedance amplifier [6] in a convenient physical package, providing a bandwidths in the 0.1-10 MHz range, depending on the trans-impedance gain set by a resistor. The photodiode can be safely operated up to incident powers of approximately 10 mW, which sets a -164 dBc/Hz shot noise limit on the RIN that can be detected. In practice, we typically operate the photodiodes with \(\approx 5\) mW of incident power. A photodiode with a bandwidth (BW) of 6 MHz is used to characterize the system, while photodiodes

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\(^4\)Strictly speaking, a \(-90\) dB phase noise is worse than specified. However, the measurement was carried out in “peak detection” mode on the spectrum analyzer, which artificially inflates the numbers by approximately 10 dB. This happens because the power at multiple frequency bands is measured within each frequency step on this plot, and in “peak detection”, the highest is reported (all noise measurements in this work were carried out in “RMS detection”, which is more suited for that purpose). The other reason that the phase noise appears worse than specified is that the dynamic range of the spectrum analyzer used is 100 dB, and we approach close to that limit.

\(^5\)The maximum attainable trap frequencies in the system are around 1.5 MHz, and parametric heating is driven by \(2\times\) the trap frequency.
Figure 3.7: PLL performance (a) The spectrum of the PLL, exhibiting phase noise of better than $-90$ dBc $100$ kHz away from the carrier. (b) The RIN of the local oscillator based on the PLL. The noise level is seen to be at or below the noise floor of the measurement device.

with a bandwidth of 330 kHz (and correspondingly higher gain) are used to perform the feedback.

The chosen photodiode (Hamamatsu G8370-01) is an InGaS based, small-area, low-noise design with a high efficiency at 1064 nm. Prior to use, the protective window is removed from the photodiode to prevent interference effects, as seen in figure 3.8. Further, to reduce the capacitance of the system, a reverse bias of 6.9 V is applied to the photodiode by a temperature-stabilized voltage reference (Linear Technology LM399). The trans-impedance circuit is shown in figure 3.6. It converts the photo-current supplied by the photodiode to a voltage signal using the low noise Texas Instruments OPA843 op-amp. To reduce electrical pickup and
Figure 3.8: **Photodiode photo** showing that the “can” of the photodiode has been cut, to prevent etalon-like behavior.

prevent ground loops, the electronic assembly is housed in a metal enclosure and mounted to the optical table using electrically insulating mica posts.

Light is focused onto the photodiode using a 25.4 mm lens such that the beam at the photodiode is significantly smaller than the photodiode diameter, to prevent pointing fluctuations from registering as amplitude fluctuations. An iris and interference filter (Semrock FF01-1020/LP25) are used to eliminate stray sources of light.

**Digital to analog converter**

The digital to analog converter (DAC, Texas Instruments DAC9881) connects the experimental digital control system to the analog control loop for the lattice. By definition, an ideal control loop would translate any noise on the analog signal from the DAC to the laser light, meaning that a poorly designed DAC would inherently limit the lattice laser performance. The noise on the DAC, when it is
Figure 3.9: **Relative intensity noise of the digital to analog converter** at a fixed output voltage and while changing values. To measure the transient RIN, a 20 ms, triangle wave with a DC offset and modulation depth of 15% of the DC offset was produced by the device. The triangle wave accounts for the series of spurs at low frequencies that fall with increasing frequencies. At frequencies above approximately 4 kHz, the spectrum is dominated by noise due to transient “glitches” that emerge when the device changes its output state.

Programmed to output a constant voltage is shown in figure 3.9, and is found to be roughly constant at a level of $-150 \text{ dBC}$ - more than acceptable. When the state of the DAC is changed, such as during a ramp, this noise level may be higher, due to the so-called “glitch” energy, as seen in the figure. The transient noise, while unfortunate, is mitigated by two factors: (1) it is only present when the lattice power is altered, which happens during lattice loading - a lattice at a fixed power will have negligible RIN contributions from the DAC. Further, (2) the loop filter will filter the noise at these frequencies.

**Loop filter**

The connection between the actuation and monitoring mechanisms of the feedback system is the loop filter, which compares the *set-point* signal, $v_s(t)$, supplied by the experimental control system and the monitoring signals $v_m(t)$, to adjust the actuation accordingly. We use a simple, purely integrating design based in three stages, as seen in figure 3.6, based on TI’s OPA211 op-amp. The first stage com-
putes and amplifies an error signal, $e(t) = v_m(t) - v_s(t)$, which is integrated by the second stage. The integral gain is set using a low-drift trim-pot. This is the case because within relevant frequency ranges, the AOM can be well approximated by a pure time delay process (with delay given by the RF travel time across the crystal $\approx 1\mu s$). In this scenario, the $P$ term must be small to avoid instability at the $\pi$ phase shift point, and a pure $I$ controller is optimal [16]. For debugging purposes, the loop filter features buffered photodiode monitor and error signal monitor outputs.

The third stage of the loop filter is used to accommodate the fact that the actuation arm is in nonlinear - the optical power transmitted by the AOM is proportional to the RF power incident on it $P_{rf} \propto v_{if}^2$, where $v_{if}$ is the actuation signal supplied to the IF port of the mixer. In effect, if the rest of the feedback system was linear, this would correspond to a quadratically increasing gain until the AOM is saturated, which could lead to slow behavior at low signal levels and ringing at higher signal levels. Even worse, since the mixer is insensitive to the sign of the voltage applied, the gain is actually negative for negative voltages, resulting in an unstable system, which thus requires a current clamp. This stage linearizes the response by increasing the gain at low signal levels and suppressing it at high signal levels by using a diode (Digi-Key BAT54S) in the feedback arm. This can be seen by considering two extreme cases - far below the diode drop, the diode is an open circuit and the gain is set by $R_{lf}$, where above the diode drop it is a closed circuit where the gain is set by the resistor $R_{hf}$. Naturally, the voltage drop over the diode is chosen such that it is approximately half the maximum desired signal level of the photodiode ($3.3 \, V$). Although a large improvement, the bandwidth still varies over the dynamic range of the loop, but only by approximately a factor of two, as seen in figure 3.10. Were it not for the linearization, the gain of the mixer would change by $10 \times$ over a dynamic range spanning two orders of magnitude. Another
Figure 3.10: **Loop bandwidth dependence on the set-point.** (a) shows the 3 dB and $\pi$ phase shift points for the X lattice (also known internally as the “northeast” lattice. (b) shows the same for the Y lattice, known as the “northwest”.

A common behavior of analog feedback systems with integration components is termed *integral wind-up* [3], and occurs when the feedback loop is manually broken, and the actuator can no longer adjust the state of the controlled parameter. In this regime, the integrator accumulates a large positive or negative value, such that when control is restored, the system is uncontrolled until the integrator reaches the desired value. In our case, *integrator wind-up* occurs when the high-
isolation RF switch is open during the state preparation procedure, and closed when the lattice is desired. Since the lattice must usually be applied adiabatically, fast transients due to this windup can result in heating. To solve this system, a bypass switch (Maxim MAX4503) is placed across the capacitor of the second stage of the feedback circuit, which siphons the charge off the capacitor when the lattice is inactive. Even when the switch is closed, its resistance is nonzero (due to a protection resistor which limits the current that can pass through the switch), the conditions leading to integral windup in an unprotected system still lead to charge accumulation on the integral capacitor, albeit at a much reduced level. Thus, in addition to the switch, when the system is inactive, the set-point is set to within ($\approx 200 \, \mu V$) of the dark signal from the photodiode, making the error signal very small.

To avoid a so-called “servo bump” in the noise spectrum, and because there is little need for fast, closed-loop control, the loop filter is tuned very conservatively, to a bandwidth of approximately 10 kHz over most of the range. However, a small amount of tuning can raise this to up to $\approx 150$ kHz, which is limited by the acoustic wave propagation delay of the AOM. Although fast, closed-loop control is impossible in the current configuration, the last stage of the loop filter features an adder, connected to an optional “feed-forward” port, which can be used to modulate the RF power at frequencies above the bandwidth.

Although it is an essential part of the system, the loop filter is also one of its major limitations. Figure 3.2 shows the noise performance of the output of the fiber amplifiers in open loop as compared to the noise in closed loop. Although noise near DC is lowered (as expected from a closed loop system), noise outside the loop bandwidth is increased in the range of 10 to 450 kHz as seen in subfigures (c) and (d). This can be explained by the Johnson noise [8] on the 1 k$\Omega$ input resistors,
amplified by the amplification stages of the loop filter\textsuperscript{6}. The sharp drop off at the 450 kHz point is due to the low-pass filter centered there, placed on the output of the loop filter. When this was determined to be a problem, and we decided that a bandwidth of higher than 10 kHz was not required in the near term, a first order low pass with a 3 dB frequency of 10 kHz, was also added, leading to the noise spectrum seen in subfigure (b), as compared to (a) in figure 3.11\textsuperscript{7}.

**Beam shaping**

After the beam has passed through the feedback optics, it must be applied to the atoms. To that end, we use a 2\textit{f} telescope of short focal length triplet collimator lenses to expand the beam, and then focus it with a long focal length lens. We focus the lattice to a 70 – 90 μm waist at the position of the atoms. In order to verify that the waist is positioned correctly, we use a temporary mirror to redirect the beam away from the glass cell and onto a camera positioned in the plane that would correspond to the position of the atoms had it not been for the temporary mirror. The resulting beam at the atoms has an \( m^2 \leq 1.4 \).

To prevent unwanted interference, the lattice beams enter the glass cell at an angle. Unfortunately, due to the angle of incidence, the beam contains both \( S \) and \( P \) polarizations, which are reflected differently, altering the polarization state of the beam. Even worse, this happens on both the initial and retro-reflected pass through the glass cell. For this reason, we use a QWP and HWP to optimize the interference contrast of each lattice\textsuperscript{8}.

\textsuperscript{6}This seems like a small quantity (-174 dBm), but there are several levels of amplification, and the voltage supplied to the mixer is small (≈ 0.1V), all of which works against the experimentalist.

\textsuperscript{7}The fiber amplifier used to take this data was different from the one used for 3.2 different fiber amplifiers, which explains the small discrepancies.

\textsuperscript{8}We do this by optimizing on the trap frequency of lattice, measured using parametric heating. This is a relatively tedious procedure.
Figure 3.11: **Laser noise of the lattice system with and without additional low pass filters** (a) Closed loop laser made a fiber amplifier (different than the one in figure 3.2. (b) Noise on the same system as (a), but with extra filters.
3.4.5 Heating rates

We have used the band mapping technique, described in 1.4.2, to characterize the heating rates in the lattice at different powers [4]. To do this, the cloud was held in a given lattice for a varied period of time, before band mapping was performed. Band mapping directly reveals the band occupations, and the lifetime of atoms in the ground band is closely related to the temperature. The results, shown in figure 3.12 revealed that lifetimes as high as tens of seconds can be achieved, but that the heating rates are consistently dominated by parametric heating induced transitions. This analysis was performed prior to adding extra 10 kHz filters to the system, and later measurements have revealed that heating rates in the $0.01 - 0.5$ W are approximately a factor of $2 - 5 \times$ lower.

3.5 Beam monitoring and alignment

Improved spatial resolution and control have given experimentalists the ability to use relatively few atoms [5, 10, 14] that are simultaneously addressed by multiple beams and held by multiple traps. Such experiments place stringent bounds on the requisite stability.
Averaged images of Mott insulators. A series of Mott insulators was created over the course of approximately one hour, and the average image is shown[7]. If the lattice fluctuated across more than a small fraction of a lattice site, the modulation contrast would be quickly washed out. The absence of this effect means that the phase of the optical lattice is very stable.

The absolute positions of lattice sites cannot be allowed to change by more than a small fraction (≈ 10%) from experimental shot to shot. Conveniently, this is relatively straightforward to ensure via careful design of the optical assembly, since the phase of a retro-reflected lattice is set by the retro-reflecting mirror, which can be close to the position of the atoms and be made very stable [9]. We have characterized the phase stability of the optical lattice by looking at a long sequence of densely populated images, and found that the phase varies by much less than one lattice site over the course of hours, as seen in figure 3.13.

The position of the atomic cloud, however, is not determined by the phase of the lattice, but by the underlying harmonic confinement. In experiments where
the entire cloud is addressed by beams auxiliary to the lattice (such as in this work, [10] or [5]), drift or fluctuation of the lattice position can pose a severe limitation.

The required positional stability is achieved through a combination of passive stability and active monitoring. Passive stability is ensured by using stable optomechanics (largely from the Thorlabs Polaris line), mounted on short optical posts, ensuring a low (2 in) beam height relative to the optical table, which is floated to minimize vibrations. In order to further improve stability, the beam is enclosed with 1 in aluminum tubes throughout its path and the entire setup is enclosed by metal plates\(^9\). To further isolate the experimental setup, the optical table is contained within an aluminum enclosure. As detailed in prior sections, care has been taken to minimize thermal lensing and drift in optics encountered by the lattice beam.

Passive stability alone has been found to be insufficient to ensure smooth operation over many hours. Changes in weather conditions, load on the watercooling systems and other external effects can lead to a slow drift in the pointing of the laser beams. The situation is further complicated by the fact that opening the enclosure changes the thermal state of the system, inducing misalignment. For these reasons, each lattice axis is fitted with a remotely actuated mirror, controlled by the experimental control software over the Ethernet network, allowing for non-invasive, digital alignment of the system. The remote actuators are Newport brand “Picomotors” (model 8302), fitted into a customized 2 in mirror mount, and work in a “fire and forget” manner, remaining passively stable when not in active use.

To prevent external influences from contaminating large data sets, we have implemented an independent monitoring system to verify appropriate pointing of both lattice laser beams and eliminate (via post-selection) experimental realizations when the system was in an undesired state. A beam-sampler (Thorlabs

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\(^9\) all plates are sanded to produce a rough finish, producing diffuse rather than specular reflections.
Figure 3.14: **Short term positional stability.** (a) A histogram of shot-to-shot step sizes along the transverse and longitudinal directions, with a Gaussian fit. (b) Correlations between the step size of subsequent shots. (c) Calibration data for the “affine fit” of the conversion from camera pixels to lattice dimensions. (d) Predicted location versus measured location along the transverse and longitudinal directions. (e,f) The measured position and predicted position of the atomic cloud.
BSF10-C) reflects a small portion of the beam shortly before it reaches the atoms and images it onto a camera located in the same plane as the atoms, producing a Gaussian image that is identical to that incident on the atoms. Naturally, the position of the atoms is dictated by the light field of both the incoming and retro-reflected beams, while the monitoring camera only observes the position of the in-going beam. To verify that the monitor camera could predict the true position of the atoms, the beam and the atoms were imaged simultaneously while a purposeful misalignment of the incoming beams was introduced. This was done by adiabatically loading one of the lattice beams ensuring that the atoms settle to its center, prior to performing site-resolved imaging [12].

Over the course of 250 sequential experimental realizations, we monitored the position of the beam on the camera and the position of the atoms. First, we characterized the passive stability of the optical axis along the transverse \(x_t\) and longitudinal \(x_l\) directions. Figure 3.14 a shows a histogram of displacements of atoms between subsequent experimental realizations, showing that the RMS displacement is \(0.54(3)(0.98(4))\) sites along the \(x_t(x_l)\) directions, where this discrepancy is consistent with the mechanical assembly of the experiment [9]. The means of both distributions are consistent with zero. If the trap followed a random walk with these step sizes, the experiment would be in trouble, since after only 100 experimental shots, the trap would move by more than 10 lattice sites. The situation is more fortunate, however, since the steps are heavily anti-correlated, as shown in figure 3.14 (b). Once this correlation is taken into account, we estimate a drift of \(8(1) \times 10^{-3}\) sites/realization in the transverse direction and \(12(2) \times 10^{-3}\) sites/realization in the axial direction, compared to a beam waist of approximately \(80 \, \mu m \approx 140\) sites.

In a real experiment, we cannot directly measure the position of the atoms and must rely on the measurement performed by the camera, related by an affine
transformation. To determine the parameters of the affine transform, we use the remote actuators to purposefully misalign the lattice beams for a small number of shots, and simultaneously measure the atomic positions and the camera reading, then perform a least-squares fit, shown in figure 3.14 c.

Unfortunately, while this fit is acceptable for a short while (≈ 30 shots), the quality of the fit degrades over time, correspondingly degrading the predictive power. The most likely culprit is thermal drift of the camera, since a displacement of approximately a pixel is very substantial to the predicted position, and each pixel is approximately 3 μm. The camera housing is not engineered for low drift mounting, and the camera produces a substantial amount of heat\(^\text{10}\), making a few μm drift very likely. To deal with this problem, we point out that the affine transform is composed of three distinct parts - the rotation, scaling and offset. Of these, only the offset is likely to drift with time. As a result, we developed a way of updating the calibration over time. To test this procedure, we analyzed the data set of camera measurements and atomic positions in the following way: we split the data set into sequential blocks of 20 shots, each followed by a block of 8 shots. The large blocks were treated as “masked” data, which we tried to predict, while the small blocks were treated as “updating” events used to update the offsets of the calibration. The results are shown in figure 3.14 (d-f), showing a large degree of tracking between the predicted positions and measured position - the average displacement between the predicted position and measured position was 0.7 lattice sites.

The purpose of developing this system was twofold - to reduce measurement noise by filtering experimental shots that suffered any sort of positional fluctuation of either lattice beam, and to minimize the frequency of such events. As it stands, for the purpose of most measurements, the experiment can perform hundreds of

\(^{10}\)It heats up by a few degrees Celsius during operation
cycles before the thermal drift becomes a problem. Further, if future experiments require the optical lattice to be more positionally stable than it is now, the monitoring and actuation system could be used in closed loop with no hardware changes to the experiment. Naturally, the transfer function of any such loop would have to be carefully engineered to account for the correlated behavior of the jumps and the timescale of the drift, but these are very solvable problems.

3.6 Long-term stability of the lattice structure

An interesting benefit of site-resolved imaging is that every measurement of the atomic distribution is also a direct measurement of the underlying lattice structure. As discussed in the supplementary material of [7, 11], the Fourier transform of an atomic distribution contains distinct peaks corresponding to the lattice structure, and these peaks can be used to extract the phase, relative angle, and spacing of the lattices. For this reason, I looked back at nine months of data spanning June 2016 through April 2017, in order to learn how these parameters change over time. Several interesting features can be seen from this figure 3.15.

1. During the summer of 2016, the lattice spacing appears to have slowly varied over as much as 10%. This can be attributed to unexplained drifts of the optical system that required daily refocusing of the imaging system using an auxiliary lens, which simultaneously changed the magnification.

2. The imaging system was simplified in September 2016, causing a sudden change in the magnification.

3. The system has been more stable in the spring of 2017 - the lattice spacing $|\nu|$ exhibits fractional fluctuations $\sigma_{|\nu|}/\mu_{|\nu|} \leq 0.005$. 

95
4. Unlike magnification, which sensitively depends on the imaging system focus, the angle is unlikely to be affected by the imaging system unless the camera is mechanically rotated. We measure that in the spring of 2017, the relative angle of the lattices has exhibited fluctuations with an RMS of $0.06^\circ$.

5. The behavior of the phase (not shown in figure 3.15) is consistent with being random, most likely due to the substantial drifts of the apparent magnitude of the lattice constant.

### 3.7 Affine transformations

In general, affine transformations are simple operations involving a linear rotation, scaling, and shift. Due to their simple form, they exceedingly useful for transforming between two planes of an imaging system, such as the atom and camera planes, of the preceding section. Thus, this section serves as a review and a numerical "recipe" for using in an optics context.

The simplest possible mapping between two planes $p$ and $q$ is an affine transformation [18]:

$$x_p = Ax_q + b,$$  \hspace{1cm} (3.4)

where $x_i$ is the coordinate in the $i$-th plane, $A$ is a transformation matrix and $b$ is an offset. For computational efficiency, this is typically reformulated as:

$$x_p = A'x_q'. \hspace{1cm} (3.5)$$

Where $A'$ is the the matrix $A$ with $b$ appended as the last column, and $x'$ is $x$ with a 1 appended as the last element.

In practice, the problem is to determine $A'$ from the locations of corresponding features in two planes. Let $X_q'$ be the $3 \times N$ dimension matrix corresponding
Figure 3.15: Long term positional stability over approximately nine months.
to the concatenation of \(N\) points representing feature locations in one plane (with 1’s in the last row). Similarly, let \(X_p\) be the \(2 \times N\) matrix representing the feature locations in the second plane, meaning that:

\[
X_p = A' x'_q. \tag{3.6}
\]

Assuming that \(N = 3\), the minimum number of points required to determine the transformation, \(A' = X_p X_q^{-1}\). More generally, \(N \neq 3\), meaning that simple inversion does not work, and a least-squares minimization is required, where the problem is exactly correspondent to a multi-dimensional, multiple regression. Specifically, it can be seen that solving for each row of \(A'\) corresponds to independent three parameter regressions, which can be performed by well known algorithms [2].

### 3.8 Bibliography


Chapter 4

Imaging a spatial light modulator

“The ships hung in the air much the way bricks don’t.”

- Douglas Adams, The Hitchhiker’s Guide to the Galaxy
4.1 Introduction

In addition to the stable lattice potential described in the previous chapter, it is desirable to have the ability to spatially modulate the potential in an arbitrary, real-time, repeatable way. Custom potentials open the way to interesting physical states by making it possible to manipulate the state at a microscopic level [23] and efficiently cool to very low temperatures [11, 12]. To this end, custom, dynamically tunable light fields can be realized using a wide variety of techniques, including (but not limited to):

- Optically shaping a beam to a desired shape using phase plates, axicons or similar optics [6].

- Using acousto-optic deflectors driven by engineered RF streams [7, 15, 17].

- Using a spatial light modulator[19, 29].

Although all of these techniques have seen a large measure of success, they require certain trade-offs to be made.

In this work, we have chosen to use a spatial light modulator (a digital micro-mirror device (DMD)) located in the image plane of the imaging system [4]. The image plane is conjugate to the atom plane, and reproduces the light field of the atoms, up to the transfer function of the imaging system (for details of the imaging system, please see [13, 22]. This architecture allows the experimentalist to apply light fields of arbitrary intensity distribution over the entire extent of the atomic cloud. Since the number of degrees of freedom of the DMD is finite, the ability to address multiple parts of the cloud simultaneously makes it more challenging to shape the applied light field at the site resolved level, a trade-off I will describe in depth. In this chapter, I will describe the experimental assembly used to spatially

\footnote{This reference, Modern Classical Optics, by Brooker, is excellent. I recommend it to everyone trying to develop an intuition for optics.}
modulate light in the image plane and describe the strengths and weaknesses of this approach. The next two chapters will demonstrate the physical effects that we analyzed using this experimental technique.

4.2 Digital micro-mirror device fundamentals

A digital micro-mirror device (DMD) is a common, commercially available tool for light modulation, used frequently in optical projectors [18]. The principal component is a $1920 \times 1080$ 2D array of 7.56 $\mu$m sided mirrors that can pivot along their diagonal by $\pm 12^\circ$. When in use, each mirror settles into one of two states, termed on and off. This platform is attractive because the state of the mirrors can be controlled programmatically and in real time. Due to its commercial applications, these arrays are typically produced at monitor resolutions, such as HD ($1920 \times 1080$) and occasionally higher.

On a more technical note, these devices are based on an extremely mature technology that has been widely adopted in the commercial world. These factors have made DMD’s extraordinarily robust and reliable, functioning continuously for more than two decades [2].

4.2.1 DMD in the image plane

The simplest approach to using a DMD, and the one we ultimately employ, is to place it into the image plane of the optical imaging system. In this configuration, the light field at the DMD is reproduced in the object plane after accounting for diffraction effects, which can be understood as a mask in the Fourier plane [9]. In the high $NA$ regime, corrections must be taken into account, but do not change the qualitative features [26]. A simple way to model the behavior of the DMD is to treat it as a binary mask applied to the incoming light field, since the tilt angle
of each mirror is much larger than the acceptance angle given by the numerical aperture.

Working in the image plane offers the experimentalist an important choice as to whether to use spatially and or temporally coherent illumination. In general, temporal incoherence can be advantageous primarily because stray reflections that differ in path length do not interfere coherently with the desired image. Temporal incoherence can be problematic, however, if strong chromatic effects are present in the system, although in practice this is typically not a problem for well-engineered systems. This is favorable to our application because the imaging system is largely achromatic, but the objective contains many uncoated glass surfaces. Spatial incoherence is also desirable because spatially coherent imaging characteristically leads to fringes in the imaged potential, particularly around sharp features [9]. However, it is highly nontrivial to produce high-power, uniform, spatially incoherent illumination [20, 24, 25].

The degree of spatial coherence strongly affects the reflection of the incident wave from the DMD, due to diffraction effects. Due to its’ diagonally pivoting mirror architecture, the DMD with pixel spacing $d_{dmd}$ behaves similarly to a saw-tooth grating along the pivoting direction, with spacing of $\sqrt{2}d_{dmd}$. This is undesirable because the numerical aperture of the system allows only one of the orders to address the system, leading to substantial loss in power. Fortunately, for an ideal saw-tooth grating, all of the light can be directed into a single order by satisfying the so-called **blazing condition** [21], which is how our DMD is positioned. In general, a saw-tooth diffraction grating illuminated at incidence angle $\theta_i$ will produce maxima at angles $\theta_b$ that satisfy

$$\sin \theta_b + \sin \theta_i = m\lambda / d,$$  \hspace{1cm} (4.1)
Figure 4.1: **Satisfying the blazing condition.** (a) Depicts the DMD architecture of pivoting mirrors, in the orientation used in the experiment. (b) Multiple diffraction orders are shown emerging from the mirror for an ingoing beam at a given incidence due to grating structure. (c) The grey and black lines show diffractive order angles for a given incidence angle. The red line shows the specular reflection. The blazing condition is satisfied at the only unique solution corresponding to angles \((\theta_i, \theta_m) = (-41.2^\circ, 17.2^\circ)\), since the other solution is the same up to a negative sign.
where \( m \) is an integer. Neglecting the effects of diffraction and assuming that the saw-tooth mirrors are tilted by angle \( \theta_t \), reflection directs the light away at angle

\[
\theta_r = \theta_i - 2\theta_t.
\] (4.2)

When equations (4.1) and (4.2) are simultaneously satisfied for some integer \( m' \), only that order has a nonzero amplitude, and the grating is said to be operated at the *blazing angle*. Despite significant power savings from operating the DMD at the blazing condition of the tilted grating (along the diagonal), the presence of nonzero Fourier components due to the lattice of mirrors typically still lead to substantial loss (approximately 50%).

The major disadvantage of placing the DMD in the image plane lies in producing small features with a large depth. Producing a few-lattice-site sized feature requires going down one of two routes: (1) placing the DMD in an image plane that has a large magnification, such that a large fraction of the DMD gets mapped to the desired lattice sites, but this may require magnifications \( M \approx 10^3 \), which is impractical. Alternatively (2), one can simply illuminate a small portion of the DMD with a tightly focused beam. Doing so will produce a potential of the desired depth, but the number of degrees of freedom will be restricted to the relatively few mirrors that illuminate the lattice sites of interest. Despite the challenges, it is possible to address individual lattice sites with an image plane DMD, as I will discuss in chapter 6.

### 4.2.2 DMD’s in the Fourier plane, an aside

Using a DMD in the Fourier plane, as compared to the image plane, can be a useful and complementary technique. A full description [29, 30] is beyond the scope of this chapter, but understanding the design criteria is important to making the right
choice in a given experiment. A Fourier plane DMD simply displays an amplitude hologram of the desired pattern, yielding two major advantages:

1. Phase control over the resulting light field, allowing fine compensation of aberrations [29].

2. Production of finely controlled potentials localized to a small number of lattice sites. Fine features will have Fourier components at many frequencies. Since the degrees of freedom of an SLM are distributed spatially, many degrees of freedom can be brought to bear on a small number of lattice sites.

These advantages have been leveraged to initialize very specific states [16, 23, 27] engineered to observe quantum phenomena of interest. Despite its attractiveness, Fourier plane DMD's require a considerable technical investment and limit the spatial extent of deep features. This technical investment primarily takes the form of careful calibration. The ability to cancel optical aberrations with extreme precision [29] relies on understanding the aberrations in the first place, which requires substantial time to measure, and which may change with time. While extremely convenient this ability may not be worth the effort for certain experiments, such as those performed in this work, making an image plane modulator a more optimal choice for our application, as will be seen in chapter 5.

4.3 Experimental assembly

4.3.1 Light source

The light source illuminating the DMD was derived from a SLED (Exalos, EXS210044), producing light centered around 649 nm with a FWHM bandwidth of 4.6 nm, based on the Gaussian fit shown in figure 4.2, leading to a coherence length of the light source of 61 μm [3]. The SLED produces a maximum of only 10 mW
of light, which is insufficient for our purposes. Consequently, it was amplified by two tapered amplifiers (TA) in series (Eagleyard, EYP-TPA-0650-00250-2007-CMT02-0000)\(^2\), producing approximately 80 mW of cleanly polarized light in a single spatial mode after an optical fiber.

Two AOM’s were used to control the intensity of the light incident on two single-mode optical fibers (Thorlabs P3-630PM-FC-10) leading to the experimental table, as shown in figure 4.2

### 4.3.2 Digital micro-mirror device optical assembly

The experimental side of the DMD assembly was designed with the following requirements:

1. Two independent DMD’s in the image plane.
2. Minimal mechanical drift between DMD’s.
3. Minimal mechanical drift between DMD’s and camera.
4. Ease of movement along the optical axis.
5. Flexibility in terms of conditioning the beam incident on each DMD.

To satisfy these constraints, the DMD assembly is composed of three components: (1) a base plate connected to couplings secured to a rail (2) a monolithic mount for the primary imaging camera and (3) a monolithically mounted breadboard holding two DMD’s and illumination optics. The optical layout of the entire system is shown in figure 4.3, and the mounted DMD is shown separately in figure 4.4.

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\(^2\)These tapered amplifiers deserve a word of caution. TA’s with the same part number can come from different production batches that have vastly different gain spectra. We bought two sets of these TA’s on separate occasions, but one of the purchased sets has almost a 2\(\times\) higher gain than the other at 649 nm, although they came from the same vendor and had the same part number. Fortunately, this is clear from the spectrum supplied on the specifications sheet, but it requires some attention.
Figure 4.2: DMD illumination light source. (a) The layout of the optics on the laser preparation tables. (b) The spectral power density of the source (solid) and a Gaussian fit (dashed).
Figure 4.3: **DMD mechanical assembly** optics layout used for illumination of the DMD and projection into the imaging system.

Figure 4.4: **Texas Instruments LC6500 DMD** mounted on custom supports and a monolithic, stable flexure mount.
The path of each beam illuminating the DMD is relatively straightforward - the fiber output is collimated, producing a beam with a beam waist of 1.6 mm (1.4 mm) for the DMD[0] (DMD[1]) path. A PBS purifies the polarization, a beam sampler (Thorlabs BSF10-B) is directs approximately 1% of the beam to a commercial photodiode, and a HWP transforms the polarization into a desired linear polarization. Further on, an easily accessible 4f telescope is used to shape the beam to a particular application necessary for a class of experiments, typically by expanding the beam. After the beam is conditioned, two low-drift, kinematic mirrors direct the beam at the DMD at the blazing angle. Since $\theta_i$, the angle of incidence on the DMD along the horizontal is set by the blazing condition, the absolute angle of the reflected beam must be set by the position of the DMD chip. In order to tune this angle, the DMD printed circuit board is mounted on a custom flexure mount made of 316 steel, providing approximately 5° of tuning range along the horizontal.

After the light is modulated by the DMD, 649 nm the beam paths are combined using a 1 inch PBS (Newport 10FC16PB.5). The 649 nm beam path is then combined with the 671 nm imaging beam path by means of a dichroic (Semrok LM01-659-25). This dichroic mirror also serves the purpose of filtering out near resonant light, such that it does not heat the cold-atom system. The small amount of leakage through the dicroic is imaged onto a dedicated camera, known as the DMD monitor, for debugging purposes. Unfortunately, the reflectivity of the dichroic is slightly dependent on the polarization. In the reference frame of the dichroic, the PBS cube produces $|S\rangle$ and $|P\rangle$ polarization. To avoid this, a half-wave plate is added between the dichroic and the PBS, thus illuminating the dichroic with $|S\rangle + |P\rangle$ and $|S\rangle - |P\rangle$.

\[ this not only affects the reflectivity, but also the transmissivity, making it much harder to debug using the DMD monitor camera, since one of the DMD’s appears much brighter than the other. \]
Since the PBS, HWP and dicroic are all relatively close to the image plane, any dust or surface features on these optics are imaged directly onto the atoms. For this reason, where possible, 20-10 scratch-dig optics were used, and the system was enclosed by a lid to prevent dust from entering (and catch stray diffraction orders).\footnote{Spraying the system with clean canned air every few months has anecdotally been found to help, however}

The illumination of the DMD’s is performed by a digital feedback loop that monitors the power using the commercial photodiodes shown in figure 4.3 and adjusts it by modulating the RF power applied to the AOM (seen in figure 4.2).

### 4.3.3 Why two DMD’s?

One of the initial design constraints was the presence of two DMD’s in the image plane, due to the following advantages, illustrated in figure 4.5: Superior coverage of the image plane. As seen in figure 4.5, placing two DMD’s in the image plane increases the area that can be addressed by one of the two DMD’s. Even better, with two DMD’s there is an area that is addressible by both of them. In this area, the experimentalist has very good control of the potential. For example, one of the DMD’s can be illuminated with a tightly focused beam, while the other is illuminated with a wider beam. The combination of these can be used to produce an optical potential with both deep features and wide features.

Due to the mechanism of switching the mirrors, any transients of the mirrors are guaranteed to take place on $\mu$s timescales, which is diabatic for most systems of interest. However, the illumination of each DMD can be controlled in an arbitrary way in real-time. For this reason, two DMD’s give the experimentalist the ability to “play movies” for the atoms in real time, by displaying subsequent “frames” on the the two DMD’s. The simultaneously turning down the illumination on one
Figure 4.5: Advantages of using two DMD’s in the image plane (a) increased coverage of the image plane (b) schematic drawing of the ramp sequence yielding adiabatic transformation of potentials.

and turning up the illumination on the other can adiabatically mold the potential between the two frames. The sudden switch of the pattern takes place when a DMD is not illuminated, and the process can, in principle, be repeated an arbitrary number of times. As of the time of this writing, we have not tried this scheme, but I see no reason why it could not work.

4.4 DMD Imaging

4.4.1 Light coherence

The coherence properties of the illumination light field are more subtle than initially advertised. Strictly speaking, the light is temporally incoherent but spatially coherent, since it is derived from an SLED and passed through a single-mode optical fiber. However, the light can be treated as being slightly spatially incoherent along one direction, due to the fact that the illumination is inclined with respect to the DMD grating. A simpler picture is to consider the light as being composed of a large number of wavelengths, each wavelength diffracting from the grating
at a different angle. Since the grating is in the image plane, this corresponds to a shift in the Fourier plane, meaning that each wavelength would be subject to a different Fourier filter. Naturally, the interference terms between different wavelengths time-average to zero, so the final image is their incoherent sum. While measurable, for the experiments performed in this work, these effects are largely negligible. Figure 4.6 shows an example of imaging a circular pattern on the DMD onto our atomic system. When the circle is much smaller than the PSF (normalized by the magnification \( M \)), the Fourier plane is entirely filled. Consequently, the produced image is very close to the PSF of the system, but with a strongly suppressed intensity (since much of the light is clipped in the Fourier plane). As the circle’s diameter is widened, the image widens while the intensity also grows (as shown in figure 4.7. The coherent imaging properties lead to “ringing” behavior which is seen to sometimes locally enhance the intensity.

### 4.4.2 Error diffusion

A clear limitation of the DMD, as compared to other spatial light modulators, is that it is a device where each spatial degree of freedom can be in only one of two states\(^5\). In practice, this can be effectively circumvented by exploiting the coarse-graining given by the diffraction limit. This can be seen by noting that the characteristic size of the point spread function in the image plane is approximately 100 \( \mu \text{m} \), whereas each mirror is 7.56 \( \mu \text{m} \) across. This means that the height of a single impulse response can be adjusted by turning on more or fewer mirrors in the PSF’s neighborhood.

\(^5\)Why not play the same trick as is used in video projectors, where every pixel is dithered in time in order to produce grey-scale? Unfortunately, to do this for cold atoms would require dithering each pixel at frequencies much faster than any relevant time-scale in the system, as we do for frequency detuned optical lattices. This would require dithering at MHz frequencies, where the pixels can only be updated \( \approx 100 \ \mu\text{s} \), which is much too slow.
Figure 4.6: Fourier optics treatment of imaging a DMD. (a-d) Show the initial and final light fields after passing through a diffraction limited imaging system. The energy distribution, as well as the filter (white circle), are shown in the last row.
Figure 4.7: **Intensity at the center of the light fields shown in figure 4.6.** The coherent nature of the light results in ringing behavior which can locally increase the local light intensity.

A clear question arises: how do we exploit this fact to efficiently transform a desired potential into a binary pattern to display on the DMD [5, 19]? The simplest answer is to apply a threshold - set every pixel below a critical value to zero, and above to 1. The limitation, naturally, is the large error induced by this technique, as well as the inability to apply fine modulation to the resulting light field. A small refinement is to randomize the threshold for every pixel, effectively applying a small amount of dithering to the system, but this too leads to large average errors. A demonstration can be seen in figure 4.8 (a)-(d).

This problem is not new, and was encountered by grey-scale and color printer manufacturers, and to solve this, the Floyd-Steinberg error diffusion algorithm was developed [8]. The key idea is that when a single pixel is binarized, an “error” \( e \) is made, \( e = b - v \), where \( b \) is the binarized value (0 or 1) and \( v \) is the original value. This error can be “diffused” to pixels that have not yet been binarized, so that the total error made in the binarization process is minimized. A formal definition
Figure 4.8: A demonstration of different types of image binarization. (a) Original demo image, “camera” from [28]. The range is fixed from 0 (black) to 1 (white). (b) Threshold at 0.5 applied to the original image. (c) Threshold applied at $0.5 + \delta$, where $\delta$ is drawn from a 0 mean normal distribution with standard deviation $\sigma = 0.3$. (d) Randomized threshold as in (b), but with $\sigma = 0.5$. (e) Non-randomized Floyd-Steinberg error diffusion. (f) Randomized error diffusion with $\sigma = 0.1$. (g) Randomized error diffusion with $\sigma = 0.3$. (h) Randomized error diffusion with $\sigma = 0.5$. 
of the algorithm is shown in 1. The main downside of the algorithm is that it is computationally difficult to parallelize, since every pixel requires information from processing the surrounding pixels. A demonstration of classical error diffusion is shown in fig4.8 (e).

```
input : Bitmap img of size r × c, float s
output: Binarized bitmap bin of size r × c
bin = zeros_like(img);
for i ← 0 to r do
    for j ← 0 to c do
        δ = Normal(μ = 0, σ = s);
        if img[i, j] + δ > 0.5 then
            bin[i, j] ← 1;
        else
            bin[i, j] ← 0;
        end
        e = bin[i, j] − img[i, j];
        img[i, j + 1] ← img[i, j + 1] − (7/16)e;
        img[i + 1, j − 1] ← img[i + 1, j − 1] − (3/16)e;
        img[i + 1, j] ← img[i + 1, j] − (5/16)e;
        img[i + 1, j + 1] ← img[i + 1, j + 1] − (1/16)e;
    end
end
```

Algorithm 1: Floyd-Steinberg error diffusion

Despite wide application to printing applications, using error diffusion for potential projection is substantially more difficult. The primary hurdle is the natural emergence of periodic structures in the binarized image, which lead to unwanted diffraction. Happily, this problem can be overcome by a simple modification to the classical algorithm - the addition of a small random term to the binarization criterion - instead of comparing the pixel value and accumulated error at that pixel to 0.5, it is compared to 0.5 + N(0, σ), where N(μ, σ) is a random number drawn from a normal distribution of mean μ and standard deviation σ. The error is diffused in the standard way once this is done, ensuring that the error over the entire image is still minimized, but breaking up the periodic structures.
Demonstrations of randomized error diffusion are shown in figure 4.8 (f-h), where in practice we use $\sigma = 0.1$, as shown in (f).

Another hurdle is that, as seen in section 4.4, the intensity of the light at a given point is not linearly proportional to the number of on pixels near that point, as assumed by the error diffusion algorithm. Various ideas for dealing with this problem have been proposed, usually involving iterative refinements of the pattern to minimize the integrated error on the potential. The experiments described in this work were thought to be sufficiently robust to errors in the potential that such procedures were not required. However, since this will likely not be the case in the future, development and implementation of such a system may be required.

### 4.4.3 The DMD, the camera and the lattice

Previous work [13] has ensured that the phase of the optical lattice drifts by significantly less than a site over the course of hours. Similarly, the monolithic, common-mode mounting of the DMD’s and the camera ensures that the relative drift between them is below the few $\mu$m level, less than a DMD pixel. The low drift nature of the setup allows for a repeatable mapping between the three planes that requires calibration only in the case of invasive changes or catastrophic misalignment.

Although determining the affine regression parameters is straightforward between the three planes is straightforward, it is an incomplete picture. First, the DMD is angled in the image plane, meaning that the magnification changes across the horizontal dimension, leading rectangles to be deformed into trapezoids, which cannot happen under an affine transformation. Further, field curvature aberrations present in the imaging system will cause straight lines in the image plane to map to curves, which is also not captured in an affine transformation. Fortunately, both of these effects are largely negligible, particularly when working with relatively small system sizes, as in this work.
4.5 Using a DMD in a cold-atom experiment

The market for DMD’s is relatively large and very much dominated by video projection applications, not cold atoms experiments. Fortunately, most important specifications, such as chip resolution, response time and reflectivity properties are equally beneficial to both applications, but this is not the case in general, and thus, there are several pitfalls to avoid. Naturally, it is possible to buy an individual DMD chip, lay out a custom PCB for it, and use a fully customized solution for a given application. The drawback is that this is an expensive proposition both in terms of price and time, so most experimentalists use general purpose evaluation boards.

The evaluation board used in our experiment is the LC6500, from TI, and I will discuss several considerations, primarily in the context of this specific device.

4.5.1 DMD communications via USB an HDMI

A typical evaluation board takes some combination of convenient inputs, such as USB, HDMI, or Ethernet and ideally comes with a convenient API. The inputs can be processed by either a dedicated ASIC or by an FPGA. In the LC6500, in order to minimize costs, an ASIC (DLPC900) parses USB and DisplayPort/HDMI inputs and drives the DMD chip using a low-level protocol [1, 14]. Basic configuration is done through the USB, which allows the user to specify pre-programmed patterns or elect to display the video feed. Real time control is possible by cycling through pre-programmed images using a TTL compatible trigger.

For cold-atom applications, the more desired behavior is to upload desired images ahead of time and activate them in real time, as opposed to streaming video. Unfortunately, real time applications were not a priority for the creators of this board, thus, for simplicity, the USB device was programmed as an human
interface device (HID). This is problematic because HID’s prioritize low latency over data throughput, limiting the bandwidth to a theoretical 64 kB/s (in practice we observe approximately 38 kB/s. These data transfer rates are only acceptable for patterns that can be compressed efficiently using run length encoding (RLE), which works by encoding long strings of identical pixels into a run length and value of that run (eg $aaabbbb \rightarrow 3a4b$). Unsurprisingly, this works best for localized patterns.

In general, patterns do not compress efficiently, and spending a minute to upload a single pattern is not acceptable. The solution is to exploit the extremely high throughput of the HDMI protocol ($\approx$ 10GB/s). To do this, a dedicated computer is connected to the DMD, and recognizes the device as it’s monitor, while the DMD is placed into “video pattern mode”, which draws the data from the HDMI stream, but allows the user some control over display parameters. The user or the experimental control system sends image files to the computer over the network, via the python remote object (PYRO) package. The image is displayed on the “effective monitor”, speeding the transmission rate by orders of magnitude. Naturally, the drawback is the lack of real time control - if multiple images needed to be displayed at specified times in the experimental sequence, the HDMI signal would have to get streamed in real time\(^6\).

Longevity is important in cold-atom experiments - since replacement and re-calibration of a degraded DMD system takes considerable time an effort. Fortunately, DMD’s are robust devices and can work for decades under the right conditions [2]. However, unlike in video projection applications, were many different patterns are applied, producing a rather “ergodic” pattern of wear and tear on the pixels, cold atom experiments tend to apply the same pattern continuously for months. To mitigate this problem, I strongly encourage practitioners to use the

\[^6\text{Although this is not currently implemented, this can be done using a fast FPGA.}\]
Figure 4.9: Observation of DMD switching noise: (a) a simple experiment to measure the switching noise. (b) reflected power as a function of time, clearly showing the periodic switching behavior and its suppression.

“idle” mode when the DMD pattern is not critical. This mode constantly randomly switches the pixels, both preventing “sticking” and artifacts from constantly using the same pattern.

4.5.2 Suppressing switching noise

In video applications, the DMD uses pulse width modulation (PWM) to control the brightness of every color. Effectively, every frame is cut into slices, where the fraction of slices that a given pixel is on depends on the desired brightness from that pixel. The eye integrates for tens of ms [10], so this slicing is not visible to humans. This is not how we control the brightness, and would be largely irrelevant, except that it is effectively hard-coded into the control IC. Every 105,\( \mu s \), the control IC releases all micro-mirrors updates the underlying SRAM, and collapses the mirrors to the new state using a so-called mirror clocking pulse (MCP). Critically, even mirrors that do not need to change state follow this procedure. From the manufacturer’s perspective, this behavior is acceptable, because (1) the mirrors are off for a negligible amount of time (3 \( \mu s \)) (2) it prevents mirrors from getting stuck in place if they remain fixed for a long period of time. From the experimentalist’s per-
spective, this is a problem because 10 kHz is a characteristic energy scale for many experiments, so driving this energy scale can lead to uncontrolled and undesired transitions, rapidly heating the system.

A simple experiment to observe this behavior was performed: the 650 nm light is reflected from a DMD displaying a flat field (every pixel on), and focused onto a sufficiently fast photodiode, as shown in figure 4.10a. The time trace default behavior is shown in red, clearly exhibiting a periodic, high-contrast dip in the power on the photodiode.

Suppression of this behavior was found to require a low level hardware intervention between the DLPC900 control ASIC and the DMD chip [1]. The mirror clocking pulse was experimentally found to pass through the DADSTRB/AF5 pin [1], conveniently accessible at test point 14 on the PCB. To suppress this pulse, we put a MOSFET (part number BSS138CT-ND, on Digi-key) between the TP14 and ground. When the FET is closed, the pulse does not reach the DMD chip, and the mirrors remain still frozen, and when open, normal operation resumes. As a technical aside, the pulse is fast only $\approx 5$ ns long - thus, connections to the FET must be short ($< 1$ cm).

This workaround for suppressing switching noise is effective but can be problematic. Freezing the DMD for $\approx 100$ ms approximately 1000 times per day for 9 months (as of Spring 2017) has not led to any observed degradation. However, leaving the DMD frozen for hours or days has anecdotally led to mirrors “sticking” or getting deformed. To combat this risk, Klaus Hueck has designed a refinement of this technique that prevents unwarranted freezing [14].
Figure 4.10: **Effects of DMD switching noise on atoms** (a) atomic cloud prepared with the DMD without suppressing switching noise. (b) atomic cloud prepared while suppressing DMD switching noise.

Figure 4.11: Preparing atoms in specified configurations. Averaged images showing the selective reduction of occupation on specified lattice sites. (a) Atomic symbol of lithium. (b) A cartoon face (perhaps that of a tired graduate student?).
4.6 Manipulating single atoms

Although Fourier plane DMD’s are in superior for producing fine potentials, image plane systems are also sufficient for many applications. The simplest use for our blue-detuned light is to locally raise the chemical potential on an array of sites and prepare a controlled array of holes, which will be discussed in detail in chapter 6. Figure 4.11 shows averaged images of Mott insulator clouds with two sample patterns that can be prepared in this way - the atomic symbol for lithium and a cartoon face. On a more serious note, we can selectively cut out a single line of atoms, as seen in figure 4.12. This can be done with > 95% fidelity, but requires careful alignment between the projected line and the optical lattice.

4.7 Conclusion

I have described our approach to applying external potentials to trapped atoms by directly imaging a digital micro-mirror device. This technique has been found to
be an extremely robust and flexible way to apply light fields spanning hundreds of lattice sites. Although this setup opens many experimental possibilities, there is dramatic room for improvement. One major improvement would be to implement an error diffusion algorithm that accounts for the propagation through the imaging system. In a similar vein, optimizing the pattern applied to the DMD via an iterative feedback algorithm [5, 19], could dramatically improve our degree of control over the applied potential. More aggressive upgrades could include adding new wavelengths to the system - the ability to apply both red- and blue-detuned potentials would improve the effective dynamic range of the change to the chemical potential. The combination of site-resolved imaging and addressing opens the way to studying physics in previously inaccessible regimes, as we will explore in the final two chapters.

4.8 Bibliography


Chapter 5

Antiferromagnetism in the Hubbard Model

“Good news, everyone!”

- Prof. Farnsworth, Futurama.
5.0 Chapter origin

This chapter focuses on the recent experimental production of an ordered Fermi-Hubbard antiferromagnet. For that reason, it is based on and includes verbatim passages from the following papers [44, 49]:


There is also some overlap of material and reliance upon previous thesis projects [35, 48, 57].

5.1 Introduction

Quantum simulation [17, 20, 38, 45, 59, 61, 64] with ultracold fermions in optical lattices offers the potential to answer open questions about the doped Hubbard Hamiltonian [4, 19, 26, 29, 33, 37, 42, 56] and it has recently been advanced by the advent of quantum gas microscopy [2, 5, 8, 12, 13, 14, 18, 25, 28, 46, 49, 50, 58]. As discussed in chapter 1, a system of cold atoms in an optical lattice is well described by the Hubbard model [34] (equation (1.5)) and, in the limit of strong repulsive interactions at half filling, by the Heisenberg model (equation (1.33)). At half-filling, this system is expected to exhibit antiferromagnetic correlations that increase in strength with decreasing temperature. Away from half-filling, the coupling between motional and spin degrees of freedom is expected to give rise to a rich many-body phase diagram (as described in chapter 1). As we have seen,
these systems can be difficult to analyze numerically due to the fermion sign problem [60, 62], which is typically NP hard. This chapter is focused on the production of finite-size, ordered antiferromagnets within an optical lattice.

### 5.2 Detecting antiferromagnetism

Transitioning from exploring the charge sector, as in [25], to exploring the spin sector of the Hubbard phase diagram poses an obvious challenge - in addition to measuring the spatial lattice occupation, it becomes necessary to measure the spin of every constituent. Unfortunately, for technical reasons, this is incompatible with the technique we use for site resolved detection [50].

The solution to this problem relies on two facts:

1. The average degree of correlation between atoms does not change between experimental realizations, assuming a constant chemical potential \( \mu \).

2. It is possible to selectively remove one of the spin states by applying resonant light to the system without affecting the spatial distribution of the other spin.

Selective removal of one of the spin states can partially translate spin correlations (which we cannot measure) into charge correlations (which we can [25]). Multiple measurements of independent experimental realizations, measured with and without removal pulses can be combined to estimate the degree of spin correlation at the percent level\(^2\), as shown in figure 5.1. This technique was originally demonstrated in [12, 48, 49] and used to measure short-ranged antiferromagnetic correlations in our system.

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\(^1\)The system is optically pumped at 0 G, where the hyperfine levels are degenerate, scrambling the spin information.

\(^2\)For the proof, please see references.
Figure 5.1: **Detecting antiferromagnetism with a quantum gas microscope.** Reproduced from [49].

Another subtlety is “parity imaging” - due to the imaging process, we cannot measure the exact occupation of every site, but only the parity, since both 0 particles and 2 particles on a single site appear as empty sites due to light-assisted collisions [1, 21, 48, 49]. However, close to half-filling and at temperatures significantly below the interaction energy, this problem can be partially overcome because the Hubbard model exhibits a linear relation between a change of the singles occupation \( \delta_{\text{singles}} \) and a change of the true density, \( \delta \). Using numerical data obtained from the dynamical cluster approximation method [41] at \( U/t = 7.2 \) and \( T/t = 0.25 \), we obtain a fitted slope of \( \delta = 1.22(1) \times \delta_{\text{singles}} \). The relation we obtain is consistent with results obtained from a resummed numerical linked-cluster expansion (NLCE) method [47] for dopings less than 6%, above which the resummed NLCE data becomes unstable. This result allows us to estimate the hole doping given the measured single-particle occupation.
5.3 Cooling via entropy redistribution

The production and high-resolution imaging and detection of spin correlations in a Mott insulator was first done in a square optical lattice with a harmonic trap [5, 13, 29, 49]. However, temperatures in these works were in the range of $T/t \approx 0.5$ - too high to find correlations over a longer range than between nearest neighbors.

We experimentally show that by carefully shaping the underlying trap, the temperature can be reduced by approximately a factor of two, using a key idea known as “entropy redistribution”. Our cold atom system is loaded into a trap isolated from the environment, meaning that the atom number $N$ and total entropy $S$ are fixed (prior to irreversible operations). Typically, a given trap contains a coexistence of phases, which can be seen most easily as being due to the local density approximation (LDA), discussed in chapter 1 and reference [25]. This effect can be exploited such that some part of the system takes on a disproportionately large fraction of the total entropy, leaving the local entropy per particle $s$ in other parts of the system to be $s < S/N$, so long as

$$S \leq \sum_{i}^{N} s. \tag{5.1}$$

Consequently, this procedure results in a lowered temperature [30, 31].

Cooling to a sufficiently low temperature is not the only challenge, however. The preceding discussion ignored the fact that the LDA only holds if the range of correlations in the system is shorter than the characteristic length of variation of the system, which is not the case in this work. To prevent order over many lattice sites from becoming corrupted when $\mu$ substantially varies over the correlation length, any ordered state of interest must be produced in a region of constant chemical potential. We address both challenges simultaneously by utilizing the image-plane spatial light modulator, which makes it possible to reshape the trap [43].
neer the potential to split the system into two subsystems: a central disk-shaped region \( \Omega \) containing \( > 75 \) sites, surrounded by a large reservoir at much lower density, see figures 5.2 and 5.3. Additionally, the potential within \( \Omega \) is shaped to cancel the underlying harmonic potential, ensuring a highly uniform and tunable filling.

The desired trap potential is created with a 2D piecewise defined function optimized experimentally, see figure 5.4. The reservoir is created by a combination of a broad paraboloid that compensates the underlying harmonic confinement and a gradient term that compensates any residual potential gradients in the system. The central region \( \Omega \) is created by a depression in the blue-detuned light field and is curved to ensure the total potential seen by atoms within \( \Omega \) is flat. Variants of the DMD-engineered potential are shown in 5.4, simulated by applying a Fourier-optics-based transfer function to the input signal and accounting for an idealized model of the mode incident on the DMD. The flatness of the potential within \( \Omega \) is critical to the realization of uniform antiferromagnetic LRO because both hole and particle doping is theoretically and empirically seen to strongly suppress magnetic correlations. We characterize the flatness of the potential by measuring the atomic density distribution within \( \Omega \), shown in figure 5.5. Azimuthal averaging reveals that the resulting density is flat to within \( < 4\% \) over approximately 80 sites. This is not an ideal metric to use, since the repulsive interaction suppresses the variance of the filling (this is taken to an extreme in a Mott insulator), but we are in a relatively compressible state, so this is acceptable. In order to explore controlled doping levels, the absolute offset of the central potential is tuned by varying the depth of the central depression in the DMD pattern, as seen in figure 5.4.

The light field applied to the atoms is shown in figure 5.4, and the resulting atomic distribution is shown in figure 5.5.
Figure 5.2: Probing antiferromagnetism in the Hubbard model with a quantum gas microscope. a, Schematic view of the 2D Hubbard phase diagram, including predicted phases. This chapter explores the trajectories traced by the red arrows for a $U/t = 7.2(2)$ Hubbard model. The strongest antiferromagnetic order is observed at the starred point. b, Experimental setup. We trap $^6$Li atoms in a 2D square optical lattice. We use the combined potential of the optical lattice and a DMD to trap the atoms in a central sample $\Omega$ of homogeneous density, surrounded by a dilute reservoir. c, Exemplary raw and processed images of the atomic distribution of single experimental realizations, with both spin components present (upper) and one spin component removed (lower). The observed checkerboard pattern in the spin-removed images indicates the presence of an antiferromagnet.

5.3.1 State preparation

The low-temperature Fermi gas is prepared using a sequence similar to previous work [25, 48, 49], where a balanced mixture of the two lowest hyperfine states of $^6$Li with repulsive interactions is adiabatically loaded into a 2D optical dipole trap. Prior to loading the lattice from the dipole trap we ramp to the final magnetic bias field used in this experiment, 576 G, corresponding to a scattering length of 210 $a_0$, and interaction energy $U/h = 6.50(3)$ kHz. This includes a fast ramp over the narrow $s$-wave resonance at 543 G to avoid heating and loss. We then perform a final
Figure 5.3: **Raw images of the AFM states.**  
- **a,** an image of the antiferromagnet with no spin removal, clearly showing Ω, the region of interest, and the surrounding sparse reservoir.  
- **b,** an image of the antiferromagnet with only the $|↑⟩$ remaining, showing the characteristic checkerboard pattern.
Figure 5.4: **Amplitude of light fields applied to atoms a**, The computed light field generated by the DMD, applied to the atoms for half-filled samples. A gradient compensates residual gradients in the lattice. The rim of the reservoir provides sharp walls for the inner subsystem. A broad, shallow paraboloid in the center flattens the potential when combined with the optical lattice. The cartoon shows a schematic view of a radial cut of the potential, including the contribution of the lattice. **b**, The amplitude of the light field with an offset in the center of the trap, used to dope the system with a finite population of holes.
Figure 5.5: **Average density profile in the system.**

**a,** The average singles density map for a sample at half-filling shows a central region of uniform density, surrounded by a ring of low density. The dotted white circle indicates our system size, excluding edge effects. **b,** The azimuthal average of the singles density shown in **a,** for the system as well as the inner edge of the donut where the density drops off to the reservoir density. The vertical dotted lines denote the boundary of the system. **c,** Azimuthal average of singles densities for three values of the hole doping used in the experiment, indicating uniformity of atom number across our system to within 4%. The horizontal lines are at the system-wide average densities.
stage of evaporation immediately prior to loading the lattice, under a magnetic
gradient.

Once the magnetic gradient is removed, we adiabatically load the atomic
cloud within 40 ms into a square optical lattice spaced by $a = 569$ nm. The lat-
tice is isotropic ($t_x/h = 9.1(1) \times 10^2$ Hz and $t_y/h = 9.0(1) \times 10^2$ Hz) with a depth
of $7.4(1) E_R$, corresponding to Hubbard parameters of $t/h = 0.90(2)$ kHz$^3$ and
$U/h = 6.50(3)$ kHz, leading to $U/t = 7.2(2)$. The lattice depth was calibrated as
in [49], using parametric lattice modulation spectroscopy [39, 55], and the interaction
energy was calculated based on the scattering length and lattice parameters.

The blue-detuned illumination of the DMD is increased concurrently with
loading the optical lattice. The populated layer lies at the focus of the high resolu-
tion microscope, which allows site-resolved detection of the lattice occupation and,
at the same time, enables us to augment the harmonic lattice trap by projecting an
approximately ring shaped potential onto the atoms from a DMD in the image
plane. The ring center contains the correct potential to prepare the subsystem $\Omega$,
while the rim of the ring is shaped to reduce the filling of the reservoir [43].

We can vary the temperature of the sample by holding the atomic gas in the
combined lattice and blue-detuned potential for a variable time. The final evap-
oration setpoint is chosen such that the final state is at half-filling after heating
(i.e. initially load more atoms when heating to higher temperatures). For the cold-
est temperature samples (zero hold time), approximately 400 atoms remain in the
trap at a temperature $T \approx 0.1 T_F$, where $T_F$ is the Fermi temperature. Near half-
filling we can actually directly measure the temperature from the level of nearest
neighbor correlation [47, 49].

The system doping can be varied by adjusting the DMD potential in the mid-

---

$^3t_{x,y}$ are the Hubbard tunneling energies along the two directions, and $t = \frac{t_x + t_y}{2}$. Within error bars, the system is isotropic, so the remainder of the discussion uses $t$. 138
dle reduces the filling. Interestingly, we speculate that the temperature stays approximately the same across levels of doping. Clearly, the size of $\Omega$ increases with increased doping, which would lead one to believe that the temperature would increase (since the low-entropy region becomes a larger fraction of the system). However, with added holes, the heat capacity of $\Omega$ also increases, which would imply that the system would get colder. We speculate that the two effects approximately cancel. Unfortunately, we have no temperature probe away from half filling (since numerical data is much less reliable), so we cannot verify this speculation\textsuperscript{4}.

5.4 Characterizing the antiferromagnet

Averaging over many independent experimental realizations, we determine the spin correlator along the $z$-direction [49]

$$C_d = \frac{1}{N_d S^2} \sum_{r, s \in \Omega} \frac{d=r-s}{d} \langle \hat{S}_r^z \hat{S}_s^z \rangle - \langle \hat{S}_r^z \rangle \langle \hat{S}_s^z \rangle$$ (5.2)

where the normalization $N_d$ is the number of different two-point correlators at displacement $d$ between sites $r$ and $s$, which lie within $\Omega$, $S = 1/2$ and $\hat{S}_i^z$ is the spin along the $z$ direction on site $i$. The correlator compares the number of parallel and anti-parallel spin orientations on two sites separated by $d$, i.e. is positive (negative) if parallel (anti-parallel) spin orientations are preferred. Figure 5.6a shows $C_d$ for different temperatures. For the lowest temperature we find spin correlations across the entire disk alternating in sign even up to the largest distance of $d = |d| = 10$, as expected for an antiferromagnetic LRO state. We determine the temperature of each sample by comparing the measured nearest-neighbor correlator $C_1$ to quan-

\textsuperscript{4}A temperature probe away from half filling is currently a major “to-do” - good luck, future student.
Figure 5.6: Observing antiferromagnetic long-range order. a, The spin correlator $C_d$ is plotted for different displacements $d$ ranging across the entire sample for five temperatures $T/t$. We record > 200 images for each temperature. Correlations extend across the entire sample for the coldest temperatures, whereas for the hottest temperature only nearest-neighbor correlations remain. b, The sign-corrected correlation function $(-1)^iC_d$ is obtained through an azimuthal average. The exponential fits to the data ($d > 2$) are shown in blue, from which we determine the correlation length $\xi$, and the fit of the coldest sample is plotted in grey for comparison. c, The measured spin structure factor obtained from averaged Fourier transformations of single images. A peak at momentum $q_{\text{AFM}} = (\pi/a, \pi/a)$ signals the presence of an antiferromagnet. d, The measured correlation length $\xi$, fitted to equation (1.36), diverges exponentially as a function of temperature, and is comparable to the system size for the lowest temperature. The inset is a semi-logarithmic plot of the same quantity versus inverse temperature. e, The measured staggered magnetization $m_z$ increases drastically below temperatures $T/t \approx 0.4$. We find good agreement with quantum Monte Carlo calculations of the Hubbard model, shown in grey.

tum Monte Carlo predictions at half-filling, which gives $T/t = 0.25(2)$ for the lowest temperature [49].

As temperature increases, the strength of antiferromagnetic order disappears rapidly, until for $T/t = 0.64(6)$ only nearest-neighbor spin correlations remain. For a quantitative analysis of the spin correlations we plot in figure 5.6b a binned azimuthal average of the sign-corrected spin correlator $(-1)^iC_d$ as a function of
distance $d$. For large distances $d > 2$ the measured correlation functions exhibit an exponential scaling with distance, verified by fitting $N_0 \exp(-d/\xi)$ to each data-set, with the correlation length $\xi$ and $N_0$ as free parameters ($N_0$ the same for all fits, since this parameter should not change with temperature, as predicted by the nonlinear $\sigma$ model). For our 2D system quantum fluctuations lead to an increase in spin correlations at short distances $d \leq 2$ above the exponential dependence, most prominently visible in the nearest-neighbor correlator [24]. In figure 5.6d we show the experimentally determined correlation length as a function of temperature, which increases dramatically at temperatures around $T/t = 0.4$. For the lowest temperature we find $\xi = 8.3(9)$ sites, which is approximately equal to the system size of 10 sites, as expected for LRO.

In order to make the theory prediction in figure 5.6d, we perform determinant quantum Monte Carlo on the $10 \times 10$ periodic-boundary 2D Hubbard Model at $U/t = 7.2$ using the QUEST package [10, 22, 36].

The long-wavelength and low-temperature behaviour of our system is expected to be well described by the quantum non-linear $\sigma$ model [9], which contains three fundamental ground-state parameters: the sub-lattice magnetization $M$, the spin stiffness constant $\rho_s$ and the spin-wave velocity $c$. The spin stiffness quantifies the rigidity of an ordered spin system with respect to a twist, and has been calculated to be $\rho_s/t \approx 0.13$ for $U/t = 7$, slightly below the Heisenberg model value [16]. Since the temperatures and correlation lengths are independently determined in our experiment, we can directly obtain an experimental value of $\rho_s$ by fitting the dependence in Eq. (1.36) to the data. The data shows excellent agreement with the predicted exponential scaling of $\xi$ with $T^{-1}$ from Eq. (1.36). From the fit we determine $\rho_s/t = 0.16(1)$, which is larger than the calculated value, possibly due to finite-size effects.
Antiferromagnetic LRO in solid state systems is typically detected by neutron scattering or magnetic x-ray scattering [29]. These methods measure the spin structure factor at wavevector $q$ and along the $z$ direction, given by

$$S^z(q) = \frac{1}{N} \sum_{r,s \in \Omega} \frac{1}{S^z} \langle S^z_r S^z_s \rangle \exp(iq \cdot (r - s)).$$  \hspace{1cm} (5.3)

In a square lattice, antiferromagnetic LRO manifests as a peak in the structure factor at $q_{\text{AFM}} = (\pi/a, \pi/a)$, whose amplitude is directly related to the staggered magnetization $m^z = \sqrt{S^z(q_{\text{AFM}})}/N$. For cold atom systems the spin structure factor can be measured from noise correlations or Bragg scattering of light [29]. The site-resolved detection in our experiment allows for a direct measurement of the spin structure factor, obtained from averaging the squared Fourier transformation of individual single-spin images. The same result is obtained when summing over all contributions of the spin correlation function, see figure 5.7.

For the lowest temperature we observe a sharp peak in the structure factor at $q = q_{\text{AFM}}$, which confirms the presence of antiferromagnetic LRO, see Fig. 2c. For increasing temperatures the amplitude of this peak decreases until it disappears for $T/t \gtrsim 0.64$, indicating the decay of LRO. At these elevated temperatures a broad peak with low amplitude remains, which originates from the remaining short-range spin correlations. We quantify the ordering strength of the antiferromagnetic LRO by the corrected staggered magnetization $m^z_c(T)$, which subtracts uncorrelated contributions and is equal to $m^z$ in the thermodynamic limit (Methods). While initially small at elevated temperatures, $m^z_c$ shows a drastic increase for lower temperatures, see Fig. 2d. We compare the measured temperature dependence to \textit{ab initio} quantum Monte Carlo calculations of the Hubbard model on a $10 \times 10$ site square lattice with periodic boundary conditions and no free parameters. We find agreement over the entire range of temperatures, with residual
deviations possibly caused by the different spatial shape of $\Omega$. The largest measured value of $m_c^z = 0.25(1)$ is more than 50% of the theoretically predicted zero-temperature value in the Heisenberg model for our system size, obtained from finite-size scaling [53].

### 5.4.1 Full counting of the staggered magnetization

Full counting statistics (FCS) represent a powerful tool to characterize quantum states and phenomena in a variety of systems [6, 7, 11, 40]. For example, they have been used to observe the quantization of electrical charge in shot noise measurements [3], the observation of fractional charges in fractional quantum Hall systems [15, 23, 52], and to characterize pre-thermalization in an ultracold atomic
Figure 5.8: **Full-counting statistics of the staggered magnetization operator $\hat{m}_z$.**

**a,** Selected images with one spin component removed (checkerboard overlaid to guide the eye) show a large variation in ordering strength at the coldest temperature. This variation is a consequence of the SU(2) symmetry of the underlying Hamiltonian, which leads to different orientations of the staggered ordering vector relative to the measurement axis $z$, as shown schematically by the spin-vectors. **b,** Measured distributions of $\hat{m}_z$ are plotted at different temperatures. We find excellent agreement with quantum Monte Carlo simulations of the Heisenberg model with no free fitting parameters.

setup [27, 32, 51]. Here we determine the FCS of the staggered magnetization operator $\hat{m}_z = \frac{1}{N} \sum_i (-1)^i \text{ } \hat{S}_z^i$ from an *ab initio* quantum Monte Carlo simulation of the antiferromagnetic Heisenberg model

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j. \tag{5.4}$$

To this end we implement a stochastic series expansion quantum Monte Carlo calculation with operator loop updates [54]. We simulate a $16 \times 16$ system with periodic boundary conditions, and calculate the FCS of $\hat{m}_z$ in a smaller $9 \times 9$ region, which is of similar size as the measurement region used in the experiment. In
our model the spins outside of the measurement area serve as an effective thermal bath, mimicking the experimental setup. The presence of the bath introduces additional fluctuations compared to a system of equal size but with periodic boundary conditions, leading to a further suppression of large values of the staggered magnetization at the lowest temperatures in Fig 5.8.

As shown in figure 5.8, the distribution of measured values of $\hat{m}^z$ shows qualitatively different characteristics at high and low temperatures, imposed by the infinite and zero temperature limits. At infinite temperature, the spins take on uncorrelated random values. In a system of $N$ measured sites, the FCS has thus the same distribution as $N$ independent coin flips, which approaches a binomial distribution of width $1/\sqrt{N}$ for large system sizes.

The underlying Hubbard Hamiltonian that describes our system is SU(2) symmetric. In the absence of a symmetry-breaking field, the staggered spin-ordering vector $\hat{\mathbf{m}} = (\hat{m}^x, \hat{m}^y, \hat{m}^z)$ is expected to point in random directions on a sphere between different experimental realizations. Consequently, individual measurements of the projection $\hat{m}^z$ are expected to show a large variation. This is directly observable in our experiment, as we can measure independent values of the staggered magnetization operator $\hat{m}^z$ from single experimental realizations, see Fig. 5.8a.

The variation of the staggered ordering can be quantified from a histogram of all measured values of $\hat{m}^z$ across different experimental realizations, which corresponds to the full-counting statistics (FCS) of the operator $\hat{m}^z$. The FCS provide a powerful tool to characterize many-body systems beyond average values [32], but so far have not been measured for the antiferromagnetic phase. Fig. 5.8b shows the measured histograms of the staggered magnetization along the $z$-direction for different temperatures at half-filling, obtained from over 250 images each.
Alternative basis measurement. We optionally apply a $\pi/2$ or $\pi$ RF pulse prior to the spin removal pulse and correlation measurement. The sign-corrected spin correlation functions show an insensitivity to the presence and duration of this RF pulse, consistent with an SU(2) symmetry of the state.

All distributions are symmetric and peaked around zero with expectation values $\langle \hat{m}^z \rangle$ consistent with zero. Both observations are consistent with a randomly oriented ordering vector. The width of the distributions is characterized by the standard deviation $m^z$ defined in Eq. (1.35). At the highest temperature the distribution is consistent with the infinite temperature expectation, where the entire finite-size sample of $N$ sites is uncorrelated. There, a binomial distribution is predicted with a width $m^z(T \to \infty) = 1/\sqrt{N} = 0.1125$, which agrees with the experimentally measured value $m^z = 0.12(2)$. At lower temperatures the width of the distribution grows substantially and sensitively depends on temperature, but still remains peaked around zero. The experimental data is in excellent agreement with ab initio quantum Monte Carlo calculations of the Heisenberg model at the experimentally determined temperatures. These findings show that the lattice thermometer based on nearest-neighbor correlations employed here is correctly calibrated and accurate down to fractions of the tunnelling.

Additionally, we find consistent spin correlations when measuring along a spin direction perpendicular to the $z$-axis via a $\pi/2$-pulse, see figure 5.9. SU(2) symmetry predicts that correlations would exist along every possible measure-
ment axis. To verify this, we added a $\pi/2$ pulse prior to the selective spin removal pulse and measured correlations as before. Figure 5.9 shows that the correlations at all length scales are insensitive to the applied RF field, regardless of whether no pulse, a $\pi/2$ pulse, or a $\pi$ pulse is performed. This outcome is consistent with but not sufficient for a claim that the underlying state is SU(2) symmetric. In the future, a more elaborate measurement would entail measuring the correlations along different bases in different parts of the same cloud, and would thus be more convincing.

5.4.2 Doping the antiferromagnet

While theoretical predictions at half-filling are available down to low temperature, this is not the case for doped systems due to the exponential scaling of the fermion sign problem with inverse temperature, system size, and interactions in this regime [60]. We can directly study the effect of doping on LRO in our experiment by reducing the density of our sample and measuring the spin structure factor. Within the region $\Omega$, we add a potential offset with the DMD for controlled hole doping, which is also expected to slightly change the temperature. The hole doping $\delta$ is deduced from the measured single particle density $n_s$.

As shown in Fig. 5.10, the strongest magnetic correlations remain at $q = q_{\text{AFM}}$. Doping gradually suppresses $m^z_c$, broadens the magnetic ordering peak in $S^z(q)$ and reduces its weight. Only at $\delta \gtrsim 0.15$ we find that $m^z_c$ settles to an approximately constant, small value. This offset originates from the strong short-range correlations still present at large dopings, see figure 5.10b. When excluding the contributions of $d < 2$ from $m^z_c$, this offset partially disappears while the qualitative dependence $m^z_c(\delta)$ remains approximately the same, see figure 5.11. This suggests that for the finite size $U/t = 7.2$ Hubbard model studied here, strong magnetic correlations persist up to a critical hole doping $\delta_c \approx 0.15$. We note that
Figure 5.10: Doping the antiferromagnet. a, We move horizontally in the phase diagram by doping the system with holes (inset), where $0.0 \lesssim \delta \lesssim 0.25$. The staggered magnetization $m^z_c$ settles at $\delta_c \approx 0.15$. b, The magnitude of the sign-corrected nearest-neighbor correlator decreases less rapidly with hole doping than correlators at larger distances. For large doping, only the nearest-neighbor correlator is appreciable, so this correlation is predominantly responsible for the non-zero staggered magnetization away from the antiferromagnetic phase. c, We show the spin structure factor, as in Fig. 2c, for each doping value.

our data may still be consistent with incommensurate magnetism commonly observed in high-$T_c$ cuprates [63], since in our current experiment finite size effects and temperature broadening may prevent us from observing resolved peaks at wavevectors close to $q_{AFM}$.

5.4.3 Data analysis.

All quantities presented in this work are extracted from a circular section of 10 lattice sites in diameter, denoted $\Omega$. This disk is centred at the centre of mass of sites exceeding 80% filling, as measured from the images with no spin removal. Sites are included in $\Omega$ if the centre of the site is within the bounds of the circle. Since
Figure 5.11: **Staggered magnetization obtained from spin correlations, with and without nearest-neighbor contribution included.** To investigate the contributions to the staggered magnetization at high dopings, we consider the staggered magnetization calculated from the spin correlator. For all points shown, we omit the longest-range correlations, which have the greatest level of noise due to the low number of pairs of sites extending across the cloud. The red points shown also omit the nearest-neighbor correlations, essentially the only non-zero correlator outside of the AFM phase. In the high-doping regime, we see that the greatest contribution to the staggered magnetization is the nearest-neighbor correlation, followed by the noisy longest-range correlations. The value of the staggered magnetization without either of these contributions is plotted in red.
the centre of mass is a non-integer coordinate, our system sizes vary between 75 and 81 sites depending on the exact location of the centre within a lattice site. We find that in all cases, the filling is constant across the disk. The entire region $\Omega$ is then used for all calculations of spin correlations, spin structure factor, and staggered magnetization. We determine the temperature of each sample by comparing the largest measured nearest-neighbor correlator in $\Omega$ to quantum Monte Carlo predictions at half-filling [47].

We calculate the average site-resolved spin correlator for a given displacement, $C_{d}$, by averaging the correlator over all pairs of sites within $\Omega$ with the given displacement. We extract this quantity using the method described in previous work [49]. Displacement vectors that have less than 100 total pairs of sites across all images are discarded. To calculate the spin correlation function versus distance, the displacements are split into bins of 0.3 sites, and averaged across. Because of the non-integer centre of $\Omega$, the largest distances may appear infrequently, so we discard bins for distances of larger than 5 sites if there are less than 5 contributions in that bin. Errors on the spin correlator are calculated as in previous work [49], and the errors on the spin correlation function are propagated using conventional techniques assuming the spin correlation errors are distributed normally.

For the structure factor we first inscribe the circular section $\Omega$ into a minimal-size square. In the associated occupation matrix atoms are denoted as 1, unoccupied sites denoted as -1, and sites introduced from placing the circular section in a square array denoted as 0. We compute the magnitude squared of the Fourier
transform of this array and average across all experimental realizations,

\[
\langle |\mathcal{F}(q)|^2 \rangle = \left\langle \sum_{r,s} e^{iq \cdot (r-s)} (\hat{S}_r^z + (\hat{m}_{0,r}^z)^2 - 1)(\hat{S}_s^z + (\hat{m}_{0,s}^z)^2 - 1) \right\rangle
\]

\[
= N S^z(q) + \left| \sum_r e^{iq \cdot r} \left\langle (\hat{m}_{0,r}^z)^2 - 1 \right\rangle \right|^2
\]

\[
\implies S^z(q) = \frac{1}{N} \left( \langle |\mathcal{F}(q)|^2 \rangle - \left| \sum_r e^{iq \cdot r} \left\langle 1 - (\hat{m}_{0,r}^z)^2 \right\rangle \right|^2 \right),
\]

where \( N \) is the number of sites, \( S^z(q) \) is the spin structure factor, \( \hat{S}_r^z \) is the spin operator at site \( r \), \( (\hat{m}_{0,r}^z)^2 \) is the local moment operator, and due to spin balance \( \langle \hat{S}_r^z((\hat{m}_{0,s}^z)^2 - 1) \rangle = 0 \). Errors are calculated by assuming the distribution of \( S^z(q) \) is normal. Though there are finite bounds on the possible values of the spin structure factor, the histograms in Fig. 3 demonstrate that the assumption of normality is reasonable.

In the thermodynamic limit, the RMS staggered magnetization is

\[
m^z = \sqrt{\frac{1}{N} S(q = (\pi/a, \pi/a))}.
\]

(5.6)

For finite systems this expression is non-zero even in the paramagnetic limit. We remove the finite offset and normalize such that the minimum value is 0 in the absence of spin correlations and the maximum value is unity:

\[
m^z_c = \sqrt{|S^z(q_{AFM}) - S^z(0)| \sqrt{N/(N^2 - N)}}.
\]

(5.7)

Errors are propagated from the computed spin structure factor using standard techniques. We verify that the value resulting from the Fourier-based computation agrees with the value obtained by summing individual site-resolved spin correlations, which explicitly accounts for doublons and holes in the sample, see figure 5.7 (due to spin balance \( \hat{S}_r^z = 0 \)).
5.5 Conclusion

We have realized a quantum antiferromagnet governed by the 2D Hubbard Hamiltonian. Our architecture makes it possible to vary the doping and temperature, enabling us to explore the Hubbard phase diagram in theoretically challenging regimes. Attainable parameters are predicted to be sufficient to access the conjectured pseudogap [60] and stripe ordered [42] phases. At lower temperatures $T/t \approx 0.05$ and dopings $\delta \approx 0.15$, theoretical work indicates a transition to a d-wave superconducting state [42]. Such temperatures could be achieved through advanced entropy redistribution schemes. Furthermore, entirely novel states of matter are within reach by augmenting the Hamiltonian with alternative lattice structures, artificial gauge fields, and dipolar long-range interactions.

5.6 Bibliography


Chapter 6

Outlook and works in progress

“Highly organized research is guaranteed to produce nothing new.”

- Frank Herbert, Dune
6.1 Introduction

The goal of this work has been to demonstrate the utility of the Fermi gas microscope in addressing interesting problems in condensed matter physics, focusing on magnetic order in the Hubbard model. Although interesting, these problems are only the beginning, and this chapter will discuss the future experimental outlook for this platform and demonstrate some early results. Please note that all data shown is preliminary and should be considered only as a promising beginning.

Broadly speaking, there are three groups of experiments that can be addressed with feasible upgrades (or even no upgrades at all) to the machine:

1. **Time-dependent measurements**

2. **Measurements at lower temperatures**

3. **Hubbard model engineering**

Although these three paths are inter-related (e.g. lattice engineering may lead to lower temperatures), they promise to illuminate different aspects of many-body physics in the Hubbard model.

6.2 Time dependent dynamics: quantum walks and quantum magnetism

A class of challenging problems stemming from the Hubbard model focuses on the many-particle dynamics of the constituents. Such experiments may probe the global response of a system to a global, time-dependent perturbation (such as a change in the lattice depth or structure), or the propagation of a localized excitation, (such as a hole). Such experiments are exceedingly challenging in condensed matter architectures, since characteristic frequencies quickly exceed hun-
dreds of THz, and have only recently become possible in condensed matter platforms through the use of atto-second spectroscopy [8].

Similarly, quantum Monte-Carlo simulations - traditionally extremely powerful, struggles with dynamics [7] due to the exponentially scaling of computation time with system size. Numerical studies using the time-dependent density matrix renormalization group (tDMRG) [28, 29] have indeed have been used with great success in 1D, but still suffer from an $O(\exp L)$ scaling in 2D, where $L$ is the characteristic side length of the system under study [32]. Happily, quantum gas microscopy is uniquely well suited to these tasks, because the geometry of the potential and the lattice can be finely tunable and real-time control and readout is trivial.

The classical random walk is a prototypical scenario in statistics, applying to diverse situations from Brownian motion [9, 12] to finance [4]. Typically, a random walk is a path composed of a series of steps drawn from some well-behaved distribution. A simple variant of a discrete random walk is shown in figure 6.1a - a particle starts on a site, and, at every time step, has equal probabilities of remaining on that site, moving left and moving right. This results in the well known scaling where the average distance away from the initial site, $x_{\text{RMS}}$, scales as $x_{\text{RMS}} \propto \sqrt{t}$, a consequence of the central limit theorem (CLT).

Charge carriers in a solid can also sometimes be modeled as following a classical random walk [22]. Loosely speaking, this is not entirely surprising in the limit of strong decoherence, because decoherence will bound the “memory” of the particle, and satisfy the conditions for the CLT to apply.

---

1. Note that this is still a huge improvement over exact diagonalization, which would scale as $O(\exp L^2)$, since the number of lattice sites scales as $L^2$.
2. This is a rather arbitrarily constructed random walk meant to demonstrate qualitative behavior only. I refer the interested reader to look at Wiener processes [12].
3. Assuming independent and identically distributed (IID) steps, the variance of the sum of the steps $\sigma_T^2$ will be the sum of the step variances $N\sigma_s^2 = \sigma_T^2$. 

160
Figure 6.1: (a) Propagation of a particle performing a classical random walk. (b) Propagation of a particle performing a quantum random walk.
Quantum mechanical carrier propagation in the absence of decoherence is a harder problem that exhibits qualitatively different behavior. Let us consider the simplest situation first: that of a single particle placed in a 1D lattice. In this case, the Hamiltonian is the tight binding model:

\[
\hat{H} = -t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma}, \tag{6.1}
\]

where \(\langle i,j \rangle\) are nearest neighbors and \(t\) is the tunneling matrix element as before. Assuming that the particle started at site 0, the probability of finding it at site \(i\), time \(T\) later is given by [10]

\[
\rho_i(t) = |J_i(2tT)|^2, \tag{6.2}
\]

where \(J_i\) is the Bessel function of \(i\)-th order. This behavior is shown in figure 6.1b, and differs from the diffusive case in that the RMS displacement scales linearly with time because the system does not decohere.

Although fundamentally interesting, a single particle propagating over a fixed potential is not a full description of real materials, where a charge carrier, such as a hole, can interact with the spin background of the system, resulting in an interesting many-body state. This interaction is interesting even before any dynamics are considered, as seen in the phase diagram described in chapter 5, or in the Nagaoka theorem, where the presence of a single hole dramatically alters the ground state of a Hubbard system [26, 34].

The physics becomes even richer when dynamic behavior is considered, and this is an active field of research [7, 16]. Numerical simulation of hole dynamics in a 2D lattice system has promised several interesting features. These studies suggest that even under unitary evolution, a hole does not follow a ballistic (\(x_{\text{RMS}} \propto T\)) trajectory since interactions with the magnetic structure of the background spins cause further corrections (even if the background is disordered) [7], an idea closely
tied to that of dissipationless decoherence [11, 25]. Further, the propagation of a hole can actually impart a significant degree of correlations to the system [16].

Thus far, experimental studies of quantum walks using single or few bosons have been performed [17, 36], including at the site-resolved level [27]. These experiments measured the basic behavior described by equation (6.2), and more interesting phenomena, including Bloch oscillations [5].

Fermi gas microscopy has the ability to push this even further. The numerical approach in [7] relied on generating an appreciable fraction of the possible paths that a hole could follow, where each path contributed to the probability density of finding the hole at the endpoint. In an $n \times n$ site system, this requires $O(4^n)$ possible paths (assuming only nearest neighbor tunneling). In contrast, an experimental system would require a number of experimental realizations scaling only as $O(n^2)$. The difference between these scalings suggests that Fermi gas microscopy can reach numerically intractable regimes.

The ability to address individual lattice sites with high fidelity, as demonstrated in chapter 4, can be exploited to prepare the starting states necessary for explorations of single hole propagation. This is typically done by illuminating a small region of the DMD, corresponding to a single lattice site, and raising the local chemical potential to such a level that the site is not populated during lattice loadings. Once the lattice is loaded, this “plug” can be removed, and the hole is effectively released.

6.2.1 Preliminary experiments

Although we have yet to perform a full, careful study of hole propagation in a 2D lattice, we have performed a number of experiments in 1D. There are two reasons why 1D is an excellent starting point:
1. The 1D theory is fully understood and can serve as verification that the experimental procedure functions as advertised.

2. Many fewer experimental cycles need to be run, as multiple independent 1D systems can be created and measured in a single cycle.

As a preliminary series of experiments, we created Mott insulators in the manner of [14], while projecting a blue detuned line of light down the center, with a depth of approximately 10 kHz, above the chemical potential. The system is then made anisotropic with a ratio of \( \approx 10 \) between the tunneling in the weakly confining direction to the tunneling in the strongly confined direction. It is naively tempting to raise the tunneling along the blocked off direction as high as possible, to completely prevent tunneling along that direction. This is not practical, however, since that simultaneously raises the harmonic confinement along the tunneling direction. The factor of 10 was chosen as a compromise such that the effects of the harmonic potential were negligible over the propagation distances considered, while simultaneously limiting propagation along the forbidden direction to \( \ll 1 \) tunneling event. The blue detuned light field is then snapped off in approximately 100 ns (limited by the AOM), which is effectively instantaneous, as far as the system is concerned. The distribution of atoms at \( T = 0 \) and a few tunneling times later is shown in figure 6.2. Every experimental cycle 15 1D systems can be reliably prepared. After imaging, rows with \( \neq 1 \) hole are eliminated, with a post-selection rate of 50 – 55%.

To measure the probability density as a function of time, the experiment is prepared as described and the system is allowed to evolve for a varied amount of time (typically ranging between zero to a few tunneling times). After the occupation is measured, we post-select 1D tubes based on having exactly one hole. The resulting distribution can be estimated with a histogram of hole occupation at each measured time, and is shown in figure 6.3. Fitting the distribution to a model
Figure 6.2: **Simulating the propagation of a single hole on a 1D lattice.** (a) Hole positions immediately upon release. (b) Hole positions approximately 3 tunneling times later. Note that the data is post-selected on having exactly one hole in each row.
based on equation (6.2) results in the comparison fits shown in the figure, reflecting excellent agreement.

The correlated propagation of multiple particles is also interesting because it can be a clear manifestation of quantum statistics. In an experiment with bosons [27], a pair of weakly interacting bosonic particles prepared on adjacent sites tended to be positively correlated due to the constructive interference of correlated paths and destructive interference of anti-correlated paths, also known as bunching. The case of fermions can be considered in an analogous way, although the behavior is exactly inverted, and the interference effects lead to the constructive interference of paths that lead the particles away from each other.

The single-hole experimental procedure can easily be scaled to produce multiple holes by “plugging” several sites at once and simultaneously releasing the produced holes, as shown in figure 6.4. We can then directly measure the correlation function of a pair of holes in 1D, as shown in figure 6.5, which clearly shows that the holes exhibit strong, anti-correlated behavior.

This situation contains one subtle feature - the background particles can be in one of two spin states. In the limit of infinite spin species present in the system, each particle is effectively distinguishable, and quantum statistics would no longer play a role. In the limit of only a single species of fermions present in the background, holes can be exactly mapped onto particles [6]. Thus, although the interference contrast is reduced, a significant degree of anti-bunching exists in the two spin case studied here.

Measuring the propagation of a hole in 2D poses a more significant technical challenge, primarily due to the larger amount of data required. As previously stated, to estimate the probability density, it is necessary to analyze $O(N)$ hole propagation experiments, where $N$ is the number of lattice sites that the hole might reach. Clearly the number of lattice sites that the hole can reach scales as $O(T^d)$,
Figure 6.3: Time resolved lattice filling, showing the propagation of a single hole. (a) Quantum walk on a shallow lattice. (b) Quantum walk on a deep lattice. The behavior is observed to be essentially identical, but on very different timescales.
Figure 6.4: Propagation of a pair of holes on a 1D lattice. (a) Hole positions immediately upon release. (b) Hole positions approximately 3 tunneling times later.
where $d$ is the dimensionality. Further, performing multiple hole propagations in a single experimental cycle is more challenging, as the systems cannot be packed as densely as 1D tubes. Altogether, it means that for a fixed system size a few sites wide, $\approx 20$ times more data is required. Figure 6.6 shows the clean preparation and release of a single hole, and figure 6.7 shows a preliminary data set showing the distribution of final hole positions in a small system. The propagation time and data quality are unfortunately insufficient to make any non-trivial statements about the dynamics. Happily, the stability of the experimental system has been improved significantly since this data was taken, and thus there is a strong possibility that taking a longer data-set will be possible.

The propagation of holes on a spin background is not the only interesting experiment probing dynamics - it is easy to envision using a Fermi gas microscope
Figure 6.6: Propagation of a single hole on a 2D lattice. (a) Hole position immediately upon release. (b) Hole positions approximately two tunneling times later.
Figure 6.7: **Time resolved lattice filling**, showing the propagation of a single hole in 2D. Note that this data is preliminary to study transport [19, 20], many body localization [1, 30], or quantum quench dynamics [18], among others. Even better, many of these experiments can be carried out with either minimal or no hardware changes.

### 6.3 Entropy redistribution

At present, one of the major goals of experimental studies of the Hubbard model is the realization of a high critical temperature $T_c$ superconducting phase [24, 31]. This phase is expected at hole dopings of $\delta \approx 0.10$ and temperatures $T_c/t \approx 0.05$, currently beyond experimentally accessible regimes. Several cooling schemes have been proposed that promise to solve this problem [3, 23] using advanced entropy redistribution. Both schemes in these proposals exploit the low local entropy $s$ of the band insulating state. Although this state is not physically interesting, adiabatically changing the filling from two particles per site to half filling can, in principle, result in an exceptionally cold Mott insulator.
In practice, these schemes build on the scheme used in chapter 5, where entropy was redistributed between an AFM state and the surrounding reservoir. The efficacy of this scheme is limited because there is no energy gap between the AFM state and excitations, meaning that the excitations can cost very little energy, which limits the amount of entropy pushed into the reservoir. This is not the case for a band insulator prepared in the redistribution region instead of an AFM state. There, excitations can either take the form of three particles on a site (which is very rare, since the energy cost is equal to the bandgap), or one particle on a site (costing the energy difference between the chemical potential in the middle of the trap and the reservoir). This “gapped” behavior leads the band insulator actively expel entropy into the reservoir and achieve a much lower entropy per particle than for the AFM states shown in chapter 5.

Figure 6.8a shows an experimentally realized band insulator in the middle of an entropy reservoir. Due to the parity imaging, the band insulator manifests as a disk of empty sites. Repeated measurements allow us to estimate the single particle filling of every lattice site in the middle of the redistribution region, shown in figure 6.8, found to be \( \leq 2\% \) within a radius of 3 sites from the center. Outside this range, we find that the fidelity of the band insulator is degraded by the edge of the redistribution pattern light field. Based on 54 images, a 2\% single particle occupation bounds the entropy per particle \( s \leq 0.1k_B^4 \), and substantially lower entropies may be possible in the near future.

The challenge, of course, is to remain adiabatic as the number of lattice sites is doubled, either using a super-lattice [23], expandable ring [3] or another method. The adiabatic timescales required for all transformations pose enormous technical

\[^4\text{This is a relatively conservative upper bound - within a smaller area, we measure a single particle occupation < 0.1\%. Further, recent progress in the lab suggests that we can do an even better job of isolating individual regions of the low entropy band insulator without artifacts from the edge of the redistribution light field.}\]
challenges. Preserving the low entropy of the state may require engineering the lattice lasers for even lower noise, dynamically tuning the lattice geometry, or other highly non-trivial steps. I expect this will be challenging, but the rewards will be well worth it.

6.4 Engineering lattice geometries

Every experiment performed in relation to this work has been in a simple square lattice. Having demonstrated site-resolved imaging and addressing, the ability to dynamically control the lattice geometry is the final component that could open a qualitatively new class of studies of the Hubbard model using our experimental platform. Dynamically shaping the lattice can make it possible to cool the system, as discussed in section 6.3, dramatically alter the Hamiltonian [13, 15], and introduce frustration into the system [2, 21, 33].

6.5 Conclusion

I expect that the coming years will prove very exciting, and will see the realization of amazing quantum states and the point where quantum simulation will conclusively surpass computational studies for certain classes of problems [35]. I am equally sure that the experiments that prove most interesting are not the ones described in this chapter, but ones that will emerge naturally from trial and error.

Naturally, there will be no shortage of challenges ahead. Taking a high-level view, I expect that the major issue for our and other machines will be carefully managing added complexity and scalability - sub-systems that worked “well enough to take data” will have to be rebuilt or improved until the users can effectively forget them. High quality, continuous monitoring of all vital sub-systems
Figure 6.8: **Band insulator cooled with entropy redistribution.** Much like in the AFM case, a BI can be cooled using entropy redistribution. (a) A typical image of a single BI that lies within the central region of a redistribution potential, in exact analogy to chapter 5. (b) Averaging many lattice occupations allows the determination of the spatially resolved single particle occupation, shown here.
has to be implemented and used\textsuperscript{5} The process of making the experiment “commercial grade” has already begun, largely due to the careful engineering that went into the experiment from its inception, and that I hope will continue. While difficult and time-consuming, a disciplined and precision-engineered approach, is the one that I expect will lead to greatest success in the long run.

Overall, the future is bright for Fermi gas microscopy.

6.6 Bibliography


\textsuperscript{5}This is something that has proven very useful in recent years in our lab - when problem occur during long data-sets, our experiment contacts the users over email and Slack.


Appendix A

Analysis of site-resolved images
In order to identify site occupations in the optical lattice, we use a Wiener deconvolution from the scikit-image toolbox [2] to generate the image from which we determine the site amplitudes for binarization. An example deconvolution, histograms for images with and without spin removal, and a binarized image can be found in figure A.1.

A.1 Bibliography


\[\text{1This text is reproduced from [1]}\]
Figure A.1: Deconvolved image, reproduced from [1]
Appendix B

Water System
**Water Cooling System**

**B.0.1 Water exchange procedure**

To prevent algae from contaminating the water system, the water reservoir should be replaced once a year.

To do this:

1. Remove all the connections from the top of the 105 gal tank and remove the black cap.

2. Put the hose on the inlet of the small black “portable utility pump” through the top of the 105 gal tank. Put the hose on the outlet of the pump into the drain that’s under the DI faucet (be sure to put the hose under both grates.

3. Start the pumpout ( 7 min). This pump can leak, so have some absorbent pads around. The hose had a tendency to stick to the side of the tank, so one person should watch it at all times. Stop the pumpout when you can see the intake for the OptiTemp, but leaving it submerged.

4. Fill the tank 1/2 way with DI water. Add 2 gallons of Citrajet (2%) then fill the rest of the way. Total time 8 minutes.

5. Put the connections back on the top of the tank and start the OptiTemp.

6. Let it run for 50 min to 1 hour.

7. At the end, turn off the OptiTemp and repeat the previous steps at least one more time. Twice if you’re patient.

8. After finishing the Citrajet cleanse, pump out the tank again and fill with pure DI water. Run the OptiTemp to flush the lines of Citrajet. (Duration ≈ 30 minutes. Opinions vary about leaving Citrajet in the lines. Just optishield should be sufficient, so long as it is not expired.)
Figure B.1: Water cooling layout
9. Pump out the tank one more time. Fill with a 10% solution of OptiShield II Plus (15 gal if you want to account for the water in the lines).