Nanoscale magnetic atom chips for quantum simulation

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Nanoscale magnetic atom chips for quantum simulation

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The work described in this thesis was carried out in the group "Quantum Gases and Quantum Information", at the Institute of Physics of the University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands, where a limited number of copies of this thesis is available. A digital version of this thesis can be downloaded from http://dare.uva.nl

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To Physics,

for keeping me happy and busy for all those years.
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Introduction

The milk production at a dairy farm was low, so the farmer wrote to the local university, asking for help from academia. A multidisciplinary team of professors was assembled, headed by a theoretical physicist, and two weeks of intensive on-site investigation took place. The scholars then returned to the university, notebooks crammed with data, where the task of writing the report was left to the team leader. Shortly thereafter the physicist returned to the farm, saying to the farmer "I have the solution, but it only works in the case of spherical cows in a vacuum."

"To study material systems, theorists create "spherical-cow" models of real materials, while in cold atomic physics experimentalists actually make spherical cows", (Galitski and Spielman) [1].

Jokes about the strange abstraction that physicists make are probably around since the days of Newton. They ridicule how detached physicists may become from the nature that they study. But it is here, in the void between ill understood systems in nature and extreme theoretical abstraction where experimental quantum simulation tries to shed some light [2]. Based on abstract Hamiltonians we build systems of interacting quantum mechanical particles to mimic similar systems in nature. Most often lattices of particles are studied which are the spherical cows that arise after a strong abstraction from solid state materials [3, 4, 5]. Several problems that have been studied in the context of condensed matter physics for decades have recently been simulated in the atomic physics community [6, 7, 8, 9, 10, 11]. These simulations give more insight in the physics of complex systems and allow us to study phase diagrams, ground states, critical exponents and the dynamics of (strongly) interacting quantum systems [12, 13, 14, 15].

By building, studying and controlling quantum simulation experiments we learn about the elements that govern nature at the quantum scale. Because we build, study and control we learn about the quantum world in three different ways. I) We learn what key elements are required to simulate a certain phenomenon by building a quantum simulator out of individual particles and interactions. II) We learn about the (mis-)match between our simulations and other quantum systems in nature by studying the relations between our results and the results of measurements on for example solid state materials. III) We learn how to use quantum-mechanical tools to our advantage in industrial applications by exploring techniques to control quantum matter. The work in this thesis is motivated mainly in terms of the second aspect: the fundamental questions that we hope to study concern large systems of interacting particles in two-dimensional lattices. However, the majority of this work concerns the construction of an experimental apparatus with which we hope to do this. The thesis also contains technology on how to make nanoscale magnets that might be useful in future applications such as magnetic field sensors and hard discs. Because of these different aspects the chapters in this thesis are quite diverse in nature. With the
"spherical-cow" models in mind we theoretically design and numerically simulate several crystal geometries. Then we build crystalline potentials out of nanoscale magnets using nano-technology and consider the use of these magnets in various applications such as force sensors. Finally we assemble the experimental apparatus in which quantum simulations with ultracold atoms and magnetic nano-scale potentials will be done. To introduce the topic of magnetic lattices for quantum simulation we first consider the differences between optical and magnetic lattices. Then we show how we will exploit the benefits that magnetic lattices provide to engineer new lattice potentials and how to scale them down to create lattices at unexplored length scales.

1.1. Quantum simulation with lattices

In this thesis and in most quantum simulation studies an effort is made to create atomic lattices to simulate crystalline materials. Starting point for many of these experiments has been the optical lattice (OL) [16, 17]. Here a standing wave of laser light is used to order gaseous ultracold atoms in lattices of 1, 2 or 3 dimensions by confining the particles around the points of lowest intensity. These breakthrough experiments have led to hundreds of experiments in the last 15 years that enriched the basic cubic optical lattice with more features that enabled richer and more advanced simulations. This was done by combining the optical lattice with more optical techniques [18, 19], and by using other gases [20, 21, 22, 23], and by using combinations of gases [24, 25] and by adding other electromagnetic fields [26, 27, 28, 29]. Through these methods new lattices can be created and interactions can be tuned in both space and time with optical and magnetic fields [17, 30, 31]. The combination of all these techniques has resulted in a large toolbox for quantum simulation experiments to use.

Two topics that still drive the advancement of quantum simulators are scalability and the creation of strong interactions. Both these topics could benefit from smaller lattices since this would increase both the interactions in between lattice sites as well as the number of particles that are involved. However the optical lattice is limited by the wavelengths of lasers that are available. What all optical lattice experiments have in common is that their fundamental lattice is made by one or more lasers with a typical wavelength of approximately 900 nm and therefore a lattice constant of approximately 450 nm. This lattice spacing is fixed by the laser wavelength and is fundamentally perfectly periodic in nature. These aspects both limit the development of smaller, more versatile and non-periodic lattices. Therefore various research teams investigate other techniques to create quantum lattices.

1.2. Permanent magnetic atom chips

In our group such an alternative technique to create atomic lattices has been developed over the last ten years. To study systems of mesoscopic ensembles and interacting Rydberg atoms lattices of $22 \times 36 \mu m^2$ and later of $10 \times 10 \mu m^2$ period were realized [32, 33]. The technique that we have developed for this purpose is fundamentally different from optical lattices because it does not depend on standing wave patterns but uses permanent magnetic fields to trap the atoms. The $\mu m$-sized lattices were made by optical lithography on films of 200-300 nm thick FePt. The patterned films created strong permanent magnetic fields with which it is possible to capture hundreds of atoms per trap. By controlling external
magnetic fields we showed that the traps could be moved over several lattice periods and that the mesoscopic clouds could be cooled down to Bose-Einstein condensates [34, 35]. Atoms that are excited to a Rydberg state can be used to create interactions in between such clouds. With such interactions a quantum simulator can be built just like the optical lattice [36]. In this thesis we will not focus on the Rydberg physics but we will try to create interactions in between lattice sites in an other way.

By scaling down the magnetic patterns we plan to reach sub-micron lattices. Also lattices with smaller spacings than possible with optical lattices are created [37]. To reach these scales new lithography techniques are required and more elaborate imaging and control over the loading process is essential. This thesis contains the considerations and preparations for new experiments with smaller lattices, as well as the fabrication of these new lattices. A procedure was developed to create magnetic lattices with a minimal lattice spacing of 250 nm. To create this new experiment not only new chips were required but also a completely new vacuum system was built to house the experiment. Several new technical features were developed for this new machine such as a loadlock mechanism to load chips into the experiment and a movable in-vacuum lens to image the atoms.

1.3. Overview

In chapter 2 we will introduce magnetic lattices. We show how we can design them with mathematical tools and we develop some new geometries for trapping atoms. In chapter 3 we simulate atoms in these newly developed traps using a quantum Monte Carlo technique (QMC). These new geometries lead to experiments that are unique to magnetic-trapping based quantum simulation. The simulations using QMC provided more insight in the physics that we want to study and underline the importance and promising nature of the proposed experiments. The 4th chapter describes the fabrication of the magnetic atom chip. While fabricating this new chip a side project was started in cooperation with an experimental group in Leiden to use a single nanomagnet as a tip for sensitive magnetic field measurements. The results of that experiment and its implications for future research can be found in chapter 5. Finally, chapter 6 describes the construction of the new atom chip experiment where we combine ultracold atoms with the magnetic chip.
2 | Novel magnetic lattices for quantum simulation experiments

2.1. Introduction

Experiments with cold atoms trapped in crystal-like trapping potentials have recently offered many new insights in condensed matter phenomena [4, 5, 38, 39, 40]. It is the unprecedented control over many-body quantum systems that these quantum simulators have which allows experimentalists to study increasingly complex systems. It is the hope of many that by these means it will be possible to emulate some of the outstanding challenges of the condensed matter community like high-$T_C$ superconductivity [41], frustrated magnetism [42] and even high energy gauge theories like QCD [43]. Most results of the past decade have been obtained in optical lattice experiments where artificial crystals are created by standing waves of laser light. These experiments are mostly focused on crystals with open or harmonically confined boundaries and a single lattice type. The method of chip-based magnetic trapping provides an alternative to optical lattices where one has more freedom in the construction of trapping geometries and length scales. The first lattice of magnetic traps with magnetic film chips was created in 2007 [32]. Here the lattice was created by a series of magnetized strips with a zig-zag edge, resulting in a rhomboid lattice of $22 \times 36 \, \mu m^2$. More recent work [33] indicated that trapping superfluid gases in permanently magnetic lattices is a feasible and scalable technique. A one-dimensional lattice with a period of 10 $\mu m$ was created in Melbourne [44] and Amsterdam two-dimensional square and triangular lattices, also a period of 10 $\mu m$, were created on the same chip [33]. Currently many efforts are taken to scale the systems down further to the sub-micron regime [45] and even below the limits of optical lattices [37]. At these length scales tunneling in magnetic lattices becomes possible in depending on the lattice geometry. So far only one-dimensional lattices in which tunneling is possible were known [37, 45]. Here we create new geometries in which two-dimensional tunneling becomes possible. Also a large effort is made to exploit Rydberg interactions over several microns to create quantum simulation and quantum information experiments with mesoscopic clouds of atoms in lattices of (3-10) $\mu m$ [46, 47]. The mentioned experiments all contain triangular and square geometries in two-dimensional and elongated one-dimensional traps [44].

In this chapter we present several new geometries that can be used for trapping purposes and that will allow many new quantum simulation studies. Kagome, hexagonal (honeycomb) structures will be presented first and may be used for Rydberg experiments to study frustration and quantum magnetism in two dimensions and at interfaces. Then low-dimensional ladder and diamond-chains are introduced which may be used in Rydberg experiments to study low-dimensional magnetic phases of spin models. Tapered structures with varying length scales are presented in section 2.5. These tapered structures provide a new loading mechanism of sub-wavelength traps which will be discussed in the last section.
In the final section of this chapter new geometries are introduced in which tunneling is possible. To restrict tunneling in one-dimensional arrays magnetic fences are introduced. Both fences and tapers can also lead to experiments in their own regards like transport studies in restricted or varying geometries. Not all magnetic two-dimensional lattices can be scaled down to enable tunneling experiments. In many geometries tunneling becomes impossible due to increased Majorana losses. A new lattice geometry is presented in which two-dimensional tunneling is possible.

2.2. Magnetic fields of patterned films

We assume that the spin of a moving atom follows the local direction of the magnetic field \( \mathbf{B}(r) \) adiabatically. The magnetic potential energy \( -\mathbf{\mu} \cdot \mathbf{B}(r) \) is then proportional to the magnitude of the field, \( U(r) = \mu_B m_F g_F B(r) \). Here \( \mu_B \) is the Bohr magneton, \( m_F \) is the magnetic quantum number and \( g_F \) the Landé factor for an atomic level with total angular momentum \( F \). Atoms in a 'low-field-seeking' state (with \( m_F g_F > 0 \)), can thus be trapped in a local magnetic field minimum. Majorana losses to non trapped states can be neglected as long as the trap frequencies remain much smaller than the Larmor frequency \( \omega_L = \mu_B g_F B_{\text{bot}}/\hbar \) [48]. Here \( B_{\text{bot}} \) is the absolute value of the magnetic field at the trap bottom.

The building block for all lattice geometries below is the Ioffe-Prichard trap (IPT) [49, 50] which is a widely used technique to create magnetic field minima, both with current carrying wires and with patterned permanent magnets. The most familiar trap is based on a Z shaped wire. A magnetic field minimum in all dimensions is created above the middle of the wire by applying an external magnetic field. A similar trap can be made by a combination of two corners in a magnetic film as indicated in Fig. 2.1. Here an IPT is presented which is created by an externally applied magnetic field and a combination of two corners, or "Z"-shape, in the edge of a magnetic film (black). The out-of-plane magnetization can be described by an equivalent magnetization current \( I_M \) which runs along the edge of the film.

In this chapter we are concerned with designing magnetic trapping potentials generated by permanently magnetized films with a thickness \( h \lesssim 300 \text{ nm} \). The distance to the chip surface is typically large compared to the film thickness, \( z \gg h \), so we neglect the finite film thickness. We describe structures made out of perpendicularly magnetized films, patterned in a binary fashion, i.e. we assume that in any given location on the chip we have either the full film thickness, or no magnetic material at all. Instead of the bulk magnetization [unit: \text{A/m}] we use the two-dimensional magnetization, i.e. the magnetic dipole per unit area; \( I_M = Mh \) [unit: \text{A}]. For a 50 nm thick film of magnetized FePt which we will consider in the majority of this chapter the magnetization current is \( I_M = 0.04 \text{ A} \).

For periodic structures it is convenient to express the fields in terms of Fourier series. Furthermore, in the region of space above the chip surface, the static magnetic field can be written as the gradient of a scalar potential, \( \mathbf{B}(r) = -\nabla \Phi_M(r) \).

Taking the magnetization to be periodic: \( M_2(\rho) = M_2(\rho + a) = M_2(\rho + b) \), where \( a, b \) are the basis vectors of the lattice, the magnetization can be written as a two-dimensional Fourier series,

\[
M_2(\rho) = I_M \sum_{m,n=-\infty}^{\infty} \left[ C_{mn} \cos[(nK_1 + mK_2) \cdot \rho] + S_{mn} \sin[(nK_1 + mK_2) \cdot \rho] \right] .
\]  

(2.1)
Figure 2.1. a) Schematic representation of a magnetic film segment. Magnetic material is black and the substrate is represented by the white area. The horizontal part of the "Z" is 3 mm wide. The magnetic film is magnetized out-of-plane. The magnetization current $I_M = 0.2$ A is indicated by the white arrows. The external field is $B_{ext} = (0,3,0)$ G which creates a trap above the "Z". b) The magnetic potential above the kink in a). Here the trapping potential is cut through the potential minimum of the Ioffe-Prichard trap (IPT).

such that $M_2(\rho)/I_M$ is 0 or 1. The vectors $\mathbf{K}_1, \mathbf{K}_2$ are the basis vectors of the reciprocal lattice, defined by $\mathbf{K}_1 \cdot \mathbf{a} = \mathbf{K}_2 \cdot \mathbf{b} = 0$ and $\mathbf{K}_1 \cdot \mathbf{b} = \mathbf{K}_2 \cdot \mathbf{a} = 2\pi$. The Fourier coefficients are found by integration over one unit cell $U$ of the lattice. Defining $k_{nm} \equiv n\mathbf{K}_1 + m\mathbf{K}_2$,

$$C_{nm} = \frac{1}{I_M U} \int_{U} M_2(\rho) \cos[k_{nm} \cdot \rho] \, d^2\rho,$$

$$S_{nm} = \frac{1}{I_M U} \int_{U} M_2(\rho) \sin[k_{nm} \cdot \rho] \, d^2\rho,$$

where $U = |\mathbf{a} \times \mathbf{b}|$ is the area of the unit cell.

For the magnetic potential we obtain [51]:

$$\Phi_M(\mathbf{r}) = \frac{1}{2} \mu_0 I_M \sum_{n,m=-\infty}^{\infty} e^{-k_{nm}z} \left[ C_{nm} \cos(k_{nm} \cdot \rho) + S_{nm} \sin(k_{nm} \cdot \rho) \right]$$

$\Phi_M(\mathbf{r})$ is defined such that it is a scale invariant Fourier series. This way $B_{film}(\mathbf{r}) = -\nabla \Phi_M(\mathbf{r}) \sim a^{-1}$ and $\nabla B(\mathbf{r}) \sim a^{-2}$ where $a$ is the lattice spacing. When the field from the magnetic pattern is combined with an external field, magnetic potential wells are created which can be described by:

$$B_{tot} = B_{ext} + B_{film}$$

In Fig. 2.2 the magnetic film for the square magnetic lattice is plotted as well as the potential created by film and external field. In this case the pattern was calculated by an
optimization scheme for p2 type lattices [52]. All trap parameters depend on the value of the external field and $I_M$. Without an external field no traps exist and depending on the magnitude and sign of its components, traps can be created at different positions above a particular chip pattern. By increasing (lowering) the external field the trap frequencies can be raised (lowered).

Figure 2.2. The height above the surface is $z$ and the lattice spacing is $a$. Three-dimensional representation of the magnetic potential in arbitrary units at $z = 0.5a$ above an out-of-plane magnetized patterned layer of FePt (gray). The magnetic pattern is based on the unit cell that can produce a square lattice above the positions that are indicated by the red dots. Here $B_{\text{ext}}$ was chosen such that a square trapping potential with equal barriers heights at $z = 0.5a$ is obtained.

To create lattices of other symmetry classes than this p2 class we combine a periodic (square or triangular) pattern with designer defects. The edge of the magnetic film is changed locally to raise or lower specific potential minima. We introduce these defects as small virtual loop wires with current $I_M$, see Fig. 2.3. The field of the film is changed to:

$$B_{\text{tot}} = B_{\text{ext}} + B_{\text{film}} + B_{\text{defects}}$$  \hspace{1cm} (2.5)

This method of calculating magnetic field potentials is more accurate than calculating the sum of a finite number of loop wires. This is due to edge effects. This can be overcome in principle by taking a large enough number of loop wires. However this quickly becomes computationally expensive.

In the sections below we calculate these new potentials. For all presented lattices we calculated the bottom field and the barrier fields between the traps in the different lattice directions. We consider two lattice length scales in this chapter that are relevant for magnetic lattice experiments. First several lattices are discussed that are relevant for Rydberg experiments where Rydberg-controlled interactions can be created over several micrometers [36, 53]. The lattice distance should be smaller than the blockade radius. The second length scale under consideration is that of sub-micron lattices where the lattice spacing is of the order of 100 nm. With these lattices we hope to study the Extended-Bose-Hubbard model where second order tunneling becomes more pronounced due to the extremely small
lattice spacing [16]. For those potentials that are relevant for Bose-Hubbard physics we also give the trap depth in units of the lattice recoil $E_R = \frac{\hbar^2}{8ma^2}$. For all trapping potentials the trap frequencies can be found by making a harmonic approximation at the trap minimum [54].

2.3. Triangular lattices with designer defects: Kagome and honeycomb

While the triangular lattice has been used for many quantum lattice studies, nowadays lattices of a higher symmetry class attract more attention. When considering spin models on the two-dimensional triangular lattice no frustrated phases or quantum degenerate phases occur. On the Kagome lattice both the Heisenberg and Ising spin models predict frustrated phases [55, 56]. To create quantum spin models with ultracold atoms interactions between the various trapping sites need to be created. While tunneling interactions in these geometries would lead to exciting physics we restrict ourselves here to experiments with Rydberg atoms on the 5 $\mu$m scale. Lattices with smaller periods which support tunneling will be discussed in section 2.6.2. Rydberg atoms are the ideal candidate to create interactions between atomic clouds. Their Rydberg blockade can be used to make atoms interact over several micrometers and can be controlled optically. Rydberg atoms have been successfully used in quantum simulation where lattices of approximately 3 $\mu$m are created by optical dipole traps [57, 58]. The frustration in this geometry has motivated numerous theoretical studies [59]. Recent work predicts the observation of a spin ice phase for Rydberg p-state interactions on a Kagome lattice [60, 61]. These proposals require lattices without external harmonic confinement such that the lattice potential is perfectly periodic and has a flat envelope. The absence of a harmonically confining potential in magnetic lattices therefore provides a direct way to observe these phenomena. Recent work on gases in uniform potentials proved the feasibility of such measurements [62].

The similar honeycomb structure does not have frustration but has attracted much attention in recent years because of the presence of Dirac cones in its band structure which gives rise to the many extraordinary properties of graphene. The hexagonal lattice can be used to perform quantum simulations of graphene without external harmonic confinement and can be used to search for other nontrivial quantum phases which are predicted to arise for hard-core bosons in graphene-like geometries [63, 64]. Optical realizations of
the hexagonal lattice have been either irregular (stretched) or spin dependent while with a magnetic lattice the true graphene structure may be realized. The geometry and its band structure can still be modified by varying the external field. Using nano-fabrication techniques, even an interface between a frustrated Kagome lattice and a non-frustrated hexagonal lattice can be created.

To build these more exotic lattices the triangular lattice is introduced first. In Fig. 2.4 the triangular lattice is presented with its corresponding potential. The magnetic lattice structure is found by applying the optimization scheme for a lattice spanned by the vectors \( \mathbf{r}_1 = (1, 0) \) and \( \mathbf{r}_2 = \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) [52]. Approximate equal barriers between all the trapping positions can be found by applying the appropriate external field, as shown in Fig. 2.4. Note that three different barriers exist in the directions of \( \mathbf{r}_1, \mathbf{r}_2 \) and \( \mathbf{r}_3 = \mathbf{r}_1 - \mathbf{r}_2 \). Assuming a film thickness of 50 nm, a magnetization of 800 kA/m and a trap at the height of \( z = 0.5a = 2.5 \mu m \) one finds a trap depth of 6.6 G, a bottom field of 2.5 G and trap frequencies of (60, 58, 18) kHz. Smaller (larger) trap frequencies and barriers can be created by considering thinner (thicker) magnetic films.

2.3.1. The Kagome lattice

We can construct the Kagome lattice by modifying the triangular lattice. Starting from an optimized pattern for a triangular lattice, specific sites are raised by introducing designer defects. These are local modifications of the edge of the pattern, near the trapping position. These defects can be described by virtual wires with currents running along the loop with or against the effective magnetization current of the magnetic structure. An example is given in Fig. 2.3.

The Kagome lattice is obtained by adding these defects to a subset of the triangular lattice sites. In these lattice sites the potential wells are raised by 1.8 G when considering the 5 \( \mu m \) lattice realization that is designed for Rydberg atom experiments. The remaining non-raised potential wells then form the desired Kagome sublattice. In Fig. 2.5 the Kagome lattice structure is presented with potential raising defects on sublattice sites that are
multiples of the vectors $2r_1$ and $2r_2$. The field is calculated for traps centered around $z = 0.5a = 2.5 \mu m$ with the same external field as for the triangular lattice in Fig. 2.4.

Figure 2.5. The Kagome lattice structure. a) In black the magnetic pattern is shown with modified local shapes at the trap positions that needed to be raised. b) The potential created by pattern a) with a lattice spacing of $5 \mu m$ and trap minima at $z = 0.5a$. The same external magnetic field as in Fig. 2.4 is applied. The Kagome lattice is indicated by the white dashed lines.

2.3.2. The honeycomb lattice

The hexagonal lattice is constructed in a similar way. Again the triangular lattice is taken as a basis and defects are placed to raise the potential in selected sites. Now the tiles including defects are placed on the sublattice that is created by multiples of $r_1 + r_2$ and $2r_1 - r_2$. The bottom field of the elevated traps is raised to $4.0 \text{ G}$ while the lower traps are kept at $2.2 \text{ G}$, as for the Kagome lattice. This demonstrates the universal applicability of this technique.

2.4. Low dimensional structures: ladders and diamond chains

We can also employ our magnetic lattices to create new low dimensional structures for ultracold atoms. Many unique phases of matter have first been observed in low dimensional structures because quantum mechanical interactions become more pronounced. Quantum simulation experiments with a three-atom Rydberg spin chain have recently been performed [57]. Here we provide several geometries that can be used to simulate spin models with Rydberg atoms such as those proposed in reference [65] and [66]. The simulations of non periodic lattices that are presented here are based on finite lattice structure calculations. The magnetic film is described by calculating the field of the magnetization current $I_M$ for each pattern. In all presented potentials only a central region of a wider lattice is presented to avoid edge effects.
Figure 2.6. The honeycomb lattice structure. a) In black the magnetic pattern is shown with modified local shapes at the trap positions that needed to be raised. b) The potential created by pattern a) with a lattice spacing of 5 µm and trap minima at \( z = 0.5a \). The same external magnetic field as in Fig. 2.4 is applied. The hexagonal lattice is indicated by the white dashed lines.

2.4.1. Ladders

To construct confining barriers in two-dimensional lattice potentials we sought a method to separate traps into particular arrays. Small spin chains or two-dimensional plaquettes of \( 2 \times 2 \) traps could be produced by isolating sets of traps. Inspired by optical lattice techniques where local traps are raised by overlapping optical fields we made magnetic artifacts that could create a sharp magnetic barrier, similar to the defects presented in the previous section. By straightening out a horizontal magnetic array we were able to disrupt the lattice in the y-direction. These interrupting "fences" can be used in combination with double or triple arrays of square lattice traps to construct ladders of a fixed number of rails. To construct an one-rail ladder, or equivalent a series of double wells, we alternate two trapping arrays with one fence array. In Fig. 2.7 the corresponding potentials are presented. When considering bosons in ladder geometries the Haldane model predicts a gapped phase for odd-rail ladders while for even-rail ladders the energy bands touch \([63, 67]\).

A three rail ladder can be created by using either 3 trapping ladders, as a trivial extension of the previous figure or by trapping on the other edge of the magnetic structures by reversing the external field. This is possible because of the corners which are present on the non-flattened side of the barrier arrays. An example can be seen in Fig. 2.8.

2.4.2. Diamond chains

Another geometry of high interest are diamond chains. The alternation between the number of sites in each column has made the diamond chain an inspiring tool for spin model proposals \([68]\). For anti-ferromagnetic spin interactions, several ideas have been proposed for how frustration in complex geometries can lead to new phases of matter \([69, 70]\). Due to its presence in many material crystals it is also a highly relevant geometry for quantum simulation. Both cuprates with CuO planes \([71]\) and azurite \([72, 73]\) have been studied intensively theoretically but so far have not been realized with optical lattices. This is due
Figure 2.7. a) Magnetic film pattern with $a = 5 \mu m$ that can create a double well series, or two rail ladder. The external field is set to generate equal barriers between all ladder sites and is $B_{ext} = (-10.0, -9, -0.05) \text{ G}$.

Figure 2.8. (a) The same magnetic film pattern as Fig. 2.7. b) The potential created by the film of (a) with the reversed external field: $B_{ext} = (10.0, 9, 0.05) \text{ G}$. A three rail ladder is created by the same structure as Fig. 2.7 with reversed external field to create wells above the other edge of the magnetic structures.
Figure 2.9. (a) A single diamond chain where single traps are positioned in between double wells. b) Potential corresponding to the pattern of a) with an external field $B_{\text{ext}} = (24.4, 2.05, 0.13)$ G chosen such that traps are formed at $z = 0.45a$. Here $a = 5 \mu\text{m}$. By controlling the external field, trap barriers between the various traps can be controlled independently.

to the large number of wavelengths that one would need to combine. Their barrier heights vary in different lattice directions and modulate along the chain axes which makes them hard to describe and create. This complexity make diamond chains an ideal systems to be studied with magnetic lattices because its complex geometry can be easily handled with nano-fabrication techniques.

By combining linear stretches and shifts it is possible to create diamond chain potentials. An example is the single diamond chain shown in Fig. 2.9. Higher order chains can be created trivially by increasing the number of trapping arrays in between the blocking arrays.

### 2.5. Tapered structures

In this section we introduce tapered lattices: structures where the lattice spacing changes gradually across the lattice, see Fig. 2.10. We will consider tapers that can connect the Rydberg regime with lattices of $5 \mu\text{m}$ that we have considered so far to submicron lattices of 250 nm. Tapered lattices solve two problems; transport of atoms into sub-micron lattices and detection of atoms in sub-micron lattices. By several groups an effort is made to reduce the period of atomic lattices since the interaction energy between atoms as well as hopping rates between sites decrease quadratically with the lattice spacing. Before we address the possibility of tunneling experiments in magnetic lattices we will first address another related challenge. When loading current magnetic lattices a large millimeter-scale cloud is brought by magnetic transport into the region of the chip-based traps, after which the global trap is turned off. This direct loading leads to heavy losses due to the large mismatch between the weak confinement in the global trap and the tightly confined microtraps. From previous experiments it is known that loading ultracold atom clouds becomes increasingly inefficient if the traps are smaller and closer to the chip surface. The change of a single millimeter wide ion trap into hundreds to thousands of micron scale traps gives rise to a large change of local
trapping fields. This leads to an increased temperature of the gas which results in overall atom losses. If one scales the loading efficiency of current magnetic lattice experiments down to sub-micron lattices a filling fraction of approximately 0.25 atoms per site would be reached in a 100nm lattice [33]. Several approaches to circumvent this problem have been presented in recent years most of which introduce a slowly varying trapping field that can bring atoms from a few hundred microns to a few hundred nanometers from the surface while being protected from strongly varying fields and enhanced inter-atomic collisions [74, 75]. Here a similar solution based on permanent magnetic traps is presented.

Most experimental groups who are working in this direction use optical dipole traps which have been shown to work while loading single atom microscopes. The introduction of such an extra transportation beam is possible but hard to combine with many compact chip experiments. By using local magnetic fields on the chip instead of loading atoms by optical transport these challenges may be solved. Magnetic transport with coils or permanent magnets has been used for decades to transport clouds between vacuum chambers [76]. On a smaller scale in atom chip experiments, arrays of wires are used to move ultracold clouds inside high finesse cavities [77, 78] or to move them over surfaces as atomic probes [79]. Another strong feature of magnetic transport is its robustness. Optical lattices and moving dipole traps are very sensitive to distortions while magnets or coils perform highly repeatable.

By creating a method to transport atoms to nanoscale lattices a related problem is also tackled. This is the problem of detecting atoms within sub-wavelength potentials. Since the atomic traps are smaller than any wavelength that can be used to image rubidium atoms, it is no longer possible to observe a single well using optical detection. If we use transport through the tapered structures in the other direction we are able to move clouds from a sub-wavelength lattice up to a region where the optical resolution is sufficient to distinguish individual traps.

From a more fundamental point of view one might also consider a cloud of atoms trapped in a sub-wavelength lattice at the smallest end of a tapered structure which is then released or shifted into the widening taper. Such systems then provide a very natural quantum
simulation of a quantum gas in an expanding lattice. This idea leads to a series of quantum simulation experiments that could be performed with this unique system. One immediately thinks of cosmological theories in which particles in the early universe are considered on an inflating lattice. Experiments like this have also been proposed in the context of the Kibble-Zurek mechanism (KZM) [80, 81], which predicts the formation of domains after a homogeneous gas is released in such a geometry. Although some experiments have been done in periodic optical lattices [8] and in one-dimensional clouds [11] a two-dimensional lattice experiment with varying length scales within the lattice as proposed here has not been created. A way to study these phenomena would be to capture a gas at the center of the smallest region of a taper in the Mott insulating state and lower the trap barriers such that the atoms spread in the tapered environment.

2.5.1. Construction of tapered lattices

To combine lattices of different length scales we developed tapered lattices in which the lattice spacing is varied slowly in one direction. Here we combine two elements that are unique to magnetic lattices. I) The length scale of each trap array can be varied. The scale invariance of the permanent magnetic Ioffe-Prichard trap enables the gradual change of length scales within a particular lattice. In optical lattice systems this would require one to vary the frequency of all lattice beams in time over a wide range while with lithographic patterning one is completely free in the scope and gradient of the lattice spacings. II) By rotating the external magnetic field around the Ioffe-axis periodically it is possible to move each array of traps up one row in any of the presented lattices [35]. The combination of this shift array with the shrinking lattices will therefore allow us to capture mesoscopic clouds of hundreds of atoms in traps several micrometer apart and then move them to smaller geometries. Because each IPT is created by the combination of one magnetic unit cell and an external magnetic field, one has to limit the amount of change from one unit cell to the next such that similar traps are created in neighboring rows. This way, atoms can be transported adiabatically up and down the lattice.

It is important to check the modification of the unit cells at the edge of the taper because they can loose their original shape by the transformation. Therefore we studied the effect of straight tapers. Here the lattice deformation arises at the edge of the tapers. We compare this with rounded tapers that are created by a local transformation and rotation of the unit cell to keep the local pattern constant as shown in Fig. 2.10. While the traps along the vertical red line have the same ratio of trap frequencies, the traps at the edges of the structures, along the blue line, vary in this regard. When one considers a fixed external magnetic field which traps atoms in the middle atomic trap at \( z = 0.5a \) with equal barriers in the \( x \)- and \( y \)-direction, the traps at the edge of the two structures are both modified in a similar manner. The potential wells at the edge of the round taper are rotated with respect to the external field and therefore have another ratio of trap frequencies and barriers than those in the center. The potential wells at the edge of the straight tapers have a different unit cell with a different "Z"-shape in the edge of the unit cell above which the IPT will be formed. This different magnetic structure in combination with the unchanged external field again results in a change in trap frequencies and barriers on a similar scale as for the round taper.

If one limits the row-to-row change to 1 percent, to ensure adiabatic transport, it requires 300 shifting operations to shrink the lattice spacing by a factor of 20: \( 0.99^{300} = 0.05 \). In such a taper the fields required at the large 5 \( \mu m \) scale are approximately 7 G to trap atoms at half the lattice spacing. By linearly increasing the external field while moving the traps
Figure 2.11. a) Section of the tapered lattice structure for which the potential is presented. The taper has a slope of 5% per line and the largest lattice spacing is 5 μm. b) The potential cross-section taken at height \( z = 0.35a \) such that it cuts through the trap bottom of the horizontal array at \( y = 2a \). The white lines show points where possible trap positions can be created at the same height. By changing the external field, atoms can be moved along those lines. The external field is \( B_{\text{ext}} = (-11.2, -4.2, 0.2) \, \text{G} \).

down the taper the final trapping field reaches 203 G to trap atoms in a 250 nm lattice, 125 nm above the surface of the chip. The trap frequencies and trap depths during this transport increase from 60 kHz and 7 G to 17 MHz and 203 G. In Fig. 2.11 the potential of a tapered section is presented. Subfigure b) also shows the lines along which transport is possible. These paths can be found by calculating \( \det (\nabla B_z=\text{const}) = 0 \), which gives all points where a magnetic field minimum can be created at a fixed height [54].

2.6. Lattices with tunneling and magnetic fences

2.6.1. One-dimensional tunneling

The realization of a gas of tunneling atoms in a magnetic lattice is driving several groups to scale down their magnetic lattices. In several earlier works it has been shown how to achieve one-dimensional tunneling above magnetic films. All references consider similar magnetic films and the optimized square and triangular unit cells from reference [52] which we have used in all previous sections as well. A calculation for one-dimensional tunneling trap arrays has been presented in reference [37] for a FePt film of 25 nm thick and a lattice spacing of 100 nm and a similar calculation for a 700 nm lattice on a 2.2 nm thick Co/Pt multilayer film is presented in reference [43]. In this approach the barriers in the y-direction are lowered to create one-dimensional channels in which tunneling is possible. Here we reproduce these results for a 250 nm square lattice. We choose this lattice spacing because it is the smallest size we could make using the techniques described in chapter 4.

To allow for tunneling among magnetic traps at this length scale the barriers must be in the order of 0.5 G which corresponds to \( 16.2 E_R \). Therefore we consider a thin magnetic
Figure 2.12. a) Magnetic lattice pattern for a series of fenced one-dimensional arrays of five sites. The lattice spacing \( a \) is 250 nm. b) Potential created by the magnetic film of a). The external field is \( \mathbf{B}_{\text{ext}} = (1.56, -0.17, 1.19) \) G such that the trap minima are positioned at \( z = 0.9a \) above the chip surface. The inter-trap barriers have a height of 0.49 G. White dots indicate the trap minima.

layer of 2.5 nm above which such traps are possible with external fields of several Gauss. This allows us to create one-dimensional magnetic trap arrays at \( z = 0.9a \) with a bottom field of \( B_{\text{bot}} = 1.4 \) G so a Larmor frequency of 1.0 MHz. Several one-dimensional arrays of four unit cells with this field configuration that creates five traps can be seen in Fig. 2.12.

In Fig. 2.12 we only show several trapping arrays with five traps each in between the fences to display a closed set of traps. A magnetic configuration such as this gives several complications which larger lattices do not have. Both the fences and the finite size of the entire lattice that is considered here cause small local shifts in the bottom field of the five traps in each one-dimensional trap array. These field differences prohibit tunneling in a small system like this. An external magnetic field that minimizes these differences might exist but is hard to find since these potentials are computationally challenging. The magnetic potentials that have been created by the process described in chapter 4 and are now placed in the apparatus described in chapter 6 have lattices of 40 × 40 sites. For these larger lattices we expect the differences in bottom field to be significant only for a few unit cells near the fences. To predict an approximate tunnel rate in these potentials we have to consider the fully periodic lattice with the same external field to simplify the calculation.

We solved the Schrödinger equation numerically in a box around the trap minimum of one well in the three-dimensional periodic lattice potential with Dirichlet boundary conditions. The same external field is taken as for the potential of which a cross section is presented in Fig. 2.12 such that the traps are very similar. First we isolate a single well and solve the Schrödinger equation in this well to find the approximate ground state wavefunction \( \psi_1 \). Then we use \( \psi_1 \) to obtain an estimate for the on-site interaction parameter \( U \).

\[
U = \frac{4\pi \hbar^2 \alpha_s}{m} \int d^3r \, \psi_1^4(r)
\]

(2.6)

Here \( \alpha_s \) is the scattering length, here we take the value for \(^{87}\text{Rb} \), \( \alpha_s = 5.3 \) nm \([82]\). At \( z = 0.9a \) with the field \( \mathbf{B}_{\text{ext}} = (1.56, -0.17, 1.19) \) G we find an on-site interaction \( U/h = \)
The trap frequencies at this field configuration can also be found from this solution and are $\omega_{\text{trap}} = 2\pi \times (97.4, 71.3, 51.7) \text{kHz}$.

To calculate an estimate for the tunneling rate in this potential we consider a section of two wells. Again we solve the Schrödinger equation in this isolated environment of two wells in the lattice. From this we obtain a new wavefunction $\psi_2$ for which we calculate the first two eigenstates. The energy difference between the even and odd realization of these eigenstate wavefunctions in the two wells gives us an approximate tunnel rate. The approximate tunneling rate that we find is $t/h = 250 \text{Hz}$. These values of $U$ and $t$ are near the phase transition between a Mott insulating phase (in which atoms are localized to their traps) into a superfluid phase (in which tunneling dominates the system). This transition and the physics associated with tunneling and interacting atoms will be discussed in chapter 3. Here we will limit ourselves to the tunneling rates associated with various barriers in the lattice. The interaction parameters $t$ and $U$ can be controlled in a magnetic lattice by tuning the barriers with external magnetic fields.

In section 2.4 it was already shown how a barrier in the $y$-direction can be created to interrupt a lattice by straightening out a horizontal magnetic array. This barrier is large enough to suppress tunneling and we have implemented this barrier in the lattice potential of Fig. 2.12 to confine the gas in the $y$-direction. Superfluid gases are generally held together by a global confining trap. A sub-micron magnetic lattice with tunneling features will not keep a gas at the trapping location. Due to the hopping over small magnetic intertrap barriers the atoms will use all the available lattice sites to spread out. This will lead to a very large, effectively endless quantum gas in an infinite magnetic lattice which will not be detectable because of the very small signal that widespread single atoms give. Many-body quantum lattice experiments in general are faced with this complication and have to choose between necessary external harmonic confinement and unrestricted free behavior of particles. Only very recently an optical box potential was used to study Bose condensed gases in such a uniform potential [83]. A similar experiment can now be constructed by an one-dimensional magnetic lattice in between confining fences.

2.6.2. Two-dimensional tunneling

Analogous to lowering the $y$-barriers one might expect that this is also feasible in the $x$-direction or that an external field configuration exists in which two-dimensional tunneling becomes possible. In reality such an extension turns out to be nontrivial. If one lowers the barriers in the $x$-direction in any of the presented geometries, by changing the relevant external field component, the bottom field of the traps tends to drop as well. An other simple way to reduce the intertrap barriers would be to trap atoms at larger distances from the chip. However this also results in a low bottom field which in turn results in high losses. As was mentioned in the introduction of this chapter Majorana losses to non-trapped states can be neglected as long as the trap frequencies remain much smaller than the Larmor frequency $\omega_L = \mu_B g_F B_{\text{bot}}/\hbar$. The trap losses grow exponentially with the ratio $\omega_{\text{trap}}/\omega_L$ [48]. Recall that these unit cells were created by optimizing the pattern such that deep traps were created [52]. Therefore they might not form the ideal starting point to create lattices in which tunneling is possible. The question therefore becomes whether it is possible to create a two-dimensional superfluid gas in a magnetic lattice. Specifically, the main challenge lies in the creation of a potential with low barriers while still keeping $\omega_L \gg \omega_{\text{trap}}$.

To extend the toolbox of magnetic trapping geometries by creating trapping lattices with shallow potentials we tried several possible adaptations to the lattice geometries. To avoid
field zeros we found it necessary to use connected strips of magnetic film. By changing the unit cell of the square lattice we were able to shrink the barriers in the x-direction. We flattened out the largest corrugation in the edge of the unit cell, above which the deepest traps could be created. This lowered the barrier in the x-direction while maintaining a bottom field on the order of a Gauss. In Fig. 2.13 we present this lattice where the barrier in the y-direction has been lowered to match the barrier in the x-direction, analogous to the procedure described for Fig. 2.12, by choosing the optimal external magnetic field. The barriers $V_x$ and $V_y$ can be tuned independently by modifications to the external field or by transformations to the unit cell. The barriers for the potential that is presented in Fig. 2.13 for the x(y)-direction are $0.046(0.047)$ G. The traps are formed at a height of $z = 1.05a$ above the surface with a bottom field of $1.7$ G which corresponds to a Larmor frequency of $\omega_L = 1.2$ MHz. The inter trap barriers can be raised (lowered) by varying the external magnetic field strength such that the trap bottom becomes closer (further) away from the magnetic field. The potential that is presented in Fig. 2.13 has barriers that result in a ratio of $U/t$ that is close to the phase transition of a superfluid to a Mott insulator. The exact phase transition is predicted to occur for two-dimensional lattices at $U = 16.5 \, t$ [84].

To obtain the tunneling rate in this two-dimensional potential we used the results from Gerbier et al. [85] which have been corrected by Ho and Zhou in reference [86]. Here the band structure is calculated for the two-dimensional cubic lattice and the following approximate expressions for the hopping and on-site interaction are found:

$$\frac{t}{E_R} = 1.43 \left( \frac{V_{\text{mag}}}{E_R} \right)^{0.98} e^{-2.07 \sqrt{V_{\text{mag}}/E_R}},$$

$$\frac{U}{E_R} = \frac{5.97a_s}{2a} \left( \frac{V_{\text{mag}}}{E_R} \right)^{0.88}.$$

The recoil energy $E_R$ is $9.2$ kHz for a $250 \, \text{nm}$ lattice. These formulas have a $1\%$ accuracy in the relevant range of $V_{\text{mag}} = (8-30) \, E_R$ for the square lattice. At this height the tunneling rate in both directions is $370 \, \text{Hz}$ and $U/h = 3.0 \, \text{kHz}$. The trap frequencies at this field configuration are $\omega_{\text{trap}} = 2\pi \times (69,50,50) \, \text{kHz}$.

### 2.6.3. Outlook

A general method to generate two-dimensional magnetic lattices which are optimized for tunneling experiments remains unknown. However we have shown ad hoc that such geometries exist and that equal tunneling barriers in a square lattice can be created while maintaining a large enough bottom field. By modifying the lattice further or by implementing new defects also other two-dimensional tunneling geometries should become possible. At this point no barriers have been designed to confine the gas in the x-direction. Also other geometric effects and boundaries like tunnel junctions similar to the work recently done in the Esslinger group [87] can be designed. Radio-frequency dressing can also be used to modify permanent magnetic potentials. With this technique one might be able to create more tunneling geometries without significant losses [88]. It would be interesting to investigate whether with such a method also the potentials presented in the earlier sections which now only work on the micron scale could be scaled down.
Figure 2.13. a) Magnetic pattern for a lattice with a flattened unit cell to lower barriers in the x-direction. The lattice spacing $a$ is 250 nm. b) Potential cross section through the potential minimum at a height of $z = 1.05a$. Inter trap barriers are $0.046(0.047)$ G in the $z(y)$-direction. The external field is $B_{\text{ext}} = (0.86, -0.02, -0.12)$ G.

### 2.7. Conclusion

We have presented several new geometries that can be used in quantum simulation experiments based on permanent magnetic atom chips. With these patterns it will become possible to create magnetic lattices of Kagome and hexagonal geometry as well as low dimensional structures such as ladders and diamond chains. Also magnetic fences have been presented that can restrict atoms to certain trapping regions while avoiding extra global harmonic confinement. Furthermore tapered structures have been created that allow for new experiments in varying geometries and may be used to load sub-wavelength lattices. Lattices on sub-micron length scales have been presented in which tunneling becomes possible along the $y$-direction in between confining barriers. A non-restricted two-dimensional lattice with tunneling in two dimensions is also presented. All presented structures can be immediately implemented on magnetic atom chips and may be loaded by atoms in the nearby future.
3 Quantum Monte Carlo simulations of the Bose-Hubbard model in new magnetic potentials

3.1. Introduction

By building and controlling quantum systems out of atomic gases in the lab we hope to learn more about their nature and similarity to materials. The first and most famous realization of a quantum simulator is the optical lattice which contains interacting and tunneling atoms [16, 39]. In this chapter we will study a similar system of hopping and interacting atoms from the perspective of experiments planned in our new magnetic lattices on an atom chip. In particular, we plan to study the Bose-Hubbard model in the geometries that were introduced in the previous chapter. Numerical simulations based on the Quantum Monte Carlo (QMC) method have proven to be an extremely accurate tool to describe the Bose-Hubbard model. This method to study bosonic lattice models will be introduced below. To incorporate the new magnetic potentials an extension is made to the "Algorithms and Libraries for Physics Simulations" (ALPS) simulator which is a QMC simulation tool built by a large collective of physicists [89]. The results in this chapter were obtained by Etienne van Walsum, as part of his Master’s thesis project under joined supervision of Dr. Philippe Corboz and the author of this thesis. The goal of this project was to obtain a quantitative description of some properties of atoms in magnetic lattices. We simulated the new nanostructures that we aim to realize in the future on our magnetic atom chip, see chapter 2. We wish to predict the quantum phases which are expected to occur in our nanofabricated magnetic lattices and predict the effect of disorder and geometry on the distribution of the atoms. In this chapter we find several new features in the phase diagram of the Bose-Hubbard model, specifically for our magnetic lattice geometries. These simulations show that the magnetic potentials that were proposed in chapter 2 offer exciting prospects for realization in the experimental apparatus which is described in chapter 6. Specifically, the relations between temperature, interactions and chemical potential are studied for realistic experimental parameters. The density per lattice site which can be measured in future experiments is simulated as well.

3.2. The Bose Hubbard model

To describe ultracold bosonic atoms in a two-dimensional (2D) lattice we use the Bose-Hubbard model:

$$H = -\sum_{\langle i,j \rangle} t_{i,j} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu_i n_i. \quad (3.1)$$
The three independent energy terms describe tunneling, on-site interactions and the chemical potential. The complete set of all local chemical potentials $\mu_i$ sets the number of particles in the system and can be modified locally to account for non-uniform potential variations. To account for non-uniform lattices we consider local tunneling elements $t_{i,j}$. The interactions between the particles in the same site, $U$, do not depend on the lattice site. Eq. (3.1) describes a system of interacting and hopping particles in the Wannier basis in which the basis states $w(\mathbf{r} - \mathbf{r}_i)$ are labeled by the lattice site positions $\mathbf{r}_i$ [3, 16, 90]. The tunneling and interaction energy can be expressed as:

$$t_{i,j} = -\int d^3r \; w^*(\mathbf{r} - \mathbf{r}_i) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{lat}}(\mathbf{r}) \right) w(\mathbf{r} - \mathbf{r}_j)$$

$$U = g_{\text{int}} \int d^3r \; w^4(\mathbf{r})$$

(3.2)

The lattice is described by positions $\mathbf{r}_i = (x_i, y_i, z_i)$. The Wannier function can be approximated by a Gaussian wave function $w^0_i(\mathbf{r} - \mathbf{r}_i) = \frac{1}{\pi^{3/2} \sqrt{2\pi^2}} e^{-\left(\frac{x-x_i}{\omega_i}\right)^2/2\omega_i^2 - \left(\frac{y-y_i}{\omega_i}\right)^2/2\omega_i^2 - \left(\frac{z-z_i}{\omega_i}\right)^2/2\omega_i^2}$. Here $\omega_i = \sqrt{\frac{\hbar}{m \omega_i}}$ where $\omega_i$ are harmonic approximations of the trap frequencies in the trap reference frame and $\hat{x}, \hat{y}, \hat{z}$ are coordinates along the major axes of the microtraps. The strength of the contact potential is $g_{\text{lat}}$. $V_{\text{lat}}$ is the lattice potential, defined by a lattice spacing $a$ and a lattice depth $V_{\text{mag}}$. It is convenient to express $V_{\text{mag}}$ in terms of the lattice recoil energy $E_R = \frac{\hbar^2}{2m a^2}$. In modern experiments the periodicity is typically around 450 nm. However, with techniques described in this thesis lattices down to 100 nm can be constructed using patterned magnetic films. The lattice recoil energy is then roughly 20$^\times$ higher. The design of these lattices is introduced in the previous chapter; here we will limit ourselves to a set of lattice parameters for which Bose-Hubbard physics can be expected.

For an estimate of the numerical values of $t_{i,j}$ and $U$ in Eq. (3.2) we follow the results of Gerbier et al. [85] which are corrected by Ho and Zhou [86]. There the band structure is calculated for the cubic lattice and the following approximate expressions for the hopping and on-site interaction are found:

$$\frac{t}{E_R} = 1.43 \left( \frac{V_{\text{mag}}}{E_R} \right)^{0.98} e^{-2.07 \sqrt{V_{\text{mag}}/E_R}},$$

$$\frac{U}{E_R} = 5.97 a_s \left( \frac{V_{\text{mag}}}{E_R} \right)^{0.88}.$$  

(3.3)

Here $a_s$ is the scattering length, here we take the value for $^{87}\text{Rb}$, $a_s = 5.3$ nm [82]. These formulas have a 1% accuracy in the relevant range of $V_{\text{mag}} = (8-30) E_R$ for the square lattice. They can also serve as an estimate for the other geometries. In the following we consider a magnetic lattice spacing of 100 nm and an inter-trap barrier height in the range of 2 to 30 $E_R$. This corresponds to a lower end magnetic field barrier of 80 mG $\cong 2 E_R$ such that we can find a regime where $t$ dominates over $U$. When barriers are much larger, $U$ will dominate over $t$ and other physics is expected. In experiments with two-dimensional optical lattices a phase transition between these two regimes was found at $U = 16.9 \, t$ by Capogrosso et al. [84]. This corresponds to a barrier height of $V_{\text{mag}} = 6.2 \, E_R$ in a 100 nm lattice. The depth of the lattice sets the value of $\frac{t}{E_R}$ and can be controlled by the strength of externally applied global magnetic fields. The atoms in the experiment are considered at a finite temperature of 0.2 $\mu$K. We only consider lattices with an equal number of unit cells in the x- and y-direction. Periodic boundary conditions will be used in all simulations.
In many experiments also a global harmonic trap is needed to keep atoms together. In our experiments such an optical potential is not present. To ultimately confine atoms a magnetic box potential is proposed and simulated in the final section of this chapter.

### 3.3. Numerical methods

#### 3.3.1. Quantum Monte Carlo Simulation

To calculate the phase diagram of the Bose-Hubbard model, Eq. (3.1), and to calculate thermodynamic observables such as the energy, density (both local or global), and the mobility of the particles, it is the canonical partition function that has to be evaluated:

$$Z = \text{Tr} \ e^{-\beta H}.$$  

(3.4)

Here $\beta = 1/k_B T$ is the inverse temperature and the trace sums over all possible configurations of particles on all lattice sites. In all further calculations we take $k_B = 1$. This sum of exponentials is hard to calculate for a system of many quantum particles since its Hilbert space grows exponentially with the number of particles.

In the following steps we map our stationary two-dimensional quantum system on a three-dimensional classical system because for the latter a numerical estimation method exists. To do this transformation we discretized $\beta$ by $M$ steps of size $\Delta \tau$. In the following equations these steps $\Delta \tau$ can be recognized as an imaginary time step:

$$Z = \text{Tr} \ e^{-\beta H} = \text{Tr} \ e^{-(\Delta \tau H)M}.$$  

(3.5)

The trace is written as a sum over the complete set of position configurations:

$$Z = \text{Tr} \ e^{-(\Delta \tau H)M} = \sum_i \langle i | e^{-(\Delta \tau H)M} | i \rangle.$$  

(3.6)

Furthermore, we write the exponent as a product of $M$ exponentials and insert closure operators $\sum_i |i\rangle \langle i|$ between all evolution operators $\langle i | e^{-(\Delta \tau H)M} | i \rangle$:

$$Z = \sum_{i_1, \ldots, i_M} \langle i_1 | e^{-\Delta \tau H} | i_2 \rangle \langle i_2 | e^{-\Delta \tau H} | i_3 \rangle \cdots \langle i_M | e^{-\Delta \tau H} | i_1 \rangle = \sum_{i_1, \ldots, i_M} P(i_1, i_2) P(i_2, i_3) \cdots P(i_M, i_1).$$  

(3.7)

The states $|i_{\tau_i}\rangle \equiv |i(\tau_i)\rangle$ are two-dimensional configurations of particles on the atomic lattice sites $(x_i, y_i)$ at 'times' or realizations $\tau_i$ such that $\tau_1 \leq \tau_\nu \leq \tau_M$. It can be shown by taking the limit $\Delta \tau \to 0$ that $Z$ can be written in the Fock basis as:

$$Z = \sum_{m=0}^{\infty} \sum_{i_1, \ldots, i_m} \int_0^{\beta} d\tau_1 \cdots \int_0^{\tau_{m-1}} d\tau_m (e^{-\tau_1 e_{i_1}} V_{i_1} e^{\tau_1 e_{i_2}}) \cdots (e^{-\tau_m e_{i_m}} V_{i_m} e^{\tau_m e_{i_1}}).$$  

(3.8)

The complete derivation is beyond the scope of this thesis and can be found in references [90, 91, 92]. Here the hopping term $V_{ij} = \langle i | b_i b_j^\dagger | j \rangle$ is split off from the Bose-Hubbard Hamiltonian, Eq. (3.1). The other two terms form $H_{t_{i,j}=0}$, such that $H_{t_{i,j}=0} | i \rangle = e_{i} | i \rangle$. The hopping term changes a state by shifting only one particle at a time. Therefore the
partition function can be completely described by the evolution of occupation numbers \( n_i(\tau) \). The integrand, which we will call weight \( W \), is completely determined by \( V_{ij} \) and \( n_i(\tau) \):

\[
W = (e^{-\tau_{i1} V_{i1i2} e^{\tau_{i2}}} \ldots (e^{-\tau_{M} V_{iMi1} e^{\tau_{1}}}). \tag{3.9}
\]

The still exponentially large sum in Eq. (3.8) is not computed but a method to generate a statistical representation of this partition function is used. This estimation method is called Monte Carlo sampling. The working principle of all Monte Carlo approximations is this: One generates on a computer, a statistically representative distribution of worldline configurations, drawn from the physical probability distribution. Then one computes the desired expectation value by "measuring" from this generated distribution of thermalized configurations. We will limit ourselves to the Bose-Hubbard model, however these methods can also be used to predict, for instance, the magnetic properties of spin systems like the Ising model. In the Bose-Hubbard model particle positions in a configuration can be represented by lines which we will call worldlines.

In our simulations we build up a thermally equilibrated distribution of particle configurations. The number of samples can be chosen and this sets the error on the simulation. Thermalization is the process in which the Monte Carlo program creates an equilibrium distribution, based on the model parameters \((t_{ij}, U, \mu, T)\). Observables can be computed by averaging measurements which are done in a thermally equilibrated distribution of configurations. In order to sample from the right probability distribution one has to thermalize. Before the simulation has reached thermalization one is not sampling from the right distribution which introduces errors in the results.

A widely used method to generate statistical representations of lattice models is to let a computer repeatedly modify the worldline configurations in a weighted way. Here a random variation in the configuration is proposed and accepted/rejected based on the probabilities of the new and old configuration. This method is known as the Metropolis Algorithm [93].

To generate a representation of a state in thermal equilibrium a computer modifies a configuration of worldlines millions of times based on the model parameters. The starting configuration can be constructed out of any valid configuration of particles on the lattice sites. The computer finds a thermal equilibrium of the system by performing a large number of updates on the worldline configurations. In each update one operator which adds or subtracts one particle at a lattice site is randomly placed in the lattice. After such an operator is placed it moves through a configuration based on a set of allowed steps. We call configurations with an open worldline extended configurations. Each of these steps is an extended configuration modification that is accepted or rejected according to the Metropolis prescription. Acceptance ratios for all these moves, \( P_{\text{acc}} \), are proportional to the ratio of the value of the probability distribution which is to be sampled at the proposed over the current extended configuration. In other words, the acceptance probability of a step is given by \( P_{\text{acc}} = \frac{W(\text{proposed})}{W(\text{current})} \). This is how the Monte Carlo process reaches an equilibrium distribution based on the system parameters. An extended configuration with open and closed worldlines is illustrated in Fig. 3.1. In this representation particle positions in the lattice are tracked by lines.

Due to the periodic boundary conditions in all three lattice dimensions \((x_i, y_i)\) and \( \tau \), moving (anti-)particles can come back to their starting position. Only connected paths represent physical particles, configurations containing open worldlines do no contribute to the partition function since they do not contribute to the trace in Eq. (3.8). Therefore we call them extended configurations which can lead us to find new real configurations which contain only closed worldlines. The algorithm then keeps the trajectory that the
Figure 3.1. Example of an extended configuration in the worldlines representation for a 1-dimensional lattice. The horizontal axis shows the lattice sites $x_i$, and the vertical axis shows the $\tau$-direction with $M = 10$ and $\beta = 1$. The number of lines on each lattice site indicates the particle number, a dotted line represented no particles. All finished worldlines have to be continuous since they were created by moving a creation type wormhead that found his tail. In this example all 8 worldlines wound around the $\tau$-boundary but none wound around the lattice dimension $x_i$. At site 5 a new worm is inserted of the creation type that moves in the $+\tau$ direction and tunnels to site 6 at $\tau = 0.4$. The red dot indicates the wormhead and the blue dot the wormtail. Figure based on [92].

(anti)-particle has traveled in the lattice as a "worldline" and continues by inserting a new operator somewhere randomly. In Fig. 3.1 an extended configuration of 1-dimensional atomic lattice is shown that evolves in discrete steps $\Delta \tau$ of 0.1. It shows 8 particles, 2 of which have moved, based on a Metropolis simulation, until they ended in their original position. Also a newly added particle is shown at position 5, starting at the blue dot symbolizing a stationary annihilation operator. Its red creation operator or "wormhead" is moving in the $+\tau$ direction. This method of Metropolis based simulation of lattice models is called a worm algorithm since "worms" are used to generate new configurations. Worms are pairs of annihilation and creation operators of which one moves through the three-dimensional lattice, $(\bar{b}_i(\tau_0)\bar{b}_j(\tau) + \bar{b}_i^\dagger(\tau_0)\bar{b}_j(\tau))$ [94]. Therefore the worm is a worldline discontinuity in space and time. A moving annihilation operator can only be placed on an already excited worldline and such an anti-worm can not pass through empty sites, such that $n_i \geq 0$ for all $i$.

For each new extended configuration that is generated by a worm step the weight is calculated. $P(i, j)$ is the ratio of this proposed weight $C_{i+1}$ over the original configuration weight $C_i$ and the modification is accepted based on this ratio. The Metropolis algorithm
for the worldline representation looks as follows:

1. From the present configuration $C_i$, propose a random local update which results in an allowed configuration $C$.

2. Generate a random number $u \in [0, 1]$.

3. Accept the proposal, i.e. $C_{i+1} = C$ if $u < \frac{W(C)}{W(C_i)}$ otherwise reject: $C_{i+1} = C_i$.

4. Perform a measurement every certain large number of Metropolis steps.

Measurements should only be performed after enough of these worm loops have been taken to ensure that this thermalization process has created a thermally equilibrated distribution of particle configurations. For a given system size the thermalization time can be determined. In the Directed Worm Algorithm (DWA) only the wormhead moves and steps can only be done in the positive $\tau$ direction. This DWA is used by the ALPS simulation code. In the ALPS code input parameters such as the system size, the chemical potential, the lattice geometry and the interaction strengths can be varied.

### 3.3.2. Observables

Observables can be obtained once a thermalized distribution is generated. They are found by measurements performed on a thermal distribution of configurations. Observables we like to give special attention are the density and the superfluid density. Both follow straight from the configurations that have been generated by the directed worm algorithm. The density per site $\rho$ is computed by simply taking an average of the number of particles per site. Also a measure for the mobility can be found straight from the configurations by counting the number of windings that worldlines make around the spatial periodic boundary conditions. Since they produce wounded worldlines, worm algorithms are a very natural method to simulate systems with superfluid particles. It was shown by Pollock and Ceperley that the average winding number can be directly related to the superfluid density [95]. The superfluid density can be computed from the winding number as:

$$\rho_s = \frac{T}{2t} \langle W_{\text{lat}} \rangle^2.$$  \hspace{1cm} (3.10)

Here we defined the winding number along the atomic lattice dimensions as $W_{\text{lat}} = \sqrt{W_x^2 + W_y^2}$ [96, 97]. The superfluid stiffness is related to the superfluid density as $n_s = \rho_s \times m$. The superfluid density is proportional to the reduced temperature $T/t$ such that it can be compared easily with the density $\rho$. The superfluid density is used to find the phase transition of the superfluid phase. The critical temperature $T_C$ is given by the following linear relation [84, 97, 98, 99, 100]:

$$\rho_s(T_C) = \frac{2T_C}{\pi t},$$  \hspace{1cm} (3.11)

At the critical temperature the superfluid density jumps from zero to a finite value, given by this relation. For finite systems a correction is given by Schmid et al. [96]:

$$\rho_s = \frac{2T_C}{\pi t} (1 + \frac{1}{2 \log \left[ L_0(T_C) \right]}).$$  \hspace{1cm} (3.12)

Here $L_0$ is some characteristic length of the order of the lattice constant [101]. This equation becomes exact in the limit of $L \to \infty$. The critical temperature for such an infinite lattice
Figure 3.2. (a) Superfluid density as a function of reduced temperature $T/t$ for a Kagome lattice with an on-site interaction of $U = 5t$ at filling $\rho = 1$. The yellow dotted line denotes the relation found by Nelson et al. [100], the intersection gives the critical temperature for varying lattice sizes $L$. (b) The critical temperature as obtained from (a). The blue dotted line shows the extrapolation of the critical temperature to find $T_c(L) = 1.764(8)t$ in the limit where $L \rightarrow \infty$.

can be found by a linear extrapolation for various system sizes. In Fig. 3.2 this relation and extrapolation are shown.

Not only the superfluid density is affected by the finite system size. A large enough system should be studied to eliminate system size effects from the measurements. After the phase diagram of the Bose-Hubbard gas on a Kagome lattice is simulated a study is made of its dependence on the system size.

### 3.4. The Bose-Hubbard model on a Kagome lattice

To introduce the phase diagram of the Bose-Hubbard model we will first use the ALPS code to simulate the model on a Kagome lattice of $10 \times 10$ sites. The first extensive study of the Bose-Hubbard model with QMC methods was done by Mahmud et al. [102] for two-dimensional square lattices. Due to its relevance for our experiment and also to compare the developed code with these earlier simulations the Bose-Hubbard model on a two-dimensional Kagome lattice is simulated here. The Kagome lattice distinguishes itself in a few important aspects from the square and triangular lattice. Since each site has four neighbors it is most similar to the square lattice but the configuration of next-nearest neighbors (NNN) is different. In the square lattice four NNN sites can be reached by multiple paths whereas in the Kagome lattice all NNN sites are unique. Due to this difference the long range connectivity is different. Therefore the phase transitions are expected at different temperatures and densities. Two experimental groups have tried to observe this but have so far been unsuccessful [103, 104].

In order to adapt lattices in different ways all simulations are based on the modified square lattice which is available in the ALPS module. A triangular lattice can be formed from the square lattice by adapting the tunneling elements of the underlying square lattice to span a triangular lattice. In a graphical two-dimensional representation this can be depicted by shifting each row by half a lattice spacing, see Fig. 3.3. We define two lattice directions in this triangular lattice: $\mathbf{r}_1 = (1, 0)$ and $\mathbf{r}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$. If one then eliminates
sites on the sublattice of all odd multiples of \(2r_1\) and \(2r_2\), by setting the local chemical potential to infinity, a Kagome lattice is created, see Fig. 3.3. The number of eliminated (black) sites do not contribute to the total number of sites and therefore this Kagome lattice has 75 sites while the underlying triangular lattice has 100 sites.

### 3.4.1. The normal fluid to superfluid transition

When considering the thermodynamics of the Bose-Hubbard model the first thing to consider is the dependence of the system with respect to temperature \(T\). Naturally, when the temperature is high enough no correlation between the particles can be found. At finite temperatures there is a second order phase transition if \(\frac{U}{T}\) crosses \((\frac{U}{T})_C\). This occurs at the critical temperature \(T_C\) which tends to go to zero if \(\frac{U}{T} \to (\frac{U}{T})_C\). This behavior can be seen in Fig. 3.4 where the finite temperature phase diagram is illustrated.

If the lattice barriers are low the dominant phase in the low \(T\) regime is the superfluid phase. In the superfluid phase the fraction of superfluid particles is non zero and these superfluid particles behave as a fluid without viscosity. This phase can be described by a two-liquid fluid model, where the superfluid and the normal fluid coexist. The superfluid part of the liquid is assumed to carry zero entropy and is assumed to flow without the loss of kinetic energy, while the other part behaves as a Newtonian fluid. The phase transition at a filling of \(\rho = 1\) was simulated. First the chemical potential, \(\mu\) was determined for all possible lattice barriers and temperatures, described by \(\frac{U}{T}\) and \(T\). With this constraint a simulation was performed on a square and a Kagome lattice. The results are shown in Fig. 3.5. Here a comparison is made with the simulation of Capogrosso et al. [84]. For the square lattice the same phase transition is found. A lower transition temperature is found for the Kagome lattice because of the lower mobility in the Kagome geometry. To find this
Figure 3.4. Schematical phase diagram of the Bose-Hubbard model for any lattice at a density of $\rho = 1$, adapted from Trotzky et al. [105]. The MI phase is only defined for $T = 0$. The SF phase has a second order phase transition, indicated by the bold orange line.

phase transition the critical temperatures were calculated by the extrapolation that was introduced in Fig. 3.2.

3.4.2. The superfluid to Mott insulator transition

Also other phase transitions in this system exist. There is a transition between the superfluid regime (SF) into a regime in which no tunneling occurs due to a large $U$. This phase is called the Mott-insulating phase (MI). When the barriers of the lattice are high the system simplifies since no hopping occurs. All the lattice sites are then completely decoupled from each other. This means that each site is occupied by an integer number of atoms. The system minimizes its energy by spreading out the atoms evenly. The lowest filled lattice is called the $\rho = 1$ Mott insulator because it has one atom in each well. The MI phase is only defined at zero temperature which makes this phase different than the superfluid phase. When $t \neq 0$ tunneling is possible between the various wells and if the chemical potential allows for more atoms than sites there will be a number of superfluid atoms that can move over the $\rho = 1$ Mott insulator. If the chemical potential allows for even more atoms and when the density approaches two atoms per site this mobility goes down again until at $\rho = 2$ all sites are filled by two atoms in the next Mott insulating phase.

The phase transition between the superfluid phase and Mott-insulating phase at zero temperature is a quantum critical point (QCP). This is a phase transition at zero temperature and a special characteristic of the Bose-Hubbard model. In a 3D square lattice it is found to occur at $U = 29.34(2) t$ [105]. An interesting field of study is the dependence of this quantum critical point on geometry and disorder [105, 106]. Here we first reproduce
Figure 3.5. Simulation of the finite temperature phase transition for the \( n = 1 \) Bose Hubbard model for a square (black dots) and Kagome lattice (blue dots). The original figure is obtained from Capogrosso et al. [84]. A comparison between their results, obtained for a square lattice and our simulations is made. Our black data points fall on top of the original data. Also the new results obtained in this thesis for the Kagome lattice are shown. Error bars fall inside the data points. The dotted lines are a guide the eye. The red dashed lines stem from analytical results for the square lattice for the weakly (strongly) interacting gas near \( U = 0 \) (17)t.

the value of the critical point for a 2D square lattice at \( U = 16.9 \) \( t \) that was found by Capogrosso et al. [84].

We performed simulations in the range of \( t = (0.0-0.14) \) \( U \) for the triangular and Kagome lattice. For both lattices the first two Mott lobes can be distinguished clearly in Fig. 3.6. Mott lobes are regions in phase space where the density per site is an integer number of atoms, here \( \rho \) is 1 or 2. The Mott-insulating phases at \( \rho = 1 \) and \( \rho = 2 \) can be studied spectroscopically in future experiments because of their different potential energies. Since density per site \( \rho \) is plotted it can not be seen that the triangular lattice contains 25 % more atoms then the Kagome lattice for the same system size \( L = 10 \).

We find that for system parameters which can be created in future experiments that both the SF and the MI can be observed and that quantitative differences occur for the various geometries. When \( t \ll U \) the superfluid phase gets suppressed by the MI. The tip of the \( \rho = 1 \) Mott lobe in the triangular lattice is found at \( t = 0.05 \) \( U \), while in the Kagome lattice case this is at \( t = 0.07 \) \( U \). For comparison, the SF-MI transition for a 3D square lattice at zero temperature and unit filling lies at \( t = 0.04 \) \( U \). Similar to the superfluid-normal phase transition a lower transition to the superfluid phase is predicted for the Kagome geometry. This lower transition temperature can be attributed to a different long-range connectivity within the lattices which can be seen in the different next-nearest neighbor configurations. No other differences between the phase diagrams of triangular and Kagome lattice can be observed.
3.4.3. Finite size effects

The effect of having a finite lattice size in the simulations was studied to obtain the system size dependence of the results. The minimal lattice size that was studied is $10 \times 10$ sites, for some studies also bigger lattices were taken into account. In Fig. 3.7 we compare simulations with varying lattice sizes and temperatures. A doubling of the system size from 100 to 400 sites is compared to a doubling of the temperature. Recall that we only consider lattices with equal width and length. We observe that the lower temperature leads to a sharper phase transition at $\mu = 0.15 U$. No differences of a similar scale are found between the simulations with varying system sizes.

3.5. A Kagome superlattice

In the previous chapter magnetic potentials were introduced that can trap atomic gases in various geometries. By controlling the external magnetic field, the chip pattern and the film thickness, lattices can be made at various length scales and with varying potential depths. To create a Kagome geometry and to study disorder, local modifications to the infinite square and triangular potential patterns were made. The effect of these modifications on ultracold gases and their quantum phases were simulated by implementing local chemical potential variations in the ALPS code.

Kagome lattices were created from a triangular lattice by raising the bottom field of particular sites by 50% which corresponds to $0.5 U$. The hexagonal lattice can be created by the same method but only simulations for the Kagome lattice are shown here since the results are valid for all possible sublattices. This simulation will provide insight in how far a magnetic trap must be raised to isolate it from the rest of the lattice. First let us recall the Bose-Hubbard Hamiltonian:

$$H = - \sum_{\langle i,j \rangle} t_{ij} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu_i n_i$$

(3.13)
Figure 3.7. Comparison between simulations with different finite size and different temperature. All simulations are done for a Kagome lattice. The density is plotted for $t = 0.033 \, U$. These three simulation are compared to relate the error that is made for a small system size to that of temperature. A simulation done at $T = 0.04 \, U$ for a $10 \times 10$ lattice is plotted in green. The effects of doubling the lattice size to $20 \times 20$ (blue) and doubling $\beta$ to $(T = 0.02 \, U)$ (yellow) are plotted. A sharper phase transition is observed near $\mu = 0.15 \, U$ for lower temperatures. Lines were added as guides to the eye.

Now we define the following local chemical potential:

$$
\mu_i = \begin{cases} 
\mu + \delta \, U & \text{All odd multiples of } 2r_1 \text{ and } 2r_2 \\
\mu & \text{All other sites}
\end{cases}
$$

Here $\delta$ is the offset of the raised lattice sites. Kagome sites are the sites which are not affected by the offset. Non-Kagome sites are the sites which are raised by a value of $\delta$. The number of sites in simulations with a finite $\delta$ is the same as the underlying triangular lattice. The following simulations are done by extending the directed worm algorithm provided by the ALPS project [89] to incorporate $\mu_i$. An example of a local density simulation is presented in Fig. 3.8. Here $\delta = 6$ which results in a lower average occupation of the elevated sites.

First the full Kagome lattice is simulated and compared with the results from the previous section. A full 100% Kagome lattice can be created by setting $\delta = 20$ which we compare to simulations done with $\delta = \infty$. We find a similar phase diagram for both systems, presented for $T = 0.04 \, U$ in Fig. 3.9. After normalization to account for the varying number of particles in the system both simulations fall on top of each other, showing the same similarity as for the lattices in Fig. 3.6.

After this check was done two different superlattices were simulated. One where a sublattice was raised maximally with $\delta = 0.5$ and another where the same sites were only elevated by $\delta = 0.2$. In Fig. 3.10 it can be seen that only when the sites are raised by $\delta = 0.5$ a real sublattice is formed. The $\rho = 1$ Mott insulator for the Kagome lattice is clearly visible at a density of 0.75 atoms per site around $\mu = 0.25 \, U$. Also a MI phase in the full triangular lattice is observed at $\mu = 0.75 \, U$. The second Kagome MI phase

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Figure 3.8. Local density simulation for a Kagome super-lattice. Local chemical potential is raised by $\delta = 6$ at lattice sites which are not part of the Kagome lattice. Here $\mu = 0.41 \, U$ and $t = 0.022 \, U$ such that Kagome lattice is filled by 1 particle per site.

Figure 3.9. The phase diagram showing average density and superfluid density for the Kagome lattice with $\delta = 20$ and with $\delta = \infty$. The simulations with infinite $\delta$ have been normalized with a factor $4/3$ to account for the lower number of lattice sites. Both lattices have a hopping value of $t = 0.022 \, U$, a lattice size $L = 10$ and a temperature $T = 0.04 \, U$. One can see that the Kagome superlattice gives the same results as the pure Kagome lattice.
Figure 3.10. Average density and superfluid density simulation for $t = 0.022\,U$ and $T = 0.04\,U$ on a Kagome lattice with size $L = 10$. a) A super-lattice with $\delta = 0.2$ compared to a complete. b) A super-lattice with $\delta = 0.5$. Lines were added as guides to the eye.

does not form at this temperature but a modification to the transition between the first and second triangular insulating phase can be observed. These results show the feasibility of our proposed method to create exotic lattices by local modifications to the magnetic pattern.

3.6. Effects of disorder in nanofabricated lattices

We also simulate disordered lattices to find out how the Bose-Hubbard physics is affected by disorder. The magnetic potentials that are described in this thesis all are fabricated with nanolithography techniques. Even though one tries to limit disorder and optimizes all processes to obtain the maximum resolution, some disorder is inevitable due to the resolution of the fabrication method. At the same time, lattices with a controlled amount of disorder are interesting in itself. The presence of disorder is a fundamental difference between static magnetic and optical lattices. There are various sources of disorder in the magnetic potentials while the optical lattice is perfectly periodic. The two most important ones are discussed here. First, the magnetization of the material might vary slightly from trap to trap. It is hard to measure the local magnetization of nanoscale structures. From measurements performed on older chips we have seen a maximum variation up to 3% in trap bottom field for microtraps at 10 $\mu$m trap separation, indicating a similar variation in the local magnetic field of the chip. Second, the inter-trap separation might vary locally because of disorder in edge definition due to pattern deformations. This leads to variations in the trap position, which can result in a spread in tunneling elements because they depend exponentially on lattice spacing. Both origins of disorder are combined in the simulations because we can not treat them separately. The smallest patterns described in this thesis have a lattice spacing of 250 nm and are written with a resolution of 30 nm, created by e-beam lithography with a focused electron beam of 5 nm. The edge roughness is approximately half of the resolution which determines the detail of the entire magnetic pattern. In these lattices this combined disorder is therefore $250/(0.5 \times 30) \approx 5\%$. We
Figure 3.11. Density and superfluid density simulation for Kagome lattice at $t = 0.022 U$ and $T = 0.04 U$. Various values of $\Delta$ are simulated to study the effects of local disorder. Lines were added as guides to the eye.

will simulate these lattices and higher amounts of disorder to predict the effect on the Bose-Hubbard physics.

The resolution of the lithography process can be used to control the amount of disorder in the manufactured potential. If one wants to generate a lattice with a fixed amount of disorder, without a priori drawing this specific lattice, the lithography process can insert disorder based on the chosen resolution.

To simulate the effect that disorder can have in magnetic lattice potentials another adaptation to the local chemical potential was made. Now the chemical potential of each lattice site is assigned a randomly generated offset:

$$\mu_i = \mu + \delta_i U, \quad -\Delta \leq \delta_i \leq \Delta. \quad (3.15)$$

Several simulations were done with different magnitudes of disorder $\Delta$ to investigate both lattices that can be created with the best possible resolution and more disordered lattices. Also a simulation is made to investigate whether the MI and SF phases are influenced or broken up by increasing amounts of disorder. The simulations for a triangular and Kagome lattice are compared in Fig. 3.11.

For both geometries we observe that at $\Delta = 0.05$, a realistic amount of disorder for the potentials that are fabricated in chapter 3, no alteration of the phase diagram can be observed. For larger amounts of disorder the MI phase shrinks. The superfluid density also shrinks when we increase the disorder. In the Kagome lattice it shrinks so much that the superfluid density goes to zero at $\Delta_i = 0.2$ around $\mu = 1$. When comparing the Kagome lattice to the triangular lattice one can observe that the Kagome lattice is less affected by increasing amounts of disorder than the triangular lattice. In the triangular lattice the superfluid fraction is larger and the MI phases are generally smaller then in the Kagome lattice. A similar simulation with various different techniques to model disorder has been made by the Lewenstein group [106], the QMC method used here confirms these results.

### 3.7. Magnetic fence potentials

The last geometric adaptation that we consider here is a modification to the boundaries. So far periodic boundary conditions have been used in the simulations. An experimental
realization of such an infinite lattice would result in a completely delocalized gas which would never be observable. To circumvent this problem we have developed magnetic barriers which can enclose a lattice gas, keeping a uniform lattice potential with periodic interruptions of a particular potential height.

In the figures below a lattice of 30 × 30 lattice sites is studied. The barriers that we simulate are comparable to the fences proposed in the previous chapter. The fences are roughly twice as high as the inter trap barriers, to suppress tunneling. Since the simulation still uses periodic boundary conditions only two trap arrays are raised. These can be recognized as the lines that run along the edge of the lattice in Fig. 3.12 (black).

To investigate the local density in all the traps we have left the raised barriers out of the next four figures. Showing the barriers themselves, as in Fig. 3.12, would overshadow the effects shown in Fig. 3.13 and Fig. 3.14. We consider a gas in the MI phase and compare thermal atomic distributions of two different boundary types. The finite lattice is shown in 3.13(a). This is a lattice without periodic boundary conditions such that it simulates infinitely high fences. This is compared with a lattice where barriers of 6 U are simulated. In the superfluid phase no difference can be observed between the lattice with infinite barriers, Fig. 3.13a, and the finite realistic magnetic fences, Fig. 3.13b. Edge effects are visible since we plot the system with less atoms than lattice sites. The local density is slightly lower at the edges because the atoms occupy the outer traps on average less than the central ones. These results show that it is possible to contain a superfluid gas by magnetic fences without generating extra edge effects in the lattice.

A simulation for a gas in the MI phase is presented in Fig. 3.14. No distinction can be made between infinite and finite box potential. The atoms are spread out completely since
Figure 3.13. Simulated local density plot for a gas in the superfluid phase with \( t = 0.022 U \), \( T = 0.04 U \) and \( \mu = 0.83 U \). (a) A triangular lattice with infinitely high barriers. (b) A triangular lattice with a surrounding fence of \( \delta = 6 \).

The simulation is done in for \( \mu = 0.34 U \), for which we expect a \( \rho = 1 \) MI phase. This results in the small variations from site to site. The creation of such box potentials allows one to study gases in uniform geometries and have recently attracted much attention [62, 83]. Lattice potentials in a confining box such as those presented here have not been created.

Figure 3.14. Simulated local density plot for a gas in the Mott-insulating phase with \( t = 0.022 U \), \( T = 0.04 U \) and \( \mu = 0.34 U \). (a) A triangular lattice with infinitely high barriers. (b) Similar lattice with a smaller fence of \( \delta = 6 \).

## 3.8. Summary

The Bose-Hubbard model has been studied by means of quantum Monte Carlo simulations with the ALPS program. The directed worm algorithm method within ALPS was extended to include a site dependent chemical potential. The phase transition between the normal and the superfluid regime is predicted to occur at a lower temperature in the Kagome lattice with respect to a square geometry. The phase diagram of hopping, interaction energy, temperature and chemical potential were studied for superlattices where the local chemical potential per site was varied to construct Kagome lattices from an underlying triangular geometry. The simulations predict that the first two Kagome Mott insulating phases can be observed with magnetic superlattices. To simulate disorder, random local chemical potential variations were used. With a total variation up to 20% the SF-MI transition could still be observed. The superfluid density and the MI phase both are
affected by the disorder and shrink compared to the fully periodic lattice. At realistic amounts of disorder no change in the systems phase diagram was observed, proving the feasibility to study the SF-MI transition in uniform magnetic lattice potentials. Magnetic box potentials were simulated by studying a free lattice gas within a structure with raised chemical potential per site at the boundaries of a lattice. Simulations predict that such a box potential with a barrier such as those presented in chapter 2 will be enough to enclose a SF bosonic gas.
4 | Fabrication of magnetic lattices with varying length scales down to 200 nm in FePt

4.1. Introduction

Simulating the quantum world keeps providing us new insights into the laws of nature. Experimental simulations of condensed matter systems with atomic lattices have provided new insights on phase transitions and low dimensional systems. Moreover, atomic lattices also provide a good platform for many quantum information applications. Phenomena that are studied in these systems include tunneling and interactions between lattice sites. Hence there is a continuous effort to scale down the length scale of these lattices. With smaller lattices higher tunneling rates and stronger interactions over multiple sites may be achieved which will allow the study of more complicated models like the extended Hubbard model and long range spin models [107, 108]. The optical lattice can not be scaled down further than approximately $\lambda/2 = 300$ nm since they are limited to available laser wavelengths. Lattices made out magnetic materials however can be scaled down since their scale is only limited by the resolution of the method by which they are made. These nano-fabricated lattices can even be scaled down continuously, providing a range of length scales which can be used for loading and detection purposes. Magnetic lattice experiments therefore combine the design freedom of solid state nano-fabrication techniques and the quantum nature of ultracold gases. The fabrication of smaller magnetic structures also has an industrial application since most hard discs use magnetic islands to store bits of information [109]. FePt is often used for hard disc fabrication although structures, techniques and dimensions differ from application to application. This chapter focuses on the fabrication of small magnetic lattices to create atom traps with the smallest possible resolution, provided by electron beam lithography.

4.1.1. Previous fabrication results

In previous experiments magnetic lattices with periods of 10 $\mu$m or larger were used both in one and in two dimensions to trap ultracold gases [33, 44, 52]. These experiments used permanent magnetic films with a thickness of several hundred nanometers, patterned by optical lithography. For patterning at the sub-micron scale electron beam lithography can be used. This technique has been well developed for semiconductor applications based on Si but has not been used so far to etch FePt. In the Swinburne group a magnetic lattice with a period of 700 nm was created this way in a Co/Pt multilayer film of 2.2 nm thick [45]. In the present chapter we describe the patterning of 50 nm thick FePt films, using e-beam lithography to create lattices with periods down to 200 nm, putting us well within the
exciting regime of sub-wavelength tunneling physics. New mono-crystalline magnetic films were developed to create these atom traps. Also a new lithography process was developed to etch patterns with a resolution of 30 nm.

Special attention will be given to tapered structures because they span all the length scales at which magnetic lattices have been made. Also they are written with the highest state-of-the-art resolution of just 30 nm. The trapping potential for the atoms in all magnetic lattice experiments is created by a permanent magnetic structure and an external magnetic field. Fig. 4.1a shows a segment of such a structure. In combination with an external field the curved magnetic structures (black) form a lattice of magnetic field minima which can be used to trap ultracold atoms. In Fig. 4.1b the simulated potential that can be created by this lattice is shown. Exact field values depend on the external magnetic fields and the film parameters.

This chapter is divided into three different sections that describe the fabrication of our new atom-chip. First we describe the newly developed FePt films and their characteristics. In the second section we describe the fabrication process of the trapping arrays in the FePt film and in the last section we show the resulting magnetic patterns that were created for various quantum simulation experiments.

4.2. Molecular beam epitaxy of mono-crystalline FePt films

To create traps for ultracold atoms at various length scales one needs to carefully consider the magnetic properties of the material. Strong permanent magnetic materials are required to create stable traps. Their magnetization and coercivity must be higher than externally applied magnetic fields of up to 200 G. The remanence magnetization should withstand the bake-out procedure that is required to obtain ultra high vacuum (UHV) conditions, typically at 150 °C. The choice for FePt as strong magnetic material is based on our experience with this material in previous experiments. The alloy FePt in the $L1_0$ crystalline phase has a very high remanence magnetization and coercivity, both above 0.1 T depending on fabrication parameters [110, 111, 112].
Previously films of FePt ranging in thickness from 200-400 nm were created by sputtering techniques [113]. The sputtered films were too thick to create lattices at smaller length scales. Also their flatness and grain size are not compatible with structures smaller than 500 nm. Therefore new films were deposited by Molecular Beam Epitaxy (MBE). This technique was explored by various research groups [110, 114, 115, 116] to develop magnetic recording media from FePt and is also used for inter-phase studies in magnetic materials [112]. The slower MBE process in combination with matched substrate lattice spacing helps to create higher quality magnetic films. Our aim is to fabricate microtraps with lattice spacings ranging from several micrometers down to 200 nm. Because of this wide range of length scales films of 50 nm thick were fabricated. More details on the resulting trap parameters can be found in chapter 2.

4.2.1. MBE deposition of FePt

The films that are used to fabricate magnetic atom chips are fabricated at the KU Leuven in the group of Prof. A. Vantomme and Prof. K. Temst. To create mono-crystalline films a matched substrate of MgO is used to grow the crystal during evaporation into the desired (001) orientation, unlike the older films which were sputtered on Si and then annealed to transform them into the L10 phase. Especially thin substrates of only 150 μm thick MgO were used. Polished MgO substrates were used with a maximum roughness of less then 2 nm/μm, measured with an interferometer microscope [117].

The substrates of 20×20 mm² were pre-annealed overnight in a vacuum oven that was connected to the MBE machine. The samples were heated to 500 °C to allow direct growth into the desired (001) orientation and the L10 phase of FePt. By controlling the growth rate around 0.5 Å/s we obtained mono-crystalline films of FePt with the same flatness as the polished MgO substrate. Six batches of two substrates were created, all with an even ratio of Fe and Pt to create Fe50Pt50. The thickness of the films was controlled by timing the growth rate in situ and all films were found to be 50(2) nm thick.

4.2.2. Characterization of FePt films

Several tests were performed on the fabricated samples to check the quality of the films. X-ray spectroscopy was performed on all samples to determine the quality of the FePt crystals. We define a long range order parameter $S = \sqrt{0.45 \times I_{000}/I_{002}}$, [112]. Here $I_{000}$ and $I_{002}$ are the intensities of the X-ray peaks corresponding to the (100) direction and the (002) direction. A perfectly ordered mono-crystal will give $S = 1$. We found values of 0.65, 0.55 and 0.65 for batch 1, 2 and 3 respectively. The spectrum of batch 3 is shown in Fig. 4.2. $S > 0.5$ indicates a high mono-crystalline fraction. The chip that was fabricated to house the first nano-lattice geometries was made out of batch 3.

We also performed Mössbauer spectroscopy, the results of which are presented in Fig. 4.3. From the aspect ratio of the six peaks in this spectrum the orientation of the magnetic axes can be found. The angle between the main crystal axes (100) and the magnetic orientation $\theta$ can be fitted to the ratio of the Mössbauer peaks by the following formula, from [112]:

$$3 : 4 \times \frac{4 \sin^2 \theta}{1 + \cos^2 \theta} : 1 : 1 : 4 \times \frac{4 \sin^2 \theta}{1 + \cos^2 \theta} : 3$$  \hspace{1cm} (4.1)

For example the intensity ratio for pure $^{57}$Fe crystal which is magnetized in-plane is 3 : 4 : 1 : 1 : 4 : 3. This indicates a magnetic orientation angle $\theta = 90^\circ$. For the fabricated mono-crystalline FePt samples an angle $\theta = 0^\circ$ was measured as can be seen in Fig. 4.3.
Figure 4.2. X-ray diffraction spectrum of the grown FePt films, measured at KU Leuven. Similar to results from B. Laenen [112].

This indicates an out of plane magnetization. These measurements match the results of previous samples that were fabricated in 2007 [112].

Figure 4.3. Mössbauer spectrum of the grown FePt films, measured at KU Leuven. Arrows indicate positions of absent peaks which would be expected for a material with in plane magnetization. The red line is a fit through the data.

To determine more magnetic properties of the fabricated films, we performed SQUID measurements on the samples in Leuven at both 300 K and 350 K, without any observable difference. The 300 K hysteresis curve is given in Fig. 4.4. The curve is rectangular, indicating both a high remanence magnetization of \( M = 900 \text{kA/m} = 9 \times 10^{-4} \text{emu/cm}^3 \) and a high coercivity of 0.4 T.

Bake-out tests were performed in Amsterdam, here hysteresis curves were measured with a Magneto Optical Kerr Effect (MOKE) experiment before and after the samples were heated up to 150 °C. No loss of the magnetization could be observed from these MOKE
Figure 4.4. Hysteresis curve of the grown FePt films, using a SQUID at KU Leuven at a temperature of 300 K.

<table>
<thead>
<tr>
<th>Property</th>
<th>UvA</th>
<th>Hitachi</th>
<th>Leuven</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions (μm²)</td>
<td>22 × 36</td>
<td>10 × 10</td>
<td>0.2 × 0.2</td>
</tr>
<tr>
<td>( M_r ) (kA/m)</td>
<td>580</td>
<td>670</td>
<td>900</td>
</tr>
<tr>
<td>( M_s ) (kA/m)</td>
<td>725</td>
<td>720</td>
<td>935</td>
</tr>
<tr>
<td>( M_r/M_s )</td>
<td>0.80</td>
<td>0.93</td>
<td>0.95</td>
</tr>
<tr>
<td>( H_c ) (G)</td>
<td>9500</td>
<td>9500</td>
<td>4000</td>
</tr>
<tr>
<td>( M_r ) decrease after 3 hour bake at 150 °C</td>
<td>20 %</td>
<td>3 %</td>
<td>0 %</td>
</tr>
<tr>
<td>Estimated grain size (nm)</td>
<td>20</td>
<td>35</td>
<td>≤ 7</td>
</tr>
<tr>
<td>Surface roughness (nm)</td>
<td>1</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>Thickness (nm)</td>
<td>300</td>
<td>250</td>
<td>50</td>
</tr>
</tbody>
</table>


measurements. In previous experiments this loss was estimated to be around 3%, [118]. The MOKE tests did reproduce the SQUID hysteresis curves.

The grain size is measured with a Scanning Electron Microscope (SEM) inspection of the samples. For a comparison in Fig. 4.5 we show a SEM image of the new MBE material together with that of an older sputtered FePt film [32]. In the sputtered material grainy structures with a typical size of 40 nm can be observed. At a much higher resolution a grain pattern like this is not visible on the MBE samples. A comparison between the parameters of the MBE grown films and sputtered films, that have been used previously for magnetic atoms chips, is presented in table 4.1.
4.3. Electron beam lithography

Patterning of these films was performed at the Kavli Nanolab in Delft. Previous magnetic films were patterned by optical lithography, a process where a mask is transferred to a resist layer by exposure to ultraviolet light. This technique is limited by the wavelength of the light that is used, minimally 200 nm. To write lattices down to 100-200 nm a much higher resolution was required. Electron beam lithography allows one to use beams down to a few nm in size. In this process a resist layer crystallizes to form an etch mask. Resolution, defined as the smallest resist structure that can stand freely, is typically several electron beam spot sizes. The FePt films were found to have a large backscattering angle which required a highly sensitive correction in the writing process. Also the samples were hard to plasma etch in a controlled way. For lattices of 200 nm or less, edges of less than 40 nm wide were required to create free standing magnets. Both these challenges are discussed in more detail below.

4.3.1. General aspects of e-beam writing

The lattice patterns were written by a VISTEC e-beam pattern generator (EBPG5000+). A negative resist was used to create islands of FePt on the substrate below. First a 100 nm resist layer, twice the thickness of the magnetic material, was spin-coated on the samples. Then the sample was aligned with a precision of several μm on an e-beam sample holder and inserted into the EBPG, where a computer controlled beam of 100 keV electrons wrote the instructed pattern in the resist layer. The high energy electrons break chemical bonds within the resist upon which the resist crystallizes. This hardened resist formed a mask to protect the layer of magnetic material during the etch. The non-crystallized resist was dissolved in a base solution leaving behind the illuminated structures. Ideally, these structures have the resolution of the 100 keV electron beam. For structures of different sizes we used beams with different spot sizes because this greatly reduces the writing time. To create our patterns a beam of 150 nm was used to create larger, low-resolution structures and a 3 nm beam was used to create the smaller, high-resolution lattices. All high-resolution
lattices are surrounded by a 2 μm square background lattice of at least 50 μm wide which is written with the 150 nm beam. This ensures that no magnetic edge effects influence the fields above the high-resolution lattices.

The EBPG writes at a maximum speed of 50 MHz, so it can illuminate at most 50 million spots of a certain size per second. To cover a square millimeter at this rate the machine would need more than an hour with a 3 nm beam and less than a minute with a 150 nm beam. Because of the digital nature of an EBPG and the chemical nature of the development several complications arose. The most important parameter to optimize the writing process was the dose of electrons, measured in μC/mm², that is deposited in the resist. To create a structure of the intended size one needs to vary the electron dose and compare the created structures with intended digital ones. For a lattice that covers 50% of a surface the ideal dose can be determined by measuring the ratio between developed resist and non-developed resist. If the dose is too low more than half of the resist will be removed during the development and the mask will cover less than half of the surface.

4.3.2. Proximity dose correction

Another process parameter that needs to be tuned is the proximity correction. This is necessary because also backscattered electrons from the various layers under the resist contribute to the crystallization process. Commercial software was used to simulate the electron beam point spread function that is unique to these samples [119]. The point spread function is dominated by two contributions, due to the forward and backward scattering angles. The forward scattering angle describes the opening angle of the beam into the resist layer. Since this is a geometric effect we express this angle by the diameter of the affected area on the resist surface, here 5 nm. The backward scattering angle describes the angle under which electrons are backscattered into the resist layer, resulting in a diameter of 23 μm. By deconvolving the structure pattern with the point spread function the ideal local dose exposure is found which will create the pattern more accurately.

The proximity correction is simplified due the background lattice which surrounds all science structures. This background lattice ensures that the edges of the science structures all receive the same electron dose. Only at the edge of the background lattice the proximity corrections corrects the local dose to ensure an even electron exposure over the entire lattice. All lattices were combined and jointly underwent proximity correction based on the simulated point spread function. Then the different lattices which were written by the different beams.

4.3.3. Electron beam lithography on mono-crystalline MgO-FePt

Initial attempts were done with hydrogen silsesquioxane (HSQ), because this resist provides the highest resolution. HSQ is a resist solution with an extremely high sensitivity [120]. This sensitivity is caused by the chemical instability of the HSQ solution, which is highly sensitive to temperature fluctuations. To write structures with the highest resolution on the FePt samples a dose of 200 μC/mm² was used. On the thin mono-crystalline MgO-FePt samples two complications occurred which were not present in earlier tests with thicker Si-FePt samples. The dose required for ideal HSQ development fluctuated wildly, requiring different doses from sample to sample. Furthermore, adhesion problems resulted in many lattices (partly) detaching from the sample during development. If, in future experiments the resolution requires the sensitivity of HSQ, a bonding layer of several nanometers must be deposited to ensure a reproducible and stable development.
For these reasons we switched to AR – N.7500.08, a more stable and less sensitive resist, manufactured by ALL resists [121]. AR – N.7500.08 is a negative resist with a resolution of \( \approx 30\,\text{nm} \). It is very stable, but requires a much higher dose to crystallize than HSQ. It can also be kept much longer and can be stored at room temperature.

The recipe to create a 100 nm high etch mask with AR – N.7500.08 at its ultimate resolution is listed below.

1. Spin adhesion film hexamethyldisilazane (HDMS) at 2000 rpm
2. Bake for 2 min at 200°C
3. Spin at 4000 rpm to get a 100 nm thick film
4. Bake for 1 min at 85°C
5. Expose at a dose of 1375 \( \mu\text{C/mm}^2 \)
6. Develop for 1 min in pure MF322
7. Develop for 1 min in 1 : 9 solution of MF322 : H\(_2\)O

An optimal dose for this negative resist was found at 1375 \( \mu\text{C/mm}^2 \) which produced structures with a resolution of 30 nm, while using a beam step size of 3 nm and a 5 nm spot. With this resolution lattices were created down to 200 nm period as shown in Fig. 4.6. In Fig. 4.6b three square lattices are written with lattice spacings of 900, 600 and 200 nm. The lattices have a minimum open trench of 50 nm in the smallest 200 nm lattice.

![Figure 4.6. a) Pattern sent to the EBPG to write square lattices on three different length scales. In this view segments with a period of 900, 600 and 200 nm are visible. b) The transferred pattern in the resist using the optimal dose of 1375 \( \mu\text{C/mm}^2 \).](image)

In lattices with periods below 200 nm the resist structures connect because the width of the trenches becomes of the order of the resolution. With thinner magnetic films thinner resist masks can be used which would allow for lattices down to 100 nm. Below 100 nm the required resolution is of the order of several nanometer and different methods need to be investigated. Possible techniques are: 1) a multi step process based on a metal mask [114, 122] and HSQ as a resist, 2) ion milling with Ga\(^+\) as investigated in the next chapter or 3) ion milling with a higher resolution He\(^+\) beam.
4.3.4. Ultra low pressure plasma etching

The resist mask is transferred to the magnetic film by ion plasma etching. Two parameters are important in this process, the redeposition of removed material and the selectivity of the etch rate for the magnetic layer as compared to the mask. The mask should ideally be just thick enough since the resist which is left behind sticks to some of the removed FePt that falls back onto the sample during etching. This redeposition falls on the sides of the left-over resist and creates edge slopes in the trenches.

The crystalline phase of these redeposited FePt, and therefore their magnetic behavior, is not known. The redeposition slope $\alpha$ on the structures side is $30^\circ$ for optimal plasma parameters. With this redeposition slope and the height of the magnetic layer of 50 nm this etching technique is limited to the fabrication of lattices with a spacing of $> 200$ nm, see Fig. 4.7. A method to achieve smaller edge slopes is to use a non-focused ion beam in stead of a plasma, which can etch under an angle with the sample. By varying the angle of incidence of the ion beam with a rotating sample one can etch the edges together with the top of the pattern, such that structures with straight or under etched (negative) slopes are created.

![Figure 4.7](image)

Figure 4.7. a) Pattern for a square lattice. Lines 1 and 2 indicate the positions of smallest trench and smallest standing resist structure. b) Cross section of the pattern at position 1 before etching. c) Etch slopes as they are created by plasma etching with optimal redeposition angle $\alpha = 30^\circ$ at position 2.

An Ion Etching (IE) machine (Survival Techniques Systems), was used at a pressure of 1.6 mTorr. At these low pressures we were able to reach the etch slopes of $30^\circ$ redeposition. The following etch settings were used: exposure of 210s to a plasma of 35 SCCM Ar and the ions were accelerated from the plasma with 795 W forward power and a power of 27.9 W on the lower plate.

To limit overetching the reflection of a laser was monitored and the process was stopped several seconds after the MgO substrate became visible. Inspection of cross sections of the samples showed no significant overetching. Fig. 4.8 was etched for 5 min to show the etch slopes more clearly. Also the redeposition is visible since it sticks out above the light magnetic layers, sticking to the left over resist. The final chip patterns and their cross sections are presented in the next section.

The redeposited FePt could not be removed chemically. The leftover resist and the redeposited FePt were left on the sample. These unwanted structures in the profile of the chip are hard to remove. There is no method to completely remove the redeposited FePt. The only partially successful recipe requires chemically enhanced etching with an CH$_4$/O$_2$ plasma in combination with a Ti/N cover film, as was recently investigated in reference [115]. Since no significant gain was possible we opted to leave the redepited material on
Figure 4.8. A cross section of a 600 nm lattice as etched by the procedure described above. From top to bottom; Pt deposited locally to protect the interface during milling (grey), resist leftovers (dark), FePt (light), MgO substrate (black). The etch slope is indicated in red with an angle of 30°. The overetched trenches go up to 200 nm into the MgO substrate. On the middle magnet the redeposition against the resist is colored blue.
the chip. The structures are approximately 100 nm high before they are covered with a mirror layer. This layer is 50 nm thick and made of Pt. It is deposited to reflect optical beams in the experiments and to protect the structures underneath. The inspection which is presented in the next section was done before the samples were covered by this layer.

### 4.4. Focused Ion Beam inspection

To inspect the fabricated structures cross sections were created by focused ion beam (FIB) milling. Before these cross sections were made, Pt was deposited locally to protect the interface of the top layer. The Pt precursor gas Pt(PF₃)₄ is used to create this ≥200 nm thick Pt dome.

In Fig. 4.9 we show a cross section of an etched FePt lattice structure with 200 nm lattice spacing. This cross section was made at the position where the trench separation is at its smallest, see also Fig 4.7. By inspecting the lattice at various points and measuring the edge slope, here α = 34(2)°, we can conclude that the structures stand freely.

![Figure 4.9. Inspection of a 200 nm lattice of FePt. a) FIB cross section; One can distinguish the different materials, from the MgO substrate up: MgO(yellow), FePt (very bright), redeposited triangular shaped metal (also bright, ≈ 100 nm high), resist (dark red), Pt cover layer (gray and grains). b) A SEM image of a wider region containing the same cross section. The red dotted line indicates the direction of the cross section. Sub-figure a) is taken several micrometer to the left of b) at a point where the magnet is widest and the trench smallest.](image)

After patterning the chips were capped by a 50 nm layer of Pt. SEM pictures from all written lattices were taken after this capping layer was deposited. In Fig. 4.10 we show one of these structures which contains both large and small lattices, written at the highest resolution. A tapered structure with a lattice spacing that decreases by 1% per line from 5000 nm to 250 nm in 300 lines is shown. Writing these extended high resolution structures took 2.5 hours, after which the surrounding "background" lattice was written. The top insets shows the taper tip and the background lattice. The other insets show parts of the lattice at different length scales.
Figure 4.10. SEM image of the full magnetic tapered lattice. Insets show section up and down the taper in higher resolution.
4.5. Summary

We created lattices in permanent magnetic material to trap ultracold atoms. We created 50 nm thick mono-crystalline films of FePt in the $L1_0$ phase with high remanence magnetization of 900 kA/m. These films were then patterned with e-beam technology to created lattices ranging continuously from 5 µm to 250 nm lattice spacing. A negative high resolution resist is used as a mask for plasma etching the film with a 30 nm resolution. Ar plasma etching was performed to imprint the pattern under optimal conditions into the magnetic film. A Pt cover layer was evaporated and the resulting structures were studied by taking FIB cross sections. The structures created with this chip will be used in the nearby future to studying systems of trapped and interacting ultracold Rb atoms.
5 | Probing the magnetic moment of FePt micromagnets prepared by Focused Ion Beam milling

This chapter is an extended version of the paper Probing the magnetic moment of FePt micromagnets prepared by Focused Ion Beam milling, published in Applied Physics Letters.

5.1. Introduction

In this chapter we test a new method of fabricating magnetic atom chips, or more in general nano-scale magnets. In the previous chapter it was shown how lattices of strong permanent magnets down to 200 nm spacing are made by electron beam lithography and plasma etching. The advantages of plasma etching are its reproducibility and speed but there are some important limitations in resolution. In stead of etching with a global plasma, either in a reactive ion etching (RIE) machine or under an angle with a beam etcher, it is also possible to etch materials with a focused ion beam (FIB). A FIB was used in the previous chapter to study the etch profiles of plasma etched structures but in this chapter we use the beam itself to cut out nanometer sized magnets. First we discuss a study of the damage that is done to the magnetic material during the FIB milling process. The results of this study were published in 2015 and form the heart of this chapter [123]. In the second part of the chapter we discuss the practical implications of the FIB milling tests for the fabrication of magnetic atom chips. In the last part of this chapter we reflect on the conclusions that we have made and look into some technical applications that exist for nano-scale magnets outside of academia to which our research might contribute.

This study was conducted in the research group of Prof. Dr. Ir. T. Oosterkamp where they use small magnets as sensitive magnetic field probes, exploiting the large magnetic field gradient from a 300-nm, 0.75-T permanent magnet [124]. Therefore we look at more then just lattices in this paper and discuss single magnets on cantilevers. The fabrication and characterization of micron sized permanent magnets is necessary for a broad range of applications, such as for magnetic tweezers [125, 126], for magnetic imaging [127, 128], and for atom trapping with chips [129].

These atom chips are planar structures that generate magnetic fields, which are widely used to control ultracold atoms [35]. The incorporation of permanent magnets in atom chips offers several advantages over the use of current carrying wires [129]: they dissipate no heat and allow for more complex trap shapes. Moreover, permanent magnets can create larger field gradients, which facilitates tighter confinement of atoms [130], resulting in shorter time scales in trapping experiments. This application does require the magnets to be
patterned on small length scales. One of the materials currently under investigation is FePt in its L1₀ phase, a corrosion resistant material with high magneto-crystalline anisotropy [32, 130, 131]. FePt atom traps that are currently in use are made by optical lithography and plasma etching [32, 33]. The currently used patterns have characteristic length scales on the order of 10 μm [44].

Micron sized magnets can also be used as a field gradient source for magnetic resonance force microscopy (MRFM) [127]. This technique uses a small magnet mounted on an ultrasonic cantilever to measure the magnetic interaction with spins in a sample underneath the cantilever. It thereby combines the advantage of elemental specificity of conventional Magnetic Resonance Imaging (MRI) techniques with the local and very sensitive probing techniques of Atomic Force Microscopy (AFM) [132, 133]. Required properties for MRFM magnets are high magneto-crystalline anisotropy and a large remanent field [134]. Small dimensions of the magnet are beneficial too, as they result in large magnetic field gradients, which increase the sensitivity of measurements [135, 136]. These requirements are similar to the requirements for atom traps and are all fulfilled by the aforementioned FePt.

One of the techniques to pattern FePt films is to use a Focused Ion Beam (FIB). However, FIB milling can damage the film, possibly degrading the magnetic properties. Examples of such damage include implantation of ions and other ion beam induced alterations to the crystal structure [137, 138]. Determining the magnetic moment after FIB exposure is crucial for applications in both atom trapping and MRFM experiments.

In this chapter, the damage caused by FIB milling on an FePt film is quantified by measuring the magnetic moment of a micron sized rod, which has been milled out of the film, and comparing it to the expected magnetic moment calculated from its volume and its remanent field. The rod is attached to a cantilever and its magnetic moment is determined by cantilever magnetometry, a sensitive technique to determine small magnetic moments [139, 140]. We demonstrate that FIB milling is a suitable way to shape magnetic films for atom trapping experiments and to prepare probes for MRFM.

5.2. Fabrication

The 300(10) nm thick FePt film has been made at the Almaden Research Center of Hitachi [32]. Films of FePt have been sputtered on a Si substrate with a thin RuAl under-layer and a Pt interlayer, between RuAl and FePt, at a temperature of 400 °C. This growth process leads to FePt in its L1₀ phase, which has a particularly high out-of-plane magnetization. No rods were made with the newly grown monocrystalline FePt that was introduced in the last chapter.

As a first step to create rods, an indentation in the edge of the film is made with a FIB (Ga⁺-ions, 30 keV, 7 nA ion current, Strata 235 Dual Beam from FEI). The edge is then crenelated (Fig. 5.1(a)) (ion current 500 pA) and rods are created in the sides of the crenels (Fig. 5.1(b)). The dimension of the rods is 8.1 μm in length, 1 μm in width and 1 μm in height (consisting of 300 nm FePt and 700 nm substrate). The sample is rotated by 90° to remove the material underneath the rods. The geometry facilitates the access necessary to mount a rod onto a cantilever. Damage to the magnetic layer is therefore created on five sides on the magnetic layer and not from below.

The FePt film and a cantilever (a single-crystalline silicon beam [141]) are then placed on two stages of an in-house developed nano-manipulator [142] inside a Scanning Electron Microscope (NanoSEM 200 from FEI, USA). Using the nano-manipulator, we bring the cantilever in contact with an FePt rod (Fig. 5.2(a)). Subsequently, fixation is achieved by
an electron beam induced deposition process with Pt(PF₃)₄ as a precursor gas. The last connection between the rod and the film is broken by suddenly retracting the cantilever. The finished assembly of the cantilever and the rod is shown in Fig. 5.2(b) and 5.2(c).

**5.3. Characterization**

Prior to the fabrication of the rods, the magnetization loop has been measured for a film of size 3 mm × 3 mm × 300 nm in a SQUID magnetometer (Quantum Design MPMS-5S). The measurement has been performed at room temperature in two different geometries (Fig. 5.3): with an in-plane and an out-of-plane external field \( \mathbf{H} \). The remanent magnetization is \( \mu_0 M = 0.76(0.03) \text{T} \) for the out-of-plane geometry, while it is \( \mu_0 M = 0.50(0.03) \text{T} \) for the in-plane geometry. In Fig. 5.3, the remanent magnetic moment shows negligible dependence on the external magnetic field. This is expected for FePt, as the coercivity increases when the lateral size decreases [143]. Therefore, the external field used in the cantilever magnetometry experiment should not affect the magnetic moment of the rod.

The rods are magnetized in a 3T field at room temperature along the out-of-plane direction (i.e. along the direction of motion of the cantilever), to achieve a higher remanent field.

Subsequently, dynamic-mode cantilever magnetometry is performed at room temperature at a pressure of \( 10^{-5} \text{mbar} \). The external magnetic field is provided by a Helmholtz coil of approximately 300 turns, generating magnetic fields up to 2 mT. The external magnetic field points along the direction of motion of the cantilever. To determine the magnetic moment \( \mu \) of the rod, the resonance frequency is measured as a function of magnetic field.
Figure 5.2. Fixation of a rod to a cantilever: (a) the cantilever is brought in position using a nano-manipulator. After an electron beam induced deposition (EBID) process to fix the rod to the cantilever, the connection to the film is broken by retracting the cantilever (b). The widening on the cantilever works as a mirror for laser interferometry. (c) the cantilever-magnet assembly.

Figure 5.3. Magnetization of the film as a function of external magnetic field strength for two different orientations of the sample. For the out-of-plane orientation the remanent field $\mu_0 M = 0.76(0.03)$ T and for the in-plane orientation it is $\mu_0 M = 0.50(0.03)$ T.
strength. A fiber optic interferometer working at a wavelength of 1550 nm is used to detect the cantilever motion. The resonance frequency is determined by fitting the thermal motion of the cantilever's fundamental mode to a Lorentzian curve [144]. A ring-down measurement, shown in Fig. 5.4(b), provides a more accurate measure of the quality factor Q.

The resonance frequency as a function of magnetic field is shown in Fig. 5.4(a). For the low magnetic field regime, the frequency shift $\Delta f$ as a function of magnetic field $H$ is given by [145]:

$$\Delta f = \frac{f_0}{2k} \left( \frac{\alpha}{l} \right)^2 \mu \mu_0 H$$  \hspace{1cm} (5.1)

where $f_0$ is the resonance frequency in the absence of a magnetic field, $l = 200 \mu m$ is the length of the cantilever, $\alpha = 1.377$ is a constant factor derived for beam cantilevers, and $k = 3.3(0.2) \times 10^{-5} N/m$ is the stiffness of the cantilever, determined by the "added-mass method" [146].

Making use of equation 5.1, the magnetic moment of the cantilever is deduced to be $\mu = 1.1(0.1) \times 10^{-12} Am^2$. Given the remanent magnetization of the FePt film and the volume of the magnet of $(1.00(0.02) \mu m \times 8.10(0.02) \mu m \times 0.30(0.01) \mu m)$ we would have expected a magnetic moment of $\mu = 1.5(0.1) \times 10^{-12} Am^2$, if the magnet had been unaffected by the FIB process. The comparison shows that roughly 60 to 80% of the magnetic moment is preserved during the FIB process. As both SQUID magnetometry and cantilever magnetometry allow only for the determination of the overall magnetic moment, we cannot precisely determine the damage profile.

Figure 5.4. (a) Resonance frequency as a function of the external magnetic field determined from the cantilever’s thermal spectrum. The slope of the curve implies a magnetic moment of $1.1(0.1) \times 10^{-12} Am^2$, which means a volume of $0.8(0.1) \mu m^3$ has been damaged by the FIB. (b) The quality factor as a function of the external magnetic field as determined by a ring-down measurement.
The quality factor seems not to depend on the magnetic field strength. Ng et al. [147] did report on a decrease of the quality factor in a magnetic field ranging up to 6 T. This change is negligible in the 2 mT magnetic field range we studied and will use during normal operation with MRFM and magnetic atom trapping.

More FePt magnets have been attached to cantilevers by the procedure described above. However, the orientation of the out-of-plane direction of the FePt film with respect to the direction of motion of these cantilevers was different. Though beneficial for MRFM experiments [145], these probes are unfit for cantilever magnetometry experiments.

5.4. Discussion

We believe MRFM would benefit from the described force sensor. Since the force exerted by a spin in the sample on the cantilever is proportional to the gradient of the magnetic field, it is beneficial to use small magnets. In earlier experiments performed in the Oosterkamp group, NdFeB spheres with a diameter of 3 μm were used [124]. The field gradient cannot be increased by using smaller NdFeB particles, because they seem to lose their magnetization when scaled down further [148]. Even though FePt has a remanent magnetization which is roughly half as large as that of NdFeB, the possibility to create smaller magnets is promising for the sensitivity of MRFM experiments. The larger magnetic field gradient is not the only improvement that small FePt magnets would yield. It has been observed that the quality factor of MRFM cantilevers can drop drastically when approaching the sample surface [124]. This is most likely due to a dissipative interaction of spins in the sample with the magnet. A smaller magnet interacts with fewer spins and therefore suffers less from this unwanted damping. A forthcoming experiment will enable us to quantify the improvement in the resolution provided by the FePt rods.

Concerning atom trapping, the factor limiting the resolution of FePt traps created by optical lithography and plasma etching is the redeposition of the etched material, the magnetic properties of which are unknown [118]. SEM images show that this redeposition can be of the order of several hundreds of nanometers. From SEM images made after FIB milling, we conclude that for the FePt rods described in this paper redeposition of FePt is negligible compared to the loss of magnetic volume caused by the FIB milling process. Furthermore, the damage induced can possibly be reduced by using a helium FIB. Hence FIB milled patterns could have an advantage over patterns created by optical lithography and plasma etching, when aiming for trap sizes on the order of 1 μm [37, 149]. For the formation of such traps a better understanding of the shape of the damaged region of magnetic films would be needed. FIB milling of FePt will probably not suffice to go to an atom trap scale of the order of 100 nm. Electron beam lithography is the most suitable technique when aiming for sub-micrometer sizes [37]. This method is currently used in various groups and was discussed in the previous chapter.

When we assume that the damage to the magnetization only occurs in the edge of the magnets because of local changes in the crystal structure created by the FIB milling, a region with a thickness of 50(5) nm is effected. This 50 nm makes the fabrication of structures at a scale less than 1 μm unfavorable. However, if we modify the pattern to a higher than 50 % FePt coverage we could still create the intended potential. This occurs if one mills away less material and thus create a lattice with a binary pattern where there is more FePt than trenches. This would affect the smaller lattices in particular. For example, in a triangular lattice with 200 nm spacing the smallest gap between structures is 70 nm making it impossible to add an extra 50 nm layer around the magnets. Thus we conclude
that FIB milling does not yield a higher spatial resolution compared to e-beam lithography and plasma etching.

A second consideration is the writing time that would be required for a slow, low current, tightly focused ion beam to mill out these structures. The process will never be able to compete with high-speed global plasma etchers that etch a chip down in several minutes. However, if it is possible to create a chip with FIB milling within several hours the total gain in simplifying the process is already considerable. We have measured the etch rate of granular and mono-crystalline FePt by an 500 pA ion beam to be approximately 2 \( \mu \text{m}^3/\text{s} \). Many parameters may influence this speed, like material properties, ion momentum and beam focus so that this etch rate may vary by up to 200%.

Consider a 100 nm thick FePt film on which a lattice with 50% coverage is etched with a 3.6 \( \times \) 10^6 \( \mu \text{m}^2 \) surface, similar to the chip described in this thesis. The total milling time for such a chip is 24 hours. FIB milling of atom chips at this scale is therefore currently unfavorable. However, if one works with thinner films and optimizes the milling process, not to over-etch significantly, there is hope to reach the 4 hours that were required to write the e-beam mask to create the same pattern in a resist. Combining this with the technical simplification of the process and the reduced redeposition of magnetic material, FIB milling can become a competing fabrication technique for thin atom chips with micron sized lattices. Because of the reduced redeposition in the local milling process, the flatness of the atom chip will also be improved. Height differences in the chips profile have unwanted effects when atoms are imaged and they may also generate inhomogeneous stray electric fields. Both effects could be reduced by creating a magnetic atom chip by FIB milling.

5.5. Valorisation aspects

In the process of making the 250 nm lattices as well as the FePt nano-rods, we have been inspired by papers and techniques from industrial partners. FePt is a common choice for magnetic hard disk recording devices [150, 151]. For some historical perspective, already in 2000 a 2 \( \mu \text{m} \) FePt lattice was made by nano-lithography for state of the art hard disc applications [152]. The first magnetic-film atom chips, not much later, were created from material provided by Hitachi, one of the major manufacturers of hard disks. A promising perspective is the development of a commercial MRFM probe which could reach unprecedented magnetic sensitivity. Such a product, similar to that of SQUIDS which come with a closed circuit cryostat, will certainly appear on the market in the upcoming years. In this section both these paths will be briefly investigated.

5.5.1. FePt nano-magnets as memory

First we discuss the use of small magnets as bits for information storage. The size of a magnetic domain is the smallest unit that can be made to store a bit. In multigrain bits the grain size is scaled down to about 3 nm such that bits can be formed out of around 30 small grains. Together they share a magnetization direction and protect each other against demagnetization. The stability of such a multigrain bit is limited by the energy that is required to flip single grains thermally and this drops with both grain size and anisotropy. Therefore it is not enough to only scale down the bit size if one wants to create bigger, higher density hard discs. One also needs to increase the magnetization to keep the small grains stable. "Because of its very high anisotropy, L10 FePt is a choice material for the next-generation media", see Sellmeyer et al. [153]. Heat assisted magnetic recording is
a widely used technique with FePt hard drives to write information in magnetic domains [109]. This recently developed technique uses laser pulses to demagnetize a bit before it is re-magnetized by a scanning coil in the other direction. Commercial hard discs up to 10TB, manufactured by Seagate, are scheduled to appear in 2016. All these developments have led to an increased interest in the fabrication of nano-scale FePt lattices.

Since in a single domain (monocrystalline) material there can be no domain-wall movement, these materials are especially well suited to store information in classical magnetic bits. They are harder to demagnetize and therefore can save information safer than grainy materials. The ideal diameter for a single domain hard permanent magnet is in the range of 10-100 nm [154]. At this smallest scale with bits of 10 nm a data storage of 1 Tb/in² may be reached. With the techniques presented in the last two chapters it is possible to create a monocrystalline FePt 30 nm bit array which could serve as a hard discs. Modern commercial hard discs are often fabricated out of bulk small grain materials or by nano-imprinting bit patterns. Electron beam lithography which is used here is often considered too slow. However with upcoming innovations it might become more competitive [155].

5.5.2. Needle magnetometers

The main application for FePt nano-rods, as presented in this chapter, is that of high sensitivity magnetic field measurements. Sensitive measurements have provided many results in physics but also have opened up completely new markets. The effort to continuously increase the sensitivity of measurement techniques is also a generator of many modern day technologies ranging from GPS to imaging tools like MRI. While single photon sources and detectors already exist and atomic clocks can measure time with a sensitivity of $10^{-16}$ s there is still work to be done in the field of magnetic field sensors. The ultimate goal in this field would be to distinguish a single electron or even nuclear spin, or a spin fluctuation within a material. The main complication in this challenge is the resolution that is required of approximately 1 nm. The combination of magnetically sensitive probes as used in MRFM are hard to combine with high resolution tools such as scanning probe microscopes (STM, MFM, etc.). In Fig. 5.5 several techniques are compared.

The widely used technique MRI is not sensitive enough to fit on these scales. However the lack of a local probe also limits the resolution of MRI. Biological samples are highly interesting since many diseases may be detectable or even traceable by magnetic signals. Methods with a highly local resolution do not yet have the sensitivity of superconducting quantum interference devices (SQUIDs). A sensitive technique and a local probe to generate a large field gradient would combine the best of both worlds.

5.5.3. FePt nano-magnets as sensors

State of the art MRFM machines have been able to observe single spins with a 25 nm resolution, several hundred nanometers apart [157]. To understand the limitations of this technique and the opportunities that FePt nano-rods present, the magnetic sensitivity of a MRFM probe has to be defined. The coupling between a cantilever probe and a sample containing a spin is given by the spin magnetic moment $\mu$ times local magnetic field gradient [158]:

$$F_{\text{spin}} = \mu \frac{\partial B}{\partial x}$$  \hspace{1cm} (5.2)

Now we assume a typical magnetic field gradient which can be produced by a 3 $\mu$m NdFeB magnet $\nabla B = 10^5$ T/m. In this magnetic field gradient the force due to a single electron
spin is $10^{-18}$ N, and that due to a nuclear spin is much smaller still, $10^{-21}$ N. To measure these forces one can either make a higher magnetic field gradient or a better force sensor. Both these options are investigated below. The minimal magnetic force and moment which can be detected are [158]:

$$F_{\text{min}} = G \mu_{\text{min}}$$
$$\mu_{\text{min}} = \frac{1}{G} \sqrt{4 \Gamma k_b T \Delta f} = \frac{S_F}{G} \quad (5.3)$$

Here we introduce $S_F$, the power spectral density of the thermal force noise, which gives the force noise sensitivity of the cantilever due to temperature. Here $T$ is the temperature, $\Gamma$ is the cantilever damping rate and $\Delta f$ is the frequency bandwidth of the device. The field gradient is controlled by the size and the magnetization of the cantilever tip. It scales as $G \propto r^{-4}$ where $r$ is the size of the magnet and it scales linear with the magnetization. We can compare these forces with noise forces that act on the cantilever such as thermal fluctuations. These can be described by [158]:

$$F_{\text{noise}} = \sqrt{4 k_B T \Gamma} \quad (5.4)$$
Here $F_{\text{noise}}$ is given in units of $N/\sqrt{\text{Hz}}$. If we take typical values for a MRFM experiment the spectral force noise is $S_F = 10^{-18} \text{N}/\sqrt{\text{Hz}}$ at a temperature of 50 mK. A 3 μm NdFeB magnet creates a gradient of $10^5 \text{T/m}$ at 1 μm from the sample. If we combine these numbers the minimal magnetic moment that can be detected in 1 second can be found:

$$\mu_{\text{min}} = \frac{10^{-18} \text{N}}{10^5 \text{T/m}} = 10^{-23} \text{J/T}$$ (5.5)

This equals the magnetic moment of 1 electron spin, or 100 nuclear spins. To improve upon this, a more sensitive cantilever can be built, as has recently been established in the Wrachtrup and Jayich groups where NV centers in diamond were used as probes [159, 160]. Also a stronger magnetic gradient can be created like we have shown in this chapter.

Technical advantages of using permanent magnets are threefold: Their large magnetization ensures the largest possible coupling to other magnets. They are the least sensitive to degradation and they give highly reproducible results. Therefore permanent magnetic nanorods form a more practical method for industrial applications than for instance diamond NV-center sensors. Both these improvements give the ultimate sensitivity which is required to observe single nuclear spins within a measurement time of 1 second. A magnetic field gradient of $10^6 \text{T/m}$, which can be provided by a FePt nano-rod, will yield one order of magnitude. With a higher quality factor resonator such as presented by Wolf et al. [159], another order is gained. Together a sensitivity of $45 \times 10^{-21} \text{N}/\sqrt{\text{Hz}}$ may be reached, sufficient to detect a single nuclear spin.

In recent work another beneficial factor for nano-rod probes was proposed [161]. The authors describe a needle magnetometer, made from a single domain, and again calculate the sensitivity that can be reached. The benefit of using a single domain, lies in the fact that no dephasing of spins inside the material can occur. All the electron spins in the bar magnet are locked to the crystal that forms the domain. Due to this decreased dephasing factor that is not present in any of the aforementioned probes, a similar sensitivity is found for a 1 μm CoPt bar magnet. Single domain bar magnets have not been used for this purpose, the most recent article in the literature in which such a magnet is created is Ref. [162]. In this paper the example of the 1 μm CoPt bar magnet is taken. When considering this 1 μm cobalt needle the authors conclude that a sensitivity for a 1 second measurement of $B = 10^{-24} \text{T}$ can be reached, leading to unprecedented sensitivities at the $10^{-25} \text{J/T}$ scale. If we compare our 0.2 μm FePt magnet to the old and large CoPt needle another factor of 10 can be gained.

Many applications become feasible at this scale; spintronics manipulation at the single spin or atom level, the detection of nuclear spin structures in condensed matter, etc. Also outside the realm of fundamental physics there is a dire need to have better magnetic probes. MRI has been limited in resolution for many years and although MRFM requires a local probe and can therefore not be used in vivo, already studies are undertaken to use these techniques on biological samples to detect Fe atoms in brain tissue of Alzheimer patients. The ability to detect magnetic signals on the scale of nuclear spins also opens up a new world for data storage. Moore’s law was thought by many to fail at the atomic level since bits could not be stored in systems of just one atom. With technical advances like these there is hope to break this barrier and encode information inside atoms. Since, if we can detect physics on this scale, we must be able to use it to our advantage as well!
5.6. Conclusion

We have shown a fabrication process for micrometer size FePt magnets by FIB milling and a way to attach these magnets to ultrasoft cantilevers by electron beam induced deposition. This technique could in principle be used for any magnetic film. From cantilever magnetometry measurements we conclude that 60 to 80% of the magnetic moment is preserved during the FIB milling process. FIB milled magnets could therefore be used in atomic trapping experiments when aiming for a trap size on the order of a micrometer. The magnet attached to the cantilever can be used as a probe in MRFM experiments. The small dimensions of the magnet are expected to improve the sensitivity of MRFM.

Practical implications for the construction of atom chips were studied. We conclude that FIB milling now offers a competing fabrication technique for lattices down to 400 nm spacing. Major benefits over E-beam lithography are the technical simplification of the process with comparable etching time and the reduced redeposition of magnetic material. Valorisation aspects were considered of magnetic lattice arrays and nano-rod cantilevers. The construction of a FePt lattice by FIB milling or electron beam lithography may be an interesting alternative for hard disc manufacturers who search for ever smaller and stronger magnets. The construction of mono-crystalline nano-scale magnets for magnetic field measurements offers unprecedented sensitivities.
6 The new experimental setup: Magchips Nano

6.1. Introduction

Atom chip experiments are investigations where nanofabricated devices are used in combination with neutral quantum-particles like ultracold atoms. Over the past ten years our group in Amsterdam has developed her own approach to these experiments where we combine magnetic potentials generated by permanent magnetic films with ultracold and degenerate gases. For a series of quantum simulation experiments a new vacuum setup was constructed. This new experiment, see Fig. 6.1, is presented in this chapter and its new features are introduced and characterized.

6.2. Design considerations

The new experimental vacuum chamber was designed with the following considerations in mind: We will combine different geometries in the same experiment. We want to be able to switch chips and dispensers quickly without disturbing the sensitive positioning of the electromagnets and optics around the vacuum chamber. To increase the optical access and to increase the space inside the vacuum, near atom chip and atoms, the choice was made to build the new experiment around a vacuum chamber with two large 8” ports. This science chamber also has four 4.5” and four 2.75” openings. Earlier experiments were performed in a $40 \times 40 \times 70 \, \text{mm}^3$ glass cell with limited room for atom chip, dispensers and high-numerical-aperture imaging system [33]. The more spacious vacuum system also allowed us to incorporate a movable imaging lens which can be positioned under the atomic clouds and focused on the atoms from the air side. In the previous experiment this lens was fixed inside the vacuum and could only be focused outside of the vacuum. Many other parts of the experiment remain the same, e.g. the vacuum is maintained by a combination of non-evaporable getter (NEG) and an ion pump. Six coils surround the vacuum system to apply global magnetic fields in all directions. The magnetic chip is placed on a silver foil that is cut into several current carrying wires which are used for initial trapping and cooling of atomic clouds.

The main features of the setup are an octagon vacuum chamber and a vertical load lock section. Through this load lock an insert with the magnetic atom chip assembly, rubidium dispensers and antennas can be moved in and out of the experimental chamber. Due to the incorporation of this loadlock section chips and dispensers can be exchanged without venting the science chamber. This prevents not only the elaborate procedure of removing all the optics and coils around the science chamber but also ensures that the initial trapping stages of the magneto-optical trap (MOT) and silver wires will not need
to be re-calibrated. Furthermore, radio-frequency (RF) and microwave (μW) antennas are placed close to the chip inside the vacuum chamber. In the sections below all these components will be introduced and described.

### 6.3. The vacuum system

Before we give details on each of the components we present an overview of the vacuum system. The largest component in the experiment is the vacuum science chamber with two windows in the 8” ports. This spacious chamber now allows us to incorporate a scaled up chip mount assembly which enters through the top 4.5” valve. Above this valve a 4-way cross connects the main chamber to a vacuum gauge, a valve for a turbo pump connection and the loadlock section. This loadlock section is based on a 4.5”-wide, 450 mm-long bellows which provides a 300 mm travel length. The loadlock allows us to insert and retract the experimental arm. On top of this loadlock section the 4.5” feedthrough flange is placed to which the experimental arm is connected. The feedthrough accommodates all currents used in the chip mount as well as the radio frequency signals for the RF antennas. The bottom window of the chamber is an aspheric lens, mounted on an inverted bellows which can be moved by five micrometer screws for focusing. The lens allows for imaging of the atoms on a camera, as well as for admission of laser light for excitation of the atoms.

The main science chamber houses one fixed $^{87}\text{Rb}$ dispenser, two $\mu$W-antennas and a chip landing platform. A feedthrough for the microwaves and dispenser is connected to the main chamber, see Fig. 6.2. Two other enriched $^{87}\text{Rb}$ dispensers can be moved in with
Figure 6.2. Drawing of the Magchips Nano experiment with electromagnets in the (y,z)-plane. Individual components are indicated.

the experimental arm. To allow for future incorporation of a high flux atomic source such as a 2D MOT an extra valve is connected in direct line of sight of the chip. This also allows future experiments to be done with different species of atoms. Besides the turbo pump, which can be connected to the 4-way cross, a SAES NexTorr 100 L/s non-evaporable getter and ion pump is connected to the main chamber. The effective pumping speed of the pump is reduced to 23 L/s because it is placed inside a short tube extending out of the main chamber. After a low temperature bake of 120-150 °C for three weeks a pressure of $10^{-10}$ mbar can be reached after which the SAES pump will maintain this pressure when the turbo pump is valved off.

Two stainless steel ridges (gray) hold three titanium frames that contain three landing points (green), see Fig. 6.4. They are fixed with clamps to ridges inside the flanges of the vacuum chamber. These three fixation points will be used to fix the chip position when it is loaded via the loadlock. To keep the access for the loadlock completely open the clamps were home built to ensure minimal obstruction for the chip mount. The materials are chosen such that only titanium is used near the magnetically sensitive chip. The fixation points are positioned with respect to the chamber with a coordinate measurement machine with a precision of approximately 20 μm (Mitutoyo [163]). The fixation points will guide the chip mount, which contains a flexible ball joint, for self-alignment into a fixed position. The optical windows are coated with a 780-nm anti-reflection (AR) coating. One special coating, namely AR for both 780 nm and 480 nm light is used on the horizontal 4.5" window and the lens. This will allow us to excite rubidium Rydberg states, using excitation lasers
from the side and from below. All windows have tantalum glass-steel connections which
are non-magnetic. We found that the standard kovar glass-to-metal seal windows generate
permanent magnetic fields up to 5 G.
   To allow for easy optical access from below and through the various windows the main
chamber is mounted at 300 mm above the optical table. The posts that support the vacuum
system can be varied in length to level the chip with respect to the table. The vacuum
setup can also be suspended (temporarily) from the ceiling which allows one to remove the
legs when mounting the electromagnets. The post connections are welded to the chamber
and they are positioned out of any optically relevant directions.

6.3.1. Loading arm and positioning

In this section the moving arm which holds the magnetic chip is described. All components
of the experimental arm will be introduced in full detail in section 6.3.2. The chip and
wires for initial trapping are held in a chip mount, which can be brought in and out of the
science chamber through the load-lock system. The bellow allows for a 300 mm translation
of the top flange. Mounted on the top flange is a 600 mm long insert, ending with the chip
as its lowest element, as shown in Fig. 6.3. In the highest position the chip is moved above
the gate valve, which can thus be closed such that the upper part can be vented and the
chip can be exchanged. The central axis of the arm is a titanium cylinder which ends on a
ball joint. To create space for a heat pipe in the central axes of the experiment the entire
cylinder is made hollow with a hole of 8 mm.

   The chip mount is connected by the ball joint to the hollow titanium tube to give the chip
mount freedom to move and rotate slightly. The widest extension of the chip mount are its
three positioning legs. When the chip mount approaches its final position the positioning
legs on the chip mount triangle have enough rotational freedom from the ball joint to
find the slits in the fixation points inside the chamber. When the positioning slits touch
the fixed landing points the top flange can be released several millimeters such that the
atmospheric pressure presses the chip mount into its final position, as can be seen in Fig.
6.4. The chip mount can thus be brought into the same position repeatedly. A view from
below through the flange of the lens, shown in Fig. 6.5, shows the chip mount in its final
position.

6.3.2. Chip mount assembly

As discussed in the previous section, an insert of 600 mm is attached to the top 4.5”
feedthrough flange. The chip mount assembly is connected to the bottom of a heat pipe.
The heat pipe is placed in the hollow titanium cylinder and sticks out on both ends to
bring heat from the silver wires near the chip to the top feedthrough. Together the heat
pipe and titanium cylinder are the longest part of the insert. They conduct heat from the
current carrying wires behind the chip to the top flange. At the feedthrough the heat pipe
is clamped to a 10 mm stainless steel strip, welded to the feedthrough flange, which acts
as a heat sink. The performance of the heat pipe will be described in section 6.3.5. At
the top of the insert all currents and radio signals are connected to the feedthrough and
passed down to the chip mount inside the vacuum by isolated wires.

   Both the chip holder and the silver wires are mounted to the bottom of the insert.
They are joined together by three 2 mm diameter titanium bolts that attach it to the
positioning triangle. The chip holder is a boron nitride (BN) block of 40 × 30 × 8 mm³
with a 12 × 12 mm² hole in the middle in which the silver wires are positioned. The silver
Figure 6.3. Cross section of experimental arm which holds the chip mount. a-b) Cross-section in the x-z and y-z-plane though the center of the experiment. All parts which are described in the text are indicated. The silver wires can only be seen in a) since they blocked in b) by the boron nitride (BN) chip mount.

Wires are glued to a 10 × 10 mm² copper block to hold and cool them. The silver surface is positioned approximately 20 μm behind the chip. This alignment is done in an assembly frame under an optical microscope. The chip itself is aligned in position using three ceramic posts, and held in place by four clamps. Tungsten clamps are used for this purpose since they are both elastic and firm. Also their electric conductivity is used to connect one clamp to the feed-through which allows us to set an electric potential on the top Pt layer of the chip.

6.3.3. Radio-frequency and microwave antennas

Radio frequency waves are used to modify the trapping potentials, for evaporative cooling and to spectroscopically address different spin states of the rubidium atoms. Frequencies that are used fall in the range from d.c. to 50 MHz. Also a microwave signal of 6.835 GHz is required to drive transitions between the two ground state manifolds. In this section we describe the construction of all antennas and we show initial characterization. Unlike most atom chips we can not use the silver wires behind the chip to deliver RF signals to the atoms because of the capacitative coupling to the copper block underneath the chip.
Figure 6.4. Picture of the landing position for the chip mount. The titanium fixation frame (green) is indicated and fixes three points inside the vacuum chamber on which the landing triangle (orange) lands. The patch antennas (brown) can also be seen as they are also mounted from the stainless steel ridges (grey). All bolts are made from titanium. a) Situation before the chip mount is landed. b) The landing triangle (orange) is landed and chip is placed in final position.

Figure 6.5. Technical drawing looking upward into the main chamber from the lens position. The three landing triangles are shown in green, the feedthrough in orange/yellow and the chip mount and silver patches antennas are gray on lighter teflon on brown copper base. Patch dimensions are indicated in lower patch.
RF antennas are therefore positioned on both sides of the chip, see Fig. 6.6. They have a hairpin shape, are 25 mm long and 5 mm wide and have two full windings. The distance of the antennas to the atoms is 10 mm. By controlling the relative phase of the two RF signals we can optimize the local field strength at the atomic position [164]. In the x-direction, which is perpendicular to the quantization axis of the atoms that are magnetically trapped, a RF field strength of 80 mG can be created. This is an improvement of about a factor two compared to the previous magnetic chips experiment [33].

Also two microwave antennas are placed in close proximity of the atoms. They are placed in between the windows and the chip landing area, 20 mm from the atoms. These patch antennas are made out of a copper ground plate, a teflon insulator and a silver resonator patch. They are connected to their own feedthrough in the science chamber and were built in house. To calculate the dimensions of the patch antenna the following equations can be used [165]:

\[
W = \frac{c}{2f_r} \sqrt{\frac{2}{\varepsilon_r + 1}}
\]

\[
\varepsilon_{\text{eff}} = \frac{\varepsilon_r + 1}{2} + \frac{\varepsilon_r - 1}{2} \sqrt{1 + \frac{12h}{W}}
\]

\[
L = \frac{c}{2f_r \sqrt{\varepsilon_{\text{eff}}}} - \frac{0.824h(\varepsilon_{\text{eff}} + 0.3)(0.264 + W/h)}{(\varepsilon_{\text{eff}} - 0.258)(0.8 + W/h)}
\]

Here \( f_r \) is the resonance frequency of 6.835 GHz, \( \varepsilon_r = 2.1 \) is the dielectric constant of teflon and \( h = 1 \) mm is the teflon height. This gives the following patch dimensions: \( W = \)
17.70 mm and $L = 14.63 \text{ mm}$.

Since the thickness of the capacitor and its dielectric constant are not exactly known, slight modifications were made after inspection with a network analyzer. The resonance frequency $f_r$ of both patches was initially found slightly to the red. We were able to move the resonance frequency to the desired 6.835 GHz by reducing the width $W$. This was done by cutting the edges of the silver patch, for several millimeters. A reflection measurement done with both patches after cutting them to their final width is shown in Fig. 6.7. The resonance width was found to be 250 MHz wide for both antennas. It is not possible to measure with macroscopic probes the exact field strength near a surface like an atom chip because of near field effects [166]. To measure the field strength ultracold atoms are the best probe. By varying the relative phase of the antennas it was observed that the local field strength can be varied significantly. In a test configuration a difference of 16 dBm was measured between in-phase operation and out-of-phase operation of the two antennas. The generation of the RF and microwave signals is described in reference [167]. These signals are split and then separately amplified for the existing Magchips setup and the setup described here respectively.

### 6.3.4. Silver wires

To capture, hold, move and cool cold atomic clouds, several current carrying wires made from silver are positioned behind the chip. We have incorporated a comb-like structure which contains four different 3 mm long Z-wire traps and one central 6 mm long Z-wire [168]. All wires can be used to create Ioffe-Prichard traps [49, 50]. A technical drawing of the silver wires as they are cut and folded in the narrow space behind the chip can be
Figure 6.8. Schematic drawing of the silver wires. Three types of wire configurations are indicated. Pinch wires (blue), 6 mm Z + dimple-wire (red), 3 mm long h-wire (yellow). An h-wire can form both a Z- and U-wire. The drawn wire connects the wires 2, 4 and 8.

seen in Fig. 6.8. Here one Z, one U and one h wire are highlighted. To show the comb structure more clearly a composite optical microscope image is presented in Fig. 6.9. The 6 mm Z-wire trap can also be combined with an extra current through the middle wire (between connection 4 and 10) to create a dimple trap which can provide an even tighter confinement. This design creates five different scientific areas on the magnetic atom chip which are all positioned with a 20 µm accuracy below the magnetic lattices which are written on the chip. These wires were cut by spark erosion with a wire of 50 µm which created cuts of 75(5) µm. The silver foil has a thickness of 250(5) µm and the wires are 225(5) µm wide in the central region. The silver foil is cut inside a frame and then glued to the copper block using H77-S epoxy (Epotek). After gluing the wires are cut free from the holding frame.

To connect the silver wires to the feedthrough terminal blocks of $3 \times 4$ mm$^2$ wide titanium were made. By folding the wire ends as shown in Fig. 6.8, all wires were connected to copper cables with a diameter of 2.6 mm. These cables are kapton coated and contain 37 silver plated copper strands that transport a total current of maximally 20 A.

6.3.5. Cooling of chip wires

When the silver wires are used at 20 A a heating power of 2 W is produced which has to be transported out of the chamber to ensure that none of the inner parts of the chip mount overheat. In previous experiments a massive copper cylinder was used to bring this heat to the outside world. Due to the experimental arm length of 600 mm the heat conductance
of a solid copper cylinder would be insufficient to cool the chip mount. Instead, we chose to incorporate a 3 mm thick, 566 mm long heat pipe, filled with methanol, which can transport up to 9 W of power in a working range of 5 to 150 °C. Methanol has a lower freezing point than water, making it more favorable for our purpose. Long thin heat pipes have two limitations. A starting temperature at the lower, hot side must be reached to begin operation. Secondly, at low input power the heat pipe works less efficiently than expected [169]. This results in a higher temperature difference over the heat pipe.

To monitor the temperature of the chip mount, as well as the operation of the heat pipe, a thermocouple is connected to the copper block, at the lower end of the heat pipe. By measuring this temperature and the flange temperature the heat pipe operation can be checked continuously. During normal operation the silver wires are operated for half the experimental cycle, producing on average of 1 W. At this power the required starting temperature of 60 °C is reached after 30 minutes. This results in an operation temperature of the copper block after stabilization of 64 °C.

In a series of tests it was checked whether the chip could overheat by varying the input power of the silver wires but no faults were found. When trying to cool the flange with the aim of lowering the temperature of the chip a counterintuitive rise of the chip temperature was found. Heat transport through the heat pipe becomes less efficient when the flange is cooled and therefore the cooling power drops. By heating the flange to 30 °C we were able to lower the temperature of the chip from 64 to 40 °C which provides an ideal operating temperature. By measuring the temperature of the copper block and controlling the flange temperature it is possible to actively control the temperature of the atom chip. These temperature variations have no influence on the magnetization of the chip.

### 6.3.6. Imaging lens

The imaging lens is part of the vacuum system as it forms the window beneath the chip. A lens connected to a bellow was constructed to hold and move the lens while keeping the experiment under vacuum. This lens is an aspheric lens with a numerical aperture of 0.45 from Asphericon (A50-40HPX). It is coated with an anti-reflection coating for both 480 nm and 780 nm light. The diameter and focal length are both 40 mm and the working distance is 31.3 mm. Fig. 6.10 shows the flexible bellow mounting that holds the lens. It can be moved up to 2.2 mm from the middle in the radial direction, allowing us to
image all five Z-wire traps. This horizontal movement is done by two micrometer screws with a 1 µm resolution. Three differential micrometer screws with an accuracy of 0.1 µm (Mitutoyo) control the tilt and z-position. The depth of focus at 780 nm is 5 µm which makes positioning critical to image the atomic clouds at a similar distance from the chip. The glued connection and inverted bellow are inspired by an earlier design from Harvard where a 10 mm lens was used [170]. Since our 40 mm lens experiences a 16 times higher atmospheric pressure holding it in place was much more challenging. In addition, the epoxy must accommodate the considerable difference in thermal expansion of the lens and the holding ring while baking. While baking above 40 °C the epoxy undergoes a glass transition and becomes more flexible. During an initial test with a plain window it was sucked into the vacuum at this temperature. These challenges were overcome in the following way. By holding the lens in place with a metal ring, baking up to 150 °C was successfully tested several times. The main epoxy that is used to hold the lens is T7109-19 (Epotek) which out-gases slightly, as measured with a residual gas analyzer. This epoxy and the epoxy thickness of 2.2 mm is selected such that compensates the difference in thermal expansion of the lens and the stainless steel bellow. By covering it with the H77-S (Epotek) epoxy the underlying glue was encapsulated and no further out-gassing was measured.

6.4. Coil design

To trap, move and release ultracold atoms, magnetic fields of up to 200 G are required. In future experiments also several rotations of the external field within the lifetime of the
trapped gas will be required and field configurations must be switchable within milliseconds. The combination of large fields and fast switching is technologically challenging. To keep the number of windings and therefore the inductance low, coils with large diameter wires to conduct currents up to 60 A were developed in combination with power supplies that could operate in all four quadrants (±20 V, ±60 A). Also a high voltage (800 V) boost to rapidly switch between field quadrants was developed for all four power supplies.

In Fig. 6.1 and 6.2 the three different sets of coils are named. The innermost two round "small" coils parallel to the large windows provide the field in the x-direction. They operate in series and the field strength required is several tens of Gauss to trap atoms in the magnetic chip traps. The two inner racetrack shaped coils around them provide the field for the mirror-MOT which captures and cools the atoms at the start of each experimental cycle for which they must create a gradient of 20 G/cm. They also need to operate in series to create bias fields in the (+z,+y)-direction in the later Ioffe-Pritchard trapping stages. The last set of coils, which we will call the outer racetrack coils, are the largest in radius and complement the inner racetrack-coils. Together they make all possible fields in the (z,y)-plane. The fields required in these two directions are of the order of the trapping fields. When atoms trapped 100 nm from the surface in experiments such as those that were proposed in chapter 2 and reference [37] fields up to 200 G will be required. There are no analytical equations to describe the fields of three-dimensional racetrack coils, hence in all that follows the magnetic fields, inductions and resistances are calculated with the help of the Radia package [171].

6.4.1. Brass housed coils

To design the coils, simulations were done to estimate the generated heat and equilibrium temperature. A comparison between the simulations and the resulting performance of the coils will be presented in the next section. Brass was selected to house the coils because of its strength and high thermal conductivity of 100 W/Km. A thermally conductive epoxy 930-4 (Epotek) with a thermal conductivity of 1.67 W/Km was used to glue the windings in the brass house. The racetrack coils were wound with a wire of 3.55 × 2.24 mm² and the small round coils with a smaller wire of only 1.6 × 2.6 mm², both isolated with 10 µm of isolation varnish. Fig. 6.1a shows a technical drawing of one of the two smallest coils. The thickness of the brass is 3 mm and the water tube inside is also 3 mm wide. Up to 101/min can be used to cool the coils, limiting their temperature even at full power and continuous operation to 60 °C, as predicted by simulations. The maximum fields in the (x,y,z)-directions that can be created are (126,320,320) G. The other dimensions of the coils are given in table 6.1. This table also contains the measured properties of the coil sets that were manufactured.

6.4.2. Temperature analysis

We want to limit the generated power \( P = I^2R \) inside the coils such that they do not overheat. The generated power can be limited by increasing the wire surface \( A \) or lowering the maximum current that is used. To predict the thermal behavior of the coils a finite element method (FEM) analysis is used that was developed by T. Tiecke [172]. For this purpose, Marc, a commercial simulation tool [173], was used to simulate the thermal conductance of the coils. Here we present the analysis of one of the small coils. The race-track are expected to have lower maximum temperatures due to their larger wire and their smaller maximum current. The total heat flow from the inner part of the coils to the cooled
brass depends on the geometry and material properties of copper wire, isolation material, epoxy and brass housing. Two simulations were done to estimate the heat flow in the small coils. The best case simulation considers optimally wound wires and a minimal amount of epoxy such that heat is transported very well. The worst case simulation considers more space and more epoxy in between the wires which results in a much lower overall thermal conductance. These simulations lead to an effective radial thermal conductance of $k_r = 3.15(1.81)\text{W/Km}$ in the optimal (worst) scenario. With these simulations an upper bound for the temperature of the coils can be found. If we assume that the brass is kept at a fixed temperature by the water and we neglect the cooling coming from the brass base, a one-dimensional approximation can be made [174]. We can do this since the thermal conductance is dominated by transport to the brass edges because the thermal conductance is largest in that direction. This can be seen in Fig. 6.11 since transport in the x-direction is mostly done through copper and this direction also contains the least isolation varnish and epoxy. This one-dimensional approximation gives an upper bound to the maximum temperature since in three-dimensional coils heat is also transported through the base of the coil.

$$\Delta T = \frac{P_{\text{tot}} W_x}{8A k_x}$$

Here $\Delta T$ is the temperature difference due to heating, $P_{\text{tot}}$ is the total generated power, $W_x$ is the width of the coil, $A$ is the cross-sectional area of the wire and $k_x$ the thermal conductivity. For the small coils the total generated power is 324 W and their width is 15.2 mm. The worst case thermal conductance of 1.8 W/Km gives a maximal temperature increase of $\Delta T = 41\text{ K}$. The duty cycle is estimated to be 50% during normal operation, which will make the operating temperature lower. However we want the coils to work at maximum input power as well without overheating. In Fig. 6.11b an infrared image is shown of one of the two small coils which has been used for a long time at maximum input power to measure its equilibrium temperature. Its maximum temperature here is 63°C which lies within the bounds of our simulations.

### 6.4.3. Four-quadrant power supplies

In the experimental cycle we want to apply external fields in all directions. Also we have to create a gradient in one direction to make a magneto-optical trap. This makes it necessary to switch the polarity of the fields. In order to switch the polarity of fields (currents into
inductive loads), it is necessary to use four quadrant power supplies ($\pm U \pm I$). High power switches were developed in-house based on multiple h-bridges to be used in combination with single-quadrant power supplies (2000-series Delta). Four of these were built to control the current output of all power supplies, three $70 \text{ V} \times 45 \text{ A}$ models for the racetracks and one $45 \text{ V} \times 70 \text{ A}$ for the small coils. High voltage switch modules were incorporated in order to reduce the switching time per coil set. These will make it possible to switch faster between field configurations. They can be used once every three seconds and discharge a $800 \text{ V}$ capacitor to help switch a large current. Current taken from the coils is used to charge the capacitors. When the Delta supplies do not have enough voltage to produce the current slew rate that is requested, the capacitors are discharged. These boosters are designed to switch field configurations in a time of the order of 1 ms.

6.5. Laser system

To cool, pump and probe the rubidium gas via the D2 line a $780 \text{ nm}$ laser is split into three paths after which acousto-optic modulators (AOM) shift the frequency to the desired detuning per path. The cooling laser of $100 \text{ mW}$ is set at a wavelength of $\lambda = 780.2 \text{ nm}$ and is frequency locked to the $F = 2$ to $F' = 3$ transition. Also a separate $780 \text{ nm}$ repump laser is used to repump atoms which leave the cooling cycle by spontaneous decay. This laser is detuned $6.8 \text{ GHz}$ to the blue and pumps atoms from the $F = 1$ ground state back into the $F' = 2$ state. After passing through the AOMs the three $780 \text{ nm}$ laser beams are each coupled into an optical fiber that delivers them to the experimental chamber. The pumping beam is brought through the large windows. To create a mirror magneto-optical trap the cooling light is split into four beams. A pair of horizontal beams is aimed at the atoms through both large windows in the ($\pm x$)-direction. The other two beams are directed at $\pm 45$ degrees in the ($y,z$)-plane and reflect from the magnetic chip.

The imaging light is coupled out of a fiber and focused onto the back-focal point of the imaging lens which collimates the light towards the atoms. After the reflection from the chip the image of the atoms is magnified 15 times and projected onto a CCD camera (Andor iKon-M), see Fig. 6.12. A more detailed description of the laser system that is used and the locking schemes can be found in [167, 175].
Figure 6.12. Schematic of the imaging setup, based on a high NA aspheric lens, 31.3 mm from the chip.

6.6. Experimental control

To set the timing of the various magnetic and optical fields an in-house developed Python-based software program is used. This program, known as Labalyzer, is described in more detail in [175] and is available at [176]. Labalyzer converts timeframe files (comma separated values) into digital and analog commands. These address the various parts of the experiment for instance to set magnetic fields values, to switch lasers on and to vary the frequency of an AOM, etc. It also acquires the atomic images taken by the camera and shows them immediately. One can then perform simple fits and other analysis to the data. The commands and their timing are generated from a Digital In Out card with 64 channels (Viewpoint DIO64). It is split in various parts; one controls a 16bit direct digital synthesizer that generates the RF signals and 48 digital transistor-transistor logic (TTL) signals. Labalyzer also controls four National Instrument cards which in total regulate 28 analog signals. The relative timing of all devices is set by the DIO64 card which uses the TTL signals to trigger specific machines and analog output signals. The timing is referenced to a rubidium 10 MHz atomic clock for stabilization. The computer that houses this software and the various cards is shared with the original magchips experiment [33] as are the lasers and the cooling water.

6.7. Outlook

The experiment was assembled in late 2015. In Fig. 6.13 a photo is shown of the chip and chip mount after they landed in the center of the vacuum chamber. After a sufficiently low vacuum is reached by means of baking the setup at maximally 150°C the experiments described in the earlier chapters can be performed.
Figure 6.13. Core of the experiment that is described in this chapter. Image is taken through the main window, looking into the vacuum chamber showing the atom chip in the center. Red light which is reflected from structures created by nanolithography in the middle of the chip can be seen.
Summary

Nanoscale magnetic atom chips for quantum simulation

Thank you for reading my thesis, I hope I will be able to explain to you some things about quantum simulation and nanoscale magnetic potentials. This thesis consists of five chapters that describe the different things that I have done in the past few years which all concern my effort to create lattices of ultracold gaseous atoms at length-scales of approximately 100 nano-meters (a millionth of a decimeter, or 200 times smaller than the diameter of a human hair). "Why do I want to make this, and what is it good for?" These are the standard follow up questions, and although the answers are rather fundamental I hope to explain to you why quantum simulation is good for everyone.

The reason why we make lattices of cold gaseous atoms is that they behave very quantum like, which is to say that they can, at the same time, behave both like particles and waves. A lot of outstanding problems in solid state physics, chemistry and computer science are related to this quantum behavior of large numbers of particles. Exact or approximate theories still fall short and although physicists have been working on the quantum problem for over a hundred years there is still not a complete understanding of the quantum world. My own favorite problem is that of interacting electrons in super-conductive metals. They were discovered decades ago and they can be very efficient for energy transport if they would work, in their super-conductive way, at room temperature. Currently they only work up to -100 °C or at very large pressures, which makes large scale practical applications impossible. Other problems are perhaps more practical, like quantum computers in which quantum bits are created for hard computations, or to simulate large complicated molecular reactions or even to create protected quantum communication. Instead of thinking about electronic interactions, or studying materials directly, the approach for quantum simulation is to build, from the ground up, a system that is similar to the complicated systems above but completely controllable by the experimental physicists in the laboratory. And that is what I have done. The main work of this thesis concerns a new machine in which we use very small magnets to control quantum-mechanical cold atoms in ways similar to that of electrons in a metallic lattice, or like quantum bits.

In our research group we use ultracold rubidium atoms in vacuum systems for this quantum simulation. They are the building blocks of our quantum computer or lattice simulator. What is special is that we do not use lasers to create periodic lattices in the atomic clouds but we use little magnets. By shaping strong permanent ferromagnetic magnets we can create egg box like potentials, see Fig. A.1, which we shape into various geometries to study lattices of quantum particles. We do use some lasers in our lab: for the initial cooling and
trapping of the atoms and in the end, when the quantum simulation is done, to make absorption pictures of the atoms to see where the atoms were.

![Image](image.png)

Figure A.1. Heart of the experiment that is described in this thesis. a) A horizontal look into the vacuum chamber of the newly built experiment. In the bottom of the photo, behind the window, the movable lens is visible. It is positioned such that it is focused on the magnetic chip in the middle of the chamber. b) Numerical simulation of the magnetic potential above an out-of-plane magnetized patterned layer of FePt (gray). The curved structure is created to produce a square trapping potential with equal barrier heights. On the chip in a), several of these structures with different geometries are created to capture and control atomic clouds.

This thesis contains the prior considerations, initial calculations and numerical simulations of the physics that we can expect and the preparations of this new magnetic quantum simulation machine. The first chapter contains an introduction into quantum simulation with magnetic lattices. In the second chapter I introduce some of the mathematics to describe small magnets and the fields and potentials that they can produce to trap atoms. The main results are new and more advanced lattice geometries. Besides the already known square and triangular lattice we are now able to make hexagonal, Kagome and semi-periodic lattices. In the next chapter you can find the results of a collaboration with theorists within the University of Amsterdam. We have numerically studied an existing theory that can describe aspects of the quantum particles in lattices and we have used this numerical tool to make some predictions of the type of physics that we can expect in our machine. The most important results describe the tolerance to magnetic random variations (disorder) in our magnetic chip potentials. Also we simulate the new semi-periodic lattices from the previous chapter and prove that they can be used to create the systems that we are interested in. The numerical code that we used is a quantum algorithm based on the Monte Carlo approach and we have expanded this tool to be able to study our magnetic non-periodic lattices. The Monte Carlo simulations give more insight in the physics that we want to study and prove the feasibility of the proposed experiments. In chapter 4 we describe the fabrication of the nanometer sized magnet arrays. This chapter is divided in the different process steps that are necessary to create the potentials. First I describe the growth of magnetic films, which I did in Belgium at the KU Leuven. Then we create the lattices in the magnetic film by doing nanoscale electron beam lithography in the
Kavli cleanroom in Delft. Finally we show the resulting lattices and characterize them. These measurements were mostly done at the University of Amsterdam and the AMOLF institute. While fabricating the new magnetic potentials a side project was started in cooperation with an experimental group in Leiden to use a single nanomagnet as a tip for sensitive magnetic field measurements. The results of that experiment and its implications for future research can be found in chapter 5. Some of the results in chapter 4 and 5 also have practical applications outside the world of quantum simulation and fundamental physics. In the last part of chapter 5 we discuss the possibility to use single nanoscale magnets as needle like probes. With these sensitive needle magnets we can measure very small magnetic fields and hopefully even single magnetic atoms. In Leiden they already use these little tips in medical studies and other experiments to measure small magnetic fields. We show how the sensitivity of small magnets scales beneficial with its size and that the FePt magnets that we have created are among the smallest and strongest magnets that you can make with state of the art techniques. The results from chapter 4 can be seen in a more application minded technical sense as well. We have created an array of 200 nm magnets which is a length-scale that is already comparable to some commercial magnetic hard discs. In chapter 6, we describe the experimental apparatus that we have built to do the quantum simulations and we show how we bring the small magnetic chip together with ultracold rubidium atoms and several lasers. We highlight the main features of the machine such as a movable high-resolution lens, a load-lock system which we can use to quickly change magnetic chips and some smaller home-built vacuum technology that was developed to manipulate the atoms. This whole machine is the result of the work of many people who helped build and make all the parts. With the construction of the machine my thesis ends but several people have already started to continue to work with the machine I built.
B | Samenvatting

Nanoscale magnetic atom chips for quantum simulation

Bedankt voor het lezen van mijn proefschrift; ik hoop dat ik u wat uit kon leggen over quantumsimulation en nanomagneten. Dit proefschrift bevat vijf hoofdstukken die de verschillende aspecten beschrijven van mijn poging om roosters van ultrakoude gassen te maken op een lengte schaal van ongeveer 100 nanometer (een miljoenste van een decimeter, of 200 keer kleiner dan de diameter van een menselijke haar). "Waarom wil ik dit maken, en waar is dit goed voor?", dat is de vraag die altijd volgt nadat ik uitleg wat ik doe, en hoewel het antwoord nogal fundamenteel is hoop ik u uit te leggen dat quantumsimulation goed is voor iedereen!

De reden waarom wij roosters van koude gassen willen maken is omdat zij zich zeer quantummechanisch gedragen, dat wil zeggen dat ze zich tegelijkertijd gedragen als deeltjes en als golven. Veel hedendaagse vragen in de vaste-stof fysica, scheikunde en informatica gaan over dit quantumgedrag van grote aantallen deeltjes. Exacte of numerieke beschrijvingen van de quantumnatuur schieten nog te kort en hoewel fysici al decennia hebben gewerkt aan dit vraagstuk, is er nog steeds geen volledige beschrijving van de quantumwereld. Mijn favoriete probleem betreft interacties van elektronen in supergeleidende metalen. Deze materialen kunnen zeer efficiënt energie transporteren als ze zouden werken, op hun supergeleidende wijze, bij kamertemperatuur. Maar momenteel werken ze slechts tot -100 °C, of bij zeer hoge druk. Andere vragen zijn misschien praktischer, zoals vragen over quantumcomputers waarin quantum-bits zijn gemaakt om mee te rekenen. Deze qubits kunnen bijvoorbeeld gebruikt worden om grote complexe moleculaire reacties te simuleren, of om beschermde quantumcommunicatie mee te doen. In plaats van het denken over de elektronische interacties of het direct bestuderen van materialen doen wij in de quantum simulatie wat anders. Wij proberen vanaf de basis quantumsystemen op te bouwen. Zo krijgen we een systeem dat vergelijkbaar is met de eerder genoemde ingewikkelde systemen, maar volledig controleerbaar door de experimentele fysicus in het laboratorium. En dat is precies wat ik heb gedaan. Het belangrijkste werk van dit proefschrift betreft het ontwerp en de bouw van een nieuwe machine die we gebruiken om met zeer kleine magneten quantummechanische koude atomen te controleren, zodat we dit kunnen vergelijken met het gedrag van elektronen in een materiaal.

Voor quantumsimulatie maken we gebruik van ultrakoude rubidium atomen in een vacuum kamer. Zij zijn de bouwstenen van onze quantumcomputer of rooster simulator. Het bijzondere in onze groep is dat we geen lasers gebruiken om periodieke patronen en roosters te creëren in onze atoomwolken maar kleine magneten. Door het etsen van sterke

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Ferromagnetische permanente magneten kunnen we eierloospotentialen maken in de vorm van verschillende roosters waarin we de quantumdeeltjes kunnen bestuderen. We gebruiken een aantal lasers in ons laboratorium voor het initiële koelen en vangen van de atomen en uiteindelijk, na de quantumsimulatie, voor het maken van een absorptiefoto van de atomen waarop we kunnen zien waar de atomen waren.

Figuur B.1. a) Hart van het door mij gebouwde experiment. In het rode kader is een simulatie te zien van wat er op nanometer schaal gebeurt met de magnetnevelden en atomen. b) De magnetische potentiaal zoals die ontstaat door de negen magnetetjes er onder (grijs) en een extern magnetisch veld. Op de bodems van deze magnetische putjes kunnen we koude atomen vangen.

Dit proefschrift bevat enige berekeningen en numerieke simulaties van de fysica die we kunnen verwachten en beschrijft het bouwen van deze nieuwe magnetische quantumsimulatietmachine. Het eerste hoofdstuk is een korte introductie op quantumsimulatie met magnetische roosters. In hoofdstuk 2 introduceer ik de wiskunde die nodig is om kleine magneten te beschrijven en om de magnetnevelden uit te rekenen die nodig zijn om atomen te vangen. De belangrijkste resultaten zijn nieuwe, meer geavanceerde roostergeometriën. Naast de reeds bekende vierkante en driehoekige roosters zijn we nu in staat om zeshoekige roosters en semi-periodieke roosters te maken. In het volgende hoofdstuk staan de resultaten van een samenwerking met enkele theoretici binnen de Universiteit van Amsterdam. We hebben een bestaande theorie gebruikt om sommige aspecten van de quantumdeeltjes in roosters te kunnen beschrijven. We hebben dit numerieke instrument gebruikt om een aantal voorspellingen te doen over het type natuurkunde dat we kunnen verwachten in onze machine. De belangrijkste resultaten hebben betrekking op de hoeveelheid onwaarkeurigheid die we toe kunnen laten in onze magnetische chip potentialen zonder dat deze variaties het onmogelijk maken om nog quantumfysica te observeren. Tevens hebben wij de nieuwe semi-periodieke roosters gesimuleerd uit het vorige hoofdstuk en bewijzen we dat deze gebruikt kunnen worden om de natuurkundige systemen die wij interessant vinden te creëren. De code die we gebruikten is een algoritme gebaseerd op de Monte Carlo benadering. We hebben deze uitgebreid om onze magnetische niet-periodieke roosters te kunnen simuleren. De simulaties hebben meer inzicht verschaf aan de fysica die we willen bestuderen en toonden de haalbaarheid van de voorgestelde experimenten aan. In hoofdstuk 4 beschrijven we de fabricage van de nanometerschaal magneetroosters. Dit hoofdstuk is onderverdeeld in de verschillende stappen die nodig zijn om de chips te maken. Eerst
groeien we de magnetische films. Dat heb ik gedaan bij de KU in Leuven. Dan creëren we
de roosters door elektronenbundel-lithografie te gebruiken. Dit werd gedaan in de Kavli
cleanroom van de TU Delft. Tot slot laten we de resulterende roosters zien en karakteri-
seren we ze op basis van meetingen die gedaan zijn aan de Universiteit van Amsterdam en
het AMOLF instituut. Tijdens het vervaardigen van de nieuwe magnetische roosters ont-
stond een project in samenwerking met een experimentele groep in Leiden waarin we één
nanomagneetnaald maakten om zeer nauwkeurige magneetveldmetingen mee te doen. De
resultaten van dit experiment en de implicaties voor toekomstig onderzoek zijn te vinden
in hoofdstuk 5. De resultaten uit hoofdstuk 4 en 5 hebben ook praktische toepassingen
buiten de wereld van de quantumsimulatie en fundamentele fysica. In het laatste deel van
hoofdstuk 5 bespreken we de mogelijkheid om losse nanoschaalmagneten te gebruiken als
naaldvormige sensoren zodat we zeer kleine magnetische velden en zelfs enkele magneti-
sche atomen kunnen meten. In Leiden gebruikt men deze kleine naalden nu al voor onder
andere medische experimenten waarin kleine magnetische atomen gezocht worden in bio-
logische monsters. We laten zien hoe de gevoeligheid van kleine magnetoetjes schaalt met
de grootte en dat onze magneten behoren tot de kleinste en sterkste magneten die je kunt
maken met state-of-the-art technieken. Het rooster van 200 nm magneten uit hoofdstuk
4 is qua lengteschaal vergelijkbaar met wat er gebruikt wordt in magnetische harde schij-
ven. In hoofdstuk 6 beschrijven we het experimentele apparaat dat we gebouwd hebben
om de quantumsimulaties mee te doen en we laten zien hoe deze de kleine magnetische
chip samenbrengt met ultrakoude rubidium atomen en verschillende lasers. We belichten
de belangrijkste kenmerken van de machine, zoals een beweegbare hoge-resolutie lens, een
laadsysteem, dat we kunnen gebruiken om snel magnetische chips te verwisselen en en-
kele andere vacuumhoogstandjes die zijn ontwikkeld om atomen mee te manipuleren en te
meten. Deze hele machine is het resultaat van heel veel werk gedaan door verschillende
mensen. Met de constructie van dit experiment eindigt mijn proefschrift maar inmiddels
zijn er al nieuwe PhD studenten gekomen die het werk voortzetten.
Dankwoord

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