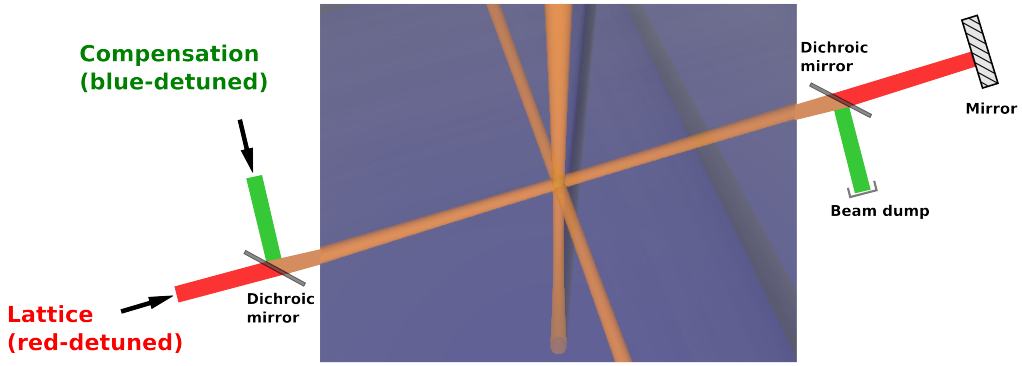


Figure 1: Simplified schematic of the compensated lattice setup

1 Compensated optical lattice

Our experiments take place in a compensated simple cubic optical lattice potential, which is formed at the intersection of three orthogonal axes, see Fig. 1. Along each axes, a 1D lattice potential is formed by retro-reflecting a red-detuned Gaussian beam, which results in a sinusoidal intensity pattern along the beam. Overlapped onto each of the lattice beams we have a compensation beam, which is blue-detuned and thus produces a repulsive potential. The compensation beam is not retro-reflected, so it does not form a standing wave potential, see Fig. 1.

The lattice beam that propagates along the x axis produces a potential of the form

$$\frac{V_L(x;y,z)}{E_R} = -s_0 \exp\left[-2\frac{y^2+z^2}{w_L^2}\right] \cos^2(k_L x) \tag{1}$$

where s_0 is the lattice depth at the center of the potential, w_L is the lattice beam waist and $k_L = 2\pi/\lambda_L$ is the wavenumber of the lattice light. The compensation beam that propagates along x produces a potential

$$\frac{V_C(x;y,z)}{E_R} = g_0 \exp\left[-2\frac{y^2+z^2}{w_C^2}\right] \tag{2}$$

where g_0 is the depth (or rather height since it is repulsive) of the compensating potential, and w_C is the beam waist of the compensation beam[1].

The combined potential of lattice plus compensation for the beams propagating along x is

$$V_{1D}(x;y,z) = V_L(x;y,z) + V_C(x;y,z) \tag{3}$$

The total potential for our simple cubic lattice is given by

$$V_{3D}(x,y,z) = V_{1D}(x;y,z) + V_{1D}(y;z,x) + V_{1D}(z;x,y) \tag{4}$$

In what follows we will study the properties of a two spin-state mixture of fermionic atoms in the compensated optical lattice potential. We are interested in the total entropy capacity of the potential, and also on the possibility of evaporative cooling in the lattice potential.

[1]We will use the letter s for the lattice depth and the letter g for the compensation depth. Both s and g are taken to be in units of the recoil energy of a lattice photon, E_R. To facilitate dimensional verification of the expressions we will explicitly indicate when a quantity is obtained in units of E_R. Note that s and g are taken always to be positive numbers.

We will use the high-temperature series expansion (HTSE), an analytical solution to the Hubbard model that is valid at high-temperatures[2]. This solution gives us the thermodynamic quantities (density, double occupancy, entropy per particle, etc.) for a homogeneous system; we then use the local density approximation (LDA) to explore the properties of the sample in the compensated lattice potential.

2 General aspects of the potential

Before we go ahead and deploy the full machinery of the LDA we will discuss some general aspects of the potential.

One of the important things to note is that at each point in space we will, in general, have three different lattice depths, associated with each of the x, y, and z lattice directions. For this reason the potential is difficult to visualize. To make thinks simpler, we can plot trap profiles along the 111 direction. Along this direction we have that the lattice depth is the same in all three directions[3]:

$$s_x(r_\mathrm{d}) = s_y(r_\mathrm{d}) = s_z(r_\mathrm{d}) = s_0 \exp\left[-\frac{4r_\mathrm{d}^2}{3w_L^2}\right] \equiv s(r_\mathrm{d}) \tag{5}$$

The bottom envelope of the lattice potential is given by

$$\frac{V_{L,\mathrm{env}}(r_\mathrm{d})}{E_R} = -3s_0 \exp\left[-\frac{4r_\mathrm{d}^2}{3w_L^2}\right] \tag{6}$$

An important aspect of a lattice potential is that the avaliable energy levels exhibit a band structure. The lowest energy of the band, E_0, measured from the potential envelope $V_{L,\mathrm{env}}$, is given by the zero-point energy of the 3D harmonic oscillator centered at the bottom of each lattice site. This harmonic oscillator result is only valid for deep lattices ($\gtrsim 10\, E_R$) but we will use it here for illustrative purposes:

$$\frac{E_0}{E_R} = \frac{\frac{3}{2}\hbar\omega_0}{E_R} = 3\sqrt{s} \tag{7}$$

We can also obtain an expression for the bandwidth W, valid in the limit of deep lattices [1]:

$$\frac{W}{E_R} = \frac{12t}{E_R} = \frac{48}{\sqrt{\pi}} s^{3/4} e^{-2\sqrt{s}} \tag{8}$$

The energy of the first excited band in the lattice corresponds to an excitation along one of the lattice directions, which adds an extra $\hbar\omega_0$ to the bottom of the band. In Fig. 2 we have plotted the lattice potential envelopes along with the envelopes of the lowest band and a line that is representative of the energy levels of the first excited band.

Also indicated in Fig. 2 is the radius, r_1, at which the energy of the lowest band is equal to band gap at the origin:

$$E_0(r_\mathrm{d} = r_1) - E_0(r_\mathrm{d} = 0) = E_1(r_\mathrm{d} = 0) - E_0(r_\mathrm{d} = 0) \tag{9}$$

In order to stay well within the single band approximation of the Hubbard model, our sample needs to have a size that is much smaller than r_1.

[2]The HTSE is very good for $T \gg t$ and works down to $T/t \sim 1.8$

[3]We will use the notation r_d to represent the distance along the 111 diagonal line.

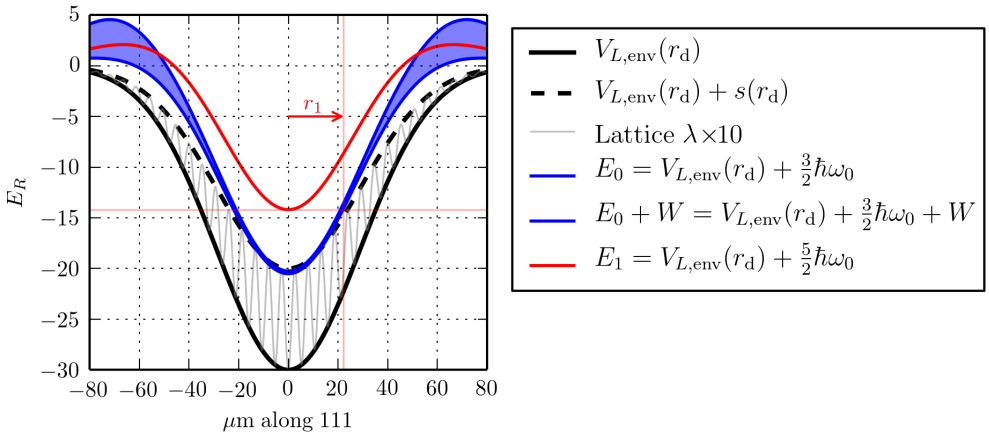


Figure 2: Diagonal profiles for a $10E_R$ lattice with $w_L = 47\,\mu$m.

2.1 Lattice locking

On occasion we will raise the lattice depth suddenly, in order to freeze out any further tunneling. This will be useful to get the maximum possible Debye-Waller factor when performing a Bragg scattering measurement, or it will also be useful to keep the density distribution frozen when sweeping across the narrow Feshbach resonance to make doublons.

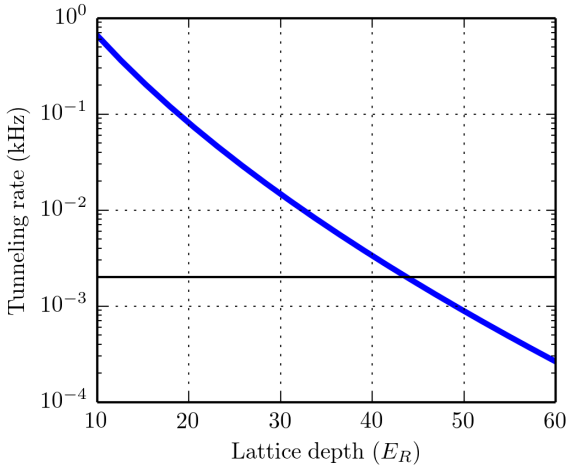
For Feshbach sweeps across the narrow resonance we have found that going across from $80\,a_0$ to $61\,a_0$ in 24 ms gives us nearly 100% conversion efficiency. For some measurements we blow away any remaining atoms with a resonant light pulse and sweep back across the resonance to dissociate the molecules. For such a procedure we require the density distribution to remain locked for times up to 48 ms. To have less than 0.1 tunneling events in 48 ms, the tunneling rate in the lattice should be less than 2 Hz.

On Fig. 3 we show the tunneling rate as a function of lattice depth, and we see that to achieve 2 Hz one needs $\approx 44\,E_R$. With that in mind we have to consider that as we lock-up the lattice to $44\,E_R$ we want to stay within the single band Hubbard model. Figure 3 also shows the atom number, N_1, corresponding to a sample with density $n = 1$ atom per site sample filled up to r_1. For atom numbers equal or greater than N_1 the single band approximation breaks down.

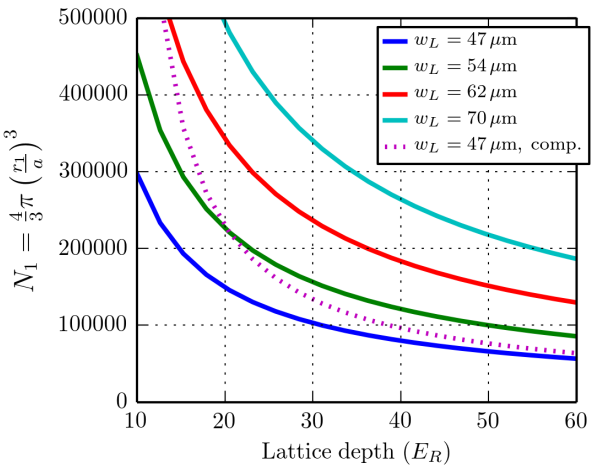
From Fig. 3 we see that for samples of $N = 300,000$ atoms and a lattice beam waist of $47\,\mu$m, the maximum lock depth to stay in the single band regime is $\approx 10\,E_R$. Currently, when doing Bragg scattering measurements, we lock the lattice up to $20\,E_R$ to get the largest possible Debye-Waller factor. In the Bragg experiment we use a compensation of $3\,E_R$ to flatten out a $7,E_R$ lattice and we leave it on during the lattice lock. Having the $3\,E_R$ of compensation gives us a maximum atom number of ≈230,000 atoms to stay in the single band regime, as is shown with the dotted line in Fig. 3.

Unfortunately, we have found that Feshbach molecules scatter green light strongly. If we have any green light on we loose them in just a few milliseconds. This means that, when considering doublon measurements, we cannot afford to have any green compensation light on.

With this in mind we see from Fig. 3 that, in order to be able to lock the lattice up to $44\,E_R$ and have the capacity to hold $N \approx 250,000$ in the single band regime, we would require a lattice beam waist as large as $70\,\mu$m.



(a) Tunneling rate. The black line is at 2 Hz, which is the rate required to keep the lattice frozen during a measurement of the double occupancy.



(b) Maximum atom number to stay in the single band regime. The dashed line includes $3\,E_R$ of compensation, with a compensation beam waist of $w_C = 40\,\mu$m.

Figure 3: Considerations to be taken when locking the lattice to freeze out tunneling.

2.2 Characteristic energy

In the previous subsection we considered the number of atoms required to fill up a sample (at zero temperature and a density of one per site) up to a certain radius. For a given number of atoms and a band shape, that band energy at that radius is (up to some constants that will be specified below) referred to as the characteristic energy of the trap, E_t.

For a sample of atoms with radius small compared to the lattice beam waists we can do a series expansion of the potential envelope and the band bottom to obtain

$$\begin{aligned} \frac{V_{L,\mathrm{env}}(r_\mathrm{d})}{E_R} &= -3s_0 + \frac{4s_0}{w_L^2} r_\mathrm{d}^2 \\ \frac{\frac{3}{2}\hbar\omega_0}{E_R} &= 3\sqrt{s_0} - \frac{2\sqrt{s_0}}{w_L^2} r_\mathrm{d}^2 \end{aligned} \tag{10}$$

The harmonic approximation to the lowest band in the lattice is then

$$\frac{E_0(r_\mathrm{d})}{E_R} = \left(\frac{4s_0 - 2\sqrt{s_0}}{w_L^2}\right) r_\mathrm{d}^2 \equiv \alpha_\mathrm{t} \left(\frac{r_\mathrm{d}}{a}\right)^2 \tag{11}$$

where $a = \lambda/2$ is the lattice spacing. This defines α_t as

$$\alpha_\mathrm{t} = \frac{4s_0 - 2\sqrt{s_0}}{(w_L/a)^2} \tag{12}$$

The characteristic energy of the trap is defined as

$$\frac{E_\mathrm{t}}{E_R} = \alpha_\mathrm{t} \left(\frac{3N}{4\pi}\right)^{2/3} \tag{13}$$

where N is the total atom number. It is seen here that the characteristic energy is the energy of the

lowest band at a radius given by

$$\frac{r_{\rm d}}{a} = \left(\frac{3N}{4\pi}\right)^{1/3} \quad \Rightarrow \quad N = \frac{1}{d^3}\left(\frac{4}{3}\pi r_{\rm d}^3\right) \tag{14}$$

This radius is simply the size occupied by the N atoms at a density of one atom per site.

Note: Usually the characteristic energy is defined using the radius of the sample at a density of two atoms per site [2]. Perhaps this is good if one wants to assess the formation of a band insulator with respect to the band gap. When dealing with Mott insulating states and comparing E_t with the Mott gap, U, a density of one atom per site on the definition is the best choice, and the one we adopt here.

The characteristic energy is a useful quantity because it provides a length-scale-free way of assessing the level of confinement in the trap[4]. Regardless of the waist of the lattice beams, for a given interaction strength U, a Mott-insulating core at the center of the sample can be achieved if $E_{\rm t} \approx U/2$. Notice that such a characteristic energy can be achieved experimentally in either of two ways: changing the confinement, $\alpha_{\rm t}$, or changing the atom number, N.

To give an example of the use of the characteristic energy, we consider our current setup with a beam waist $w_L = 47\,\mu$m. In a $7\,E_R$ lattice (without compensation)

$$\begin{aligned} \alpha_{\rm t} &= 2.909 \times 10^{-3} \\ t &= 4.88 \times 10^{-2}\,E_R \end{aligned} \tag{16}$$

With an interaction strength $U/t = 24$, the atom number required to make an insulating state with $n = 1$ at the center is

$$N = \frac{4\pi}{3}\left(\frac{U/E_R}{2\alpha_{\rm t}}\right)^{3/2} \approx 12,000 \text{ atoms} \tag{17}$$

We will see in a later section that this estimate agrees with the full machinery of the LDA.

In actual experiments typically the main constraint is the atom number. The shape and depth of the traps can be adjusted around the achievable atom number such that one can access the phases of interest. In our case these are the Mott insulator state and the antiferromagnetic Mott-insulator which both require a density of one atom per site at the center.

A plot of $E_{\rm t}/t$ as a function of lattice beam waist for a fixed atom number, N=500,000 is shown in Fig. 4. We use a black line to denote the value of $U/2t$ for a scattering legth of $650a_0$ in a $10\,E_R$ lattice. We see that achieving half-filling with the confinement provided only by the red-detuned lattice requires a lattice beam waist of $\approx 160\,\mu$m. In the next section we will see how the addition of the compensating potential can help us achieve a Mott insulating state using a smaller waist lattice for the lattice beams.

2.3 Compensation

As we have stated, we are interested in exploring the idea of evaporative cooling in a lattice and also the concept of the entropy capacity of the lattice system. We will see that for both these two ideas it

[4] As an alternative measure of the same concept, the characteristic filling is defined as [3].

$$\rho_{\rm t} = N\left(\frac{\alpha_t}{6t}\right)^{3/2} = \frac{8\pi}{3}\left(\frac{E_{\rm t}}{6t}\right)^{3/2} \tag{15}$$

Using the characteristic filling it is a little bit more cumbersome to quickly get an idea of the length-scale-free filling as one has to convert the interaction energy to an effective density in order to make a well informed comparison. It is always easier to just compare U to E_t.

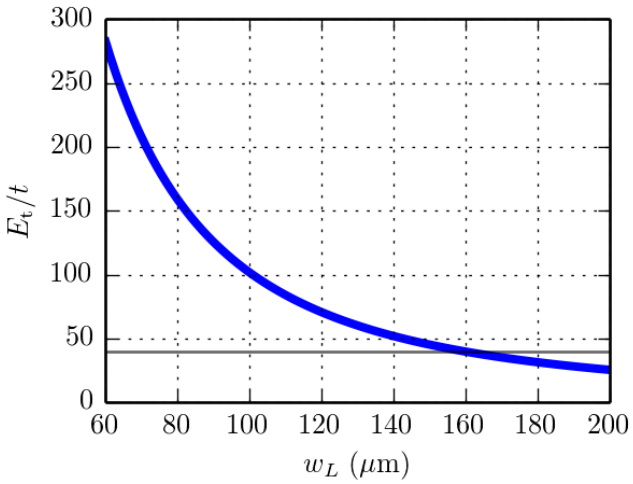


Figure 4: Characteristic energy as a function of beam waist for $N = 500,000$ atoms. The black line denotes $U/2t$, which should be the characteristic energy required to obtain a half-filled sample at the center of the potential.

will be necessary to introduce the concept of compensation. Compensation is a way of reducing α_t for a given lattice beam waist, such that large system sizes can be achieved on a smaller beam waist lattice.

For cooling it is necessary to have the boundary of the potential as close as possible to the edge of the sample and compensation helps achieve that. For entropy redistribution in the sample, one may gain advantage from the inhomogeneity in the Hubbard parameters that arises from small lattice beam waists.

With the addition of repulsive compensation beams with depth g_0 and beam waist w_C, as in Eq. 2, we can expand the lowest band of the lattice in a power series as

$$\begin{aligned}\frac{E_0(r_\mathrm{d})}{E_R} &\approx 3(g_0+\sqrt{s_0}-s_0)+\left[\frac{4s_0-2\sqrt{s_0}}{w_L^2}-\frac{4g_0}{w_C^2}\right]r_\mathrm{d}^2+\left[\frac{-8s_0+2\sqrt{s_0}}{3w_L^4}+\frac{8g_0}{3w_C^4}\right]r_\mathrm{d}^4 \\ &\equiv (A_0+A_2r_\mathrm{d}^2+A_4r_\mathrm{d}^4)/E_R\end{aligned} \tag{18}$$

Enlarging the Mott plateau We define the beam waist ratio $\alpha = w_L/w_C$ as in [4]. We see that we can completely cancel the quadratic term of the confinement by choosing

$$g_0 = \frac{4s_0-2\sqrt{s_0}}{4\alpha^2} \equiv g_\mathrm{quartic} \tag{19}$$

This choice of g_0 will be the most favorable in enlarging the size of the $n = 1$ region of the cloud because it will provide a band that is flat at the center. We point out that, for $\alpha > 1$, if we use a compensation larger than g_quartic, the band profile would have a bump in the center. We have observed epxerimentally that in that case it becomes hard to align the compensation beams such that the sample actually stays at the center of the trap.

In our current experiments we use s_0=7 and our beam waists are approximately $w_L = 47\,\mu$m and $w_C = 40\,\mu$m, which gives $\alpha = 1.175$. The necessary compensation to flatten the band would be $g_\mathrm{quartic} = 4.11$

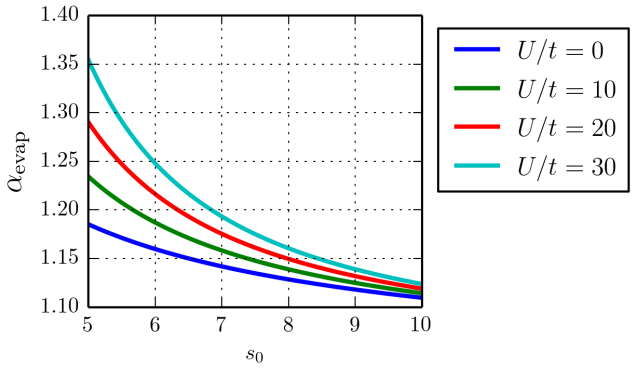


Figure 5: Optimal beam waist ratio for enlarging the central flat portion on the band and maximizing the rate of evaporative cooling.

Evaporation. We want to consider the possibility of evaporative cooling in a sample that has $n = 1$ at the center. Half-filling implies that athe radius of the cloud is $r_{\rm hf}$, such that

$$E_0(r_{\rm d} = r_{\rm hf}) - E_0(r_{\rm d} = 0) = U/2 \tag{20}$$

In order to maximize the evaporation rate for a half filled sample we need $E_0(r_{\rm hf})$ to come as close as possible to the evaporation threshold, which in our system is the energy required to escape along one of the lattice beams:

$$E_{\rm th} = (g_0 + \sqrt{s_0} - s_0)E_R \tag{21}$$

The best we can do is set $E_{\rm th} = E_0(r_{\rm hf})$ which results in

$$-2(g_0 + \sqrt{s_0} - s_0)E_R = U/2 \tag{22}$$

To maximize the size of the Mott plateau we set $g_0 = g_{\rm quartic}$, and then we solve for the beam waist ratio $\alpha_{\rm evap}$, which optimizes the evaporation rate in the lattice.

$$\alpha_{\rm evap}^2 = \frac{4s_0 - 2\sqrt{s_0}}{4s_0 - 4\sqrt{s_0} - U/E_R} \tag{23}$$

For a deep lattice ($\gtrsim 10\, E_R$) the **on-site interactions** can be expressed analytically as

$$\frac{U}{E_R} = 4\sqrt{2\pi}\frac{a_s}{\lambda}s^{3/4} \tag{24}$$

The scattering length is usually expressed in units of the Bohr radius, a_0, so it is useful to keep in mind that for our 1064 nm lattice $\lambda = 20113a_0$. In our experiment we want to avoid very large scattering lengths because they give rise to fast inelastic losses that scale as a_s^4. Reasonable values are up to $800\, a_0$. In a $7\, E_R$ lattice a scattering length $a_s = 800\, a_0$ implies an interaction strength $U/t = 30$. In Fig. 5 we show plots of $\alpha_{\rm evap}$ for various values of U/t.

We can see that for a $7\, E_R$ lattice $\alpha_{\rm evap}$ is between 1.15 and 1.20. This beam waist ratio is obtained for $g_0 = g_{\rm quartic}$ so the size of the Mott plateau is maximized, and it is chosen such that evaporation in the lattice proceeds optimally.

Atom number We now turn to examime the number of atoms required in order to achieve half-filling in the optimal setup. To get this number we need to find the half-filling radius, r_{hf}, which was defined in Eq. 20. Using a density of one atom per site we can find the atom number from the radius as $N_{\mathrm{hf}} = \frac{4}{3}\pi(r_{\mathrm{hf}}/a)^3$.

To solve Eq. 20 we can use the power series expansion of the band energy, which for $g_0 = g_{\mathrm{quartic}}$ is

$$E_0(r_{\mathrm{d}}) - E_0(0) = \left[\frac{2\sqrt{s_0} - 8s_0 + 4(2s_0 - \sqrt{s_0})\alpha^4}{3w_L^4}\right] r_{\mathrm{d}}^4 \tag{25}$$

The solution for r_{hf} is then

$$r_{\mathrm{hf}} = \frac{w_L}{\alpha}\left[\frac{3}{2}\frac{(1 - 2\alpha^4 + 2\sqrt{s_0}(\alpha^4 - 1))}{(1 - 2\alpha^4 + 4\sqrt{s0}(\alpha^4 - 1))}\right]^{1/4} \tag{26}$$

Which for $s_0 = 7$ and $\alpha = 1.17$ is $r_{\mathrm{hf}} \approx 0.7 w_L$. For a lattice beam waist $w_L = 47\,\mu$m this amounts to $N_{\mathrm{hf}} = 990,000$ atoms.

Considerations for our current setup In our current setup we have approximately $w_L = 47\,\mu$m and $w_C = 40\,\mu$m, which amounts to $\alpha = 1.175$. We use a lattice depth of $7\,E_R$. As we have seen above we should compensate this sample with $g_{\mathrm{quartic}} = 4.11$ and populate it with $990,000$ atoms. This would yiled a half-filled sample with optimal conditions for evaporative cooling in the lattice.

Unfortunately we only have ≈300,000 atoms at our disposal. This forces us to reduce the compensation below g_{quartic} in order to achieve $n = 1$ at the center. Reducing the compensation significantly affects the possibility of evaporative cooling in the lattice.

At the moment we use the following compensations for each of the three axes:

beam	1	2	3
g_0	3.65	3.90	2.9

With these values we have found empirically that we can obtain the same confinement frequencies in all three directions and that we can achieve $n = 1$ at the center with $N \approx 300,000$ atoms.

Why is our atom number 300,000? At the moment our experimental sequence consists of the following steps:

1. Evaporate into a dimple potential with a depth of $\approx 0.5\,E_R$ per axis. The cold sample in the dimple has a density of nearly one atom per site.
2. Rotate the polarization of the retro beams to go from dimple to lattice configuration. We want the sample in the dimple to have a Fermi energy $E_F < E_R$ so that we can ensure that as we rotate to a lattice potential all of the atoms will remain in the lowest band. While we rotate we add a minimal amount of compensation, $0.06\,E_R$.
3. Ramp up the lattice depth slowly up to the point where the lowest band and first excited band separate, which correponds to a lattice depth of $\approx 2.4\,E_R$. At the same time add $0.65\,E_R$ of compensation. During this time also ramp the interaction strength from the evaporation value to the value we want in the experiment.
4. Ramp up the lattice depth to $7\,E_R$ and the compensation to the final values indicated in the table above.

So far in our experiments we have tried to keep the density at one per site from the moment we start in the dimple at Step 1, up to the final sample in the lattice. Keeping the density at $n = 1$ gives us a constraint for the number of atoms that we start with in the dimple potential. We derive this below.

In the dimple, having a peak density of one per site translates into having a Fermi energy which is $E_F \approx E_R$. In fact, the local Fermi energy at the center of the trap and the density there can be related by $E_F = \frac{\hbar}{2m}(3\pi^2 n)^{2/3}$. Setting the density to one per site, $n = a^{-3}$ yields $E_F = (3/\pi)^{2/3} E_R \approx 0.97 E_R$. The local Fermi energy at the center will be the same as the global Fermi energy of the harmonic trap, so we can find the total trapped atom number from

$$E_F = \hbar\omega(3N)^{1/3} = E_R \qquad \Rightarrow \qquad N = \frac{1}{3}\left(\frac{E_R}{\hbar\omega}\right)^3 \tag{27}$$

A dimple potential with depth V_0 per axis has a trapping frequency

$$\omega = \left(\frac{8V_0}{m w_L^2}\right)^{1/2} = \frac{a\sqrt{2E_R}}{\hbar\pi}\left(\frac{8V_0}{w_L^2}\right)^{1/2} = \frac{4a}{\hbar\pi w_L}\left(E_R V_0\right)^{1/2} \tag{28}$$

so

$$N = \frac{1}{3}\left(\frac{\pi(w_L/a)}{4(V_0/E_R)^{1/2}}\right)^3 \tag{29}$$

With $V_0 = 0.5\, E_R$ and $w_L = 47\,\mu$m we obtain

$$N = 315,000 \ \text{ atoms} \tag{30}$$

Just notice that for this calculation to make sense, the depth of the dimple potential has to be larger than the Fermi energy, that is

$$2V_0 > E_F \tag{31}$$

In our setup we just match this condition since $2V_0 = 1\, E_R$ and $E_F = 1\, E_R$.

Can we load more atoms into the trap? A possible change to the experimental sequence would be to load initially a larger depth dimple. With our beam waist this will necessarily have a density larger than one atom per site, and thus a Fermi energy above $1\, E_R$, which would lead to population of higher bands when rotating into the lattice.

A simple way to circumvent this issue is to compensate the dimple before rotating the polarization of the retro beams. In that way, a larger atom number can be acomodated at a density of one atom per site, and we could proceed with the ramps that maintain the density. With a larger atom number we would find in the final sample that we would requiere a larger g_0, closer to g_{quartic} in order to have half-filling.

Why do we not do this? We go back to the first consideration of this section: locking the lattice. If we load a sample of more than $N = 230,000$ atoms the lattice lock to $20\, E_R$ compromises our mesurement by forcing atoms into the first excited band. Already at our atom number of $N \approx 300,000$ the lock to $20\, E_R$ poses somewhat of a compromise, but we have observed Bragg signals there so we are sticking with it.

Considerations for future improvements. The main bottleneck for oru setup at the moment is related to the lock. A lattice beam waist of $w_L = 70\,\mu$m would allow us to lock up to $35\, E_R$ with

a sample of $N = 300,000$ atoms. We will show with the exact calculations of the LDA, that when the atom number is a constraint one can obtain a better scenario for evaporative cooling by using a lower value of α. We will see there that a value of $\alpha \approx 1$, that is equal beam waists for lattice and compensation may be what we want to do.

3 Entropy redistribution

In the quest for producing and antiferromagnetically (AFM) ordered state with cold atoms, the entropy per particle is an important metric. It determines the number of quantum states that are accessible to each atom. At half-filling there is an average of one-particle per site[5]. If the temperature of the system is high, $T \gg U$, there is an equal probability for a site to be empty, singly or doubly occupied. If the site is singly occupied, the spin there could be up or down, so at high temperatures there are a total of four ($|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$) equally probable state at each lattice site, giving an entropy per particle[6] is equal to $s/k_{\mathrm{B}} = \ln 4 = 1.38$.

When the temperature is $T < U$, double occupancies and vacancies are suppressed and the system enters the Mott insulating state. In this case the probability of having empty sites or doubly occupied sites goes to zero. At each site, a particle can still be spin-up or spin-down with equal probability, so the entropy per particle becomes $s/k_{\mathrm{B}} = \ln 2 = 0.69$.

As the temperature of the system goes below the Néel temperature, the spin of the atoms becomes strongly determined by their position in the lattice, as they start to order antiferromagnetically. At zero temperature each site has only one possible quantum state (spin-up or spin-down depending on the lattice site) and the entropy per particle goes to zero.

For a homogeneous 3D lattice, at the Néel temperature $T_N = 0.36t$, the entropy per particle is $s = 0.4\, k_{\mathrm{B}}$. As the temperature starts dropping below T_N the entropy approaches zero very quickly in what is referred to as the AFM transition (AFM stands for antiferromagnetic order). The AFM transition has been studied theoretically for homogeneous 3D systems using quantum Monte Carlo (QMC) [5] and the dynamical cluster approximation (DCA) [6]. The results from these two approaches are shown in Figs. 6a,6b.

The theoretical calculations shown correspond to a homogeneous system, but in practice one has samples with a finite number of atoms so one is forced to confine them in order to reach half-filling. Since the confinement is typically harmonic (as opposed to a well with hard walls), the density decays as a function of distance to the center. We will show below that this inhomogeneity in the density leads to the concept of entropy redistribution. We will see that the entropy necessary to achieve a Néel state can be higher in a trapped system that in the homogeneous case.

3.1 High temperature series expansion for the Hubbard model

In this section we will plot the thermodynamic properties of the Hubbard model obtained using the high temperature series expansion (HTSE) to second order [7, 3]. The HTSE allows us to visualize the signatures of the Mott insulating state:

- The density as function of chemical potential has a plateau at $n = 1$

[5]Notice that half-filling corresponds to $n = 1$, for this reason sometimes the terms half-filling, unit filling, and unit density are used interchangeably. Here we will restrict the terminology to half-filling or we will write explicitly $n = 1$ to avoid confusion.

[6]Notice that at half-filling any quantity per particle is the same as per lattice site, since $n = 1$

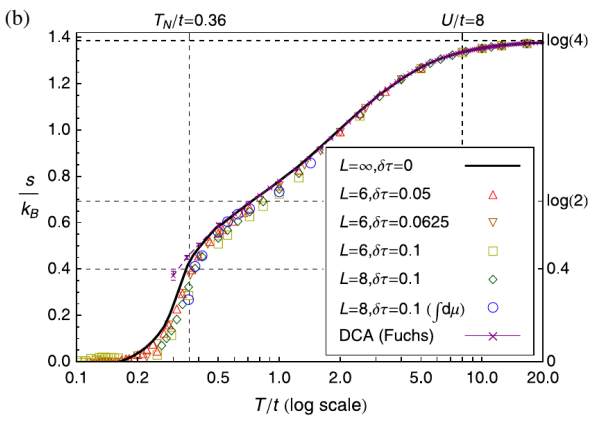


FIG. 1 (color online). (a) Energy per site of homogeneous system at half filling and $U/t = 8$, calculated by using DQMC down to $T/t = 0.1$. Statistical error bars are smaller than symbols. The solid curve is the entropy extrapolated to $L = \infty$ and $d\tau = 0$ (details in Ref. [11]). (b) Entropy per site obtained by integrating down from $T = \infty$, showing a shoulder at the Mott scale $T_{\text{Mott}} \simeq U$ and a distinct feature at the Néel temperature $T_N \approx 0.36t$ due to critical fluctuations. Errors in E/t and s/k_B are both about 0.02. Our extrapolated results are fully consistent, within error bars, with the DCA results from Fuchs *et al.* [6].

(a) Paiva [5]

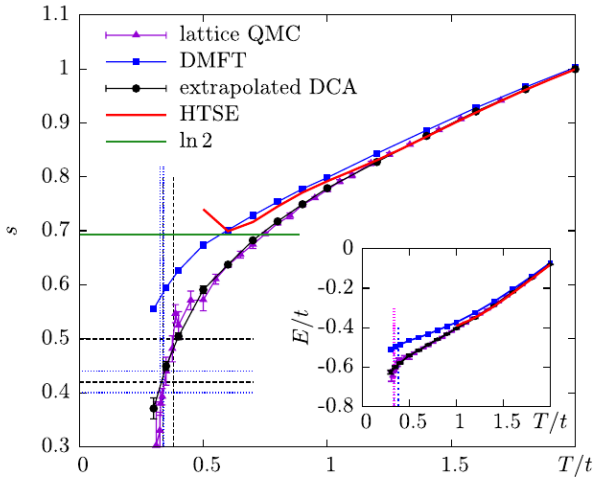


FIG. 1 (color online). Entropy per lattice site s of the Hubbard model as a function of temperature T/t, for $U/t = 8$, at half filling. Dashed vertical lines (black): T_N from Ref. [20]; dotted lines (blue): according to DMC simulations. Dashed horizontal lines (black): entropy per lattice site s at T_N [20]; dotted lines (blue): according to DMC simulations; log(2) is shown as a solid (green) horizontal line. Inset: Energy E/t per lattice site. The DMC data were extrapolated linearly in $1/L$ from the data at $L = 6, 8, 10$.

(b) Fuchs [6]

Figure 6: Calculations of entropy per lattice site versus temperature at half filling.

- The double occupancy is suppressed
- The density fluctuations are suppressed
- The entropy per site as a function of filling has a dip at $n = 1$.

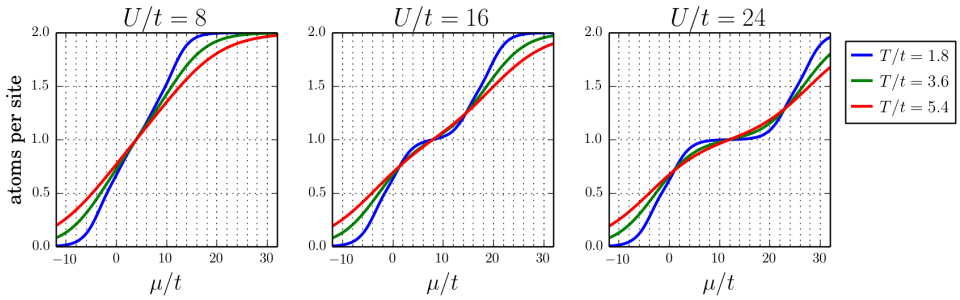
For the homogeneous Hubbard model, we show in Fig. 7 plots of the density, double occupancy, density fluctuations and entropy per site. We can see the signatures of the Mott state if we look at the variation of the thermodynamic quantities at $n = 1$. As the temperature gets lower and the interaction strength is increased these signatures become more pronounced.

3.1.1 Entropy per particle

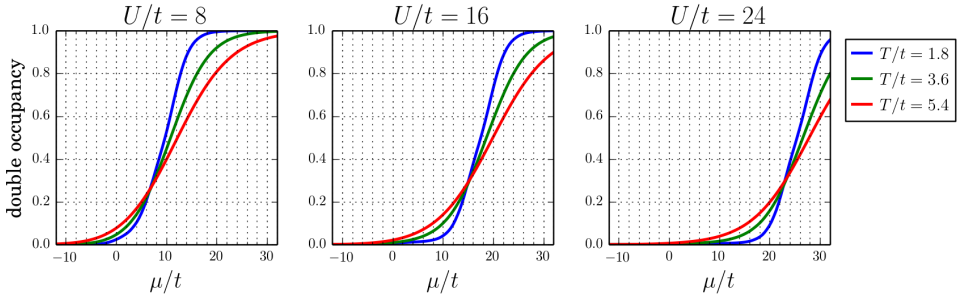
The HTSE gives us the result for the entropy per lattice site, which we can plot versus the density, as shown in Fig. 8 The interesting result arises if we divide the entropy per lattice site by the density, in order to obtain the entropy per particle. This is shown in Fig. 9. It is seen there that the entropy per particle rises significantly for lower filling values, and most importantly that the value of the entropy per particle at low filling **does not** depend strongly on temperature or interaction strength. This property is referred to as the larger entropy capacity of the metallic shell, which is at the root of the idea of entropy redistribution.

3.2 Local density approximation

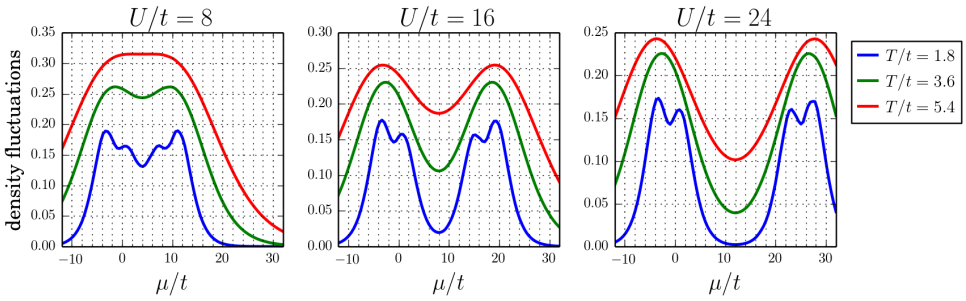
In what follows we will use the results from HTSE and the local density approximation to calculate trap profiles of the various thermodynamic quantities. A trapped gas with a finite number of atoms



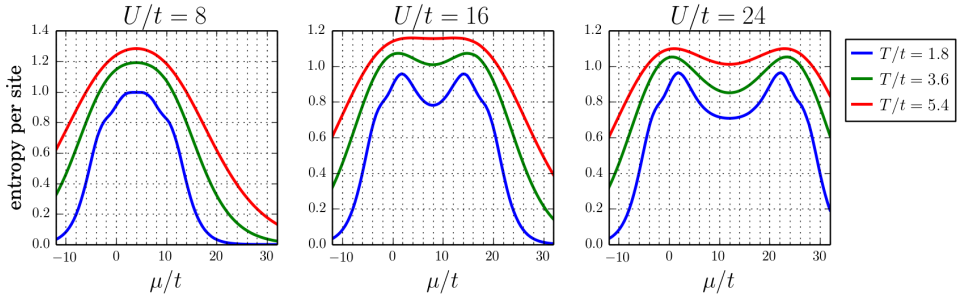
(a) Density



(b) Double occupancy



(c) Density fluctuations



(d) Entropy per lattice site

Figure 7: Thermodynamic quantities as a function of chemical potential calculated using the HTSE.

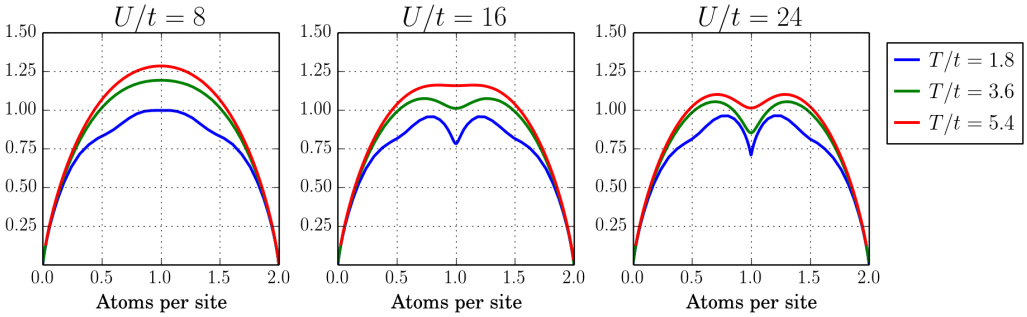


Figure 8: Entropy per lattice site versus density.

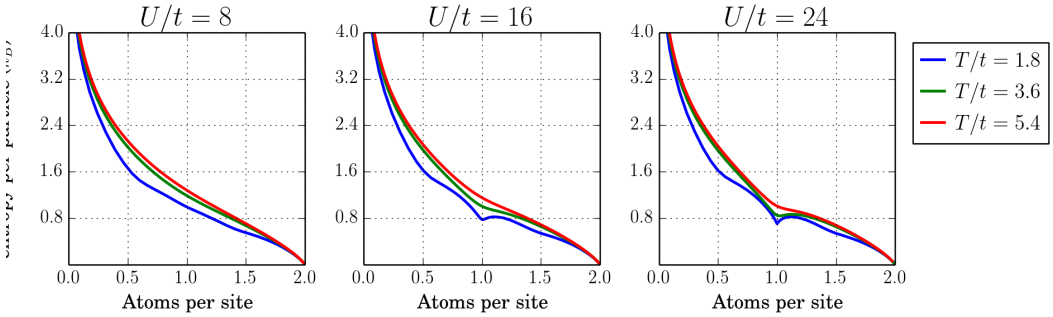


Figure 9: Entropy per particle versus density.

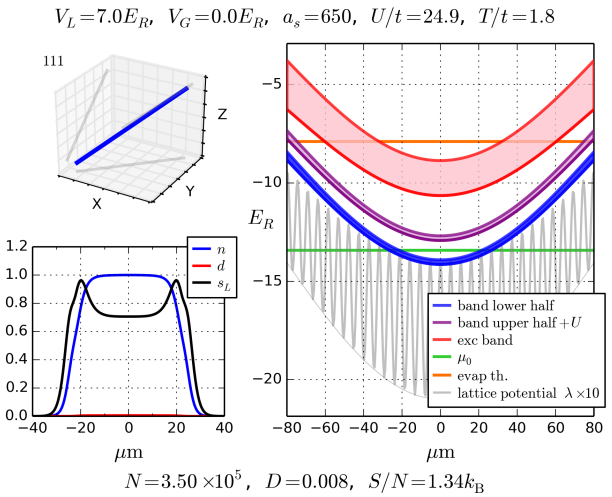
has a density that inevitably decreases as a function of distance from the center. As the density goes down, the outer shells of the cloud, which are below half-filling, will have a large entropy per particle. The overall entropy per particle of the trapped system, S/N, will be distributed such that most of it is carried by the metallic edges of the cloud.

3.2.1 Comparison between a red detuned lattice without and with compensation

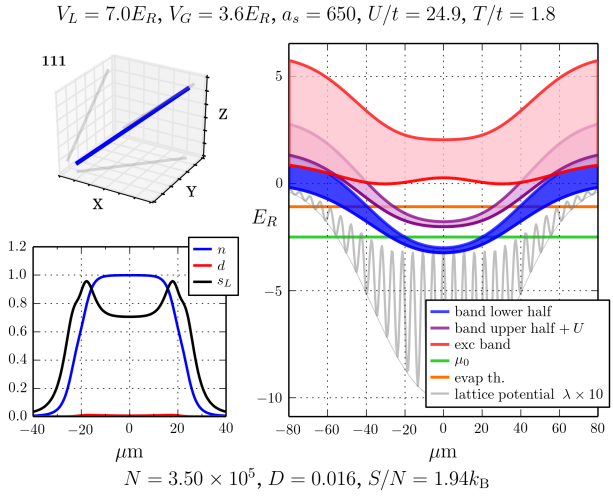
Figure 10 shows a comparison of the trap profiles for a red detuned lattice without compensation (10a) and a red detuned lattice with compensation (10b). In order to make a legitimate comparison, we set the atom number to 350,000 atoms. In the case without compensation we vary the beam waist of the lattice beams such that a density of $n = 1$ is achieved at the center of the sample. Lattice beams with smaller beam waists will produce a stronger confinement, so in general if you have a large amount of atoms and you want to achieve unit filling without compensation you must use lattice beams with a large waist. In the case with compensation we use the lattice and compensation beam waists that we currently have in our setup: $w_L = 47\,\mu$m and $w_C = 40\,\mu$m. We then adjust the depth of the compensation beams to achieve half filling with 350,000 atoms.

From looking at this figure we can see that even though the band structure profiles are very different (in the compensated case the Hubbard parameters vary strongly with radial distance), the trap profiles of the density look very similar in both cases. Despite this similarity in the density, the double occupancy and the entropy per lattice site are slightly different. The important result is that even though in both cases one has the exact same local state at the center (same filling, same U/t, same s) the overall entropy per particle can be larger for the compensated lattice by a factor of 1.5 ($1.94k_{\mathrm{B}}$to $1.34k_{\mathrm{B}}$).

This larger capacity of the compensated lattice to redistribute entropy is what can make it favorable to achieve an AFM ordered state at the center of the sample. If one looks in more detail, as is shown in Fig. 11 one realizes that the larger entropy capacity comes from a small enhancement of the double



(a) Red detuned lattice without compensation. The lattice beam waist is 146 μm for all three lattice axes. The beam waist is chosen such that the confinement produces unit filling at the center when there are 350,000 atoms in the trap.



(b) Red detuned lattice with compensation. The lattice beam waist is 47 μm and the compensation beam waist is 40 μm. These values are approximately what we use in our experimental setup. The compensation depth of 3.6 E_R is chosen so that unit filling is achieved at the center for an atom number of 350,000.

Figure 10: Full trap profiles of band structure and thermodynamic quantities for a lattice without and with compensation. For both cases the atom number is chosen to be 350,000 atoms, and the filling at the center is $n = 1$. Not that despite the very different band structure profiles, the density profiles are very similar for both cases. Even though the local Hubbard parameters and the filling are set to be the same at the center of the sample, the overall entropy per particle can be 1.5 times larger in the compensated case (1.94k_B) than in the uncompensated case (1.34k_B).

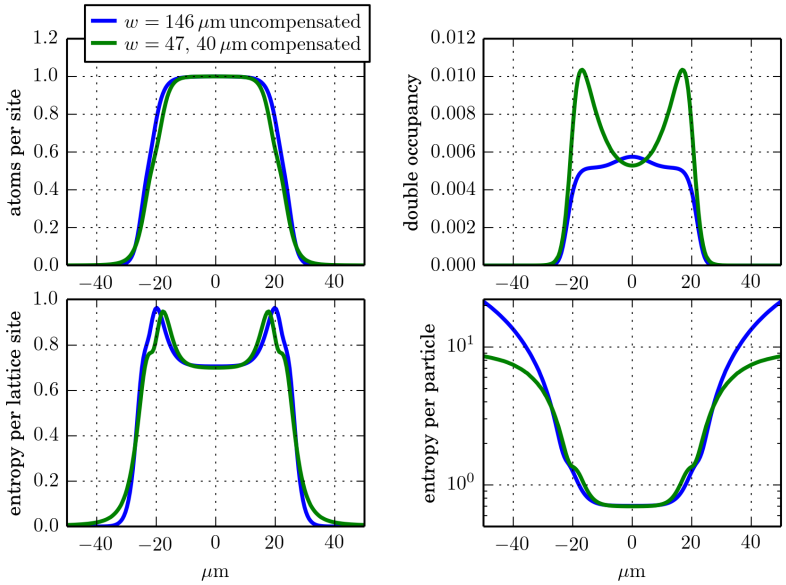


Figure 11: Detailed comparison of the thermodynamic quantities for the large beam waist uncompensated lattice and the small beam waist compensated lattice. The density is very similar for both cases. The double occupancy is quite different, which leads to a very slightly larger entropy per particle across a large range of radii in the trap.

occupancy (on the half-a percent level) which leads to a slightly larger entropy per particle on the region from about $5\,\mu$m to $25\,\mu$m radius. This radii encompass a large volume of the trap, which can make a difference on the overall entropy capacity even though the extra entropy per particle plotted radially looks very small.

The profiles that are shown in Fig. 10 are calculated at a temperature $T = 1.8t$, which is near the lowest temperature value accessible with the HTSE. The chemical potential, measured from the lowest energy level available to the system (the bottom of the band) is set to $\mu = 6t + U/2$ to guarantee half-filling at the center. [7] We used a value of $U = 24.9t$, given by the scattering length, which is set at $650a_0$.

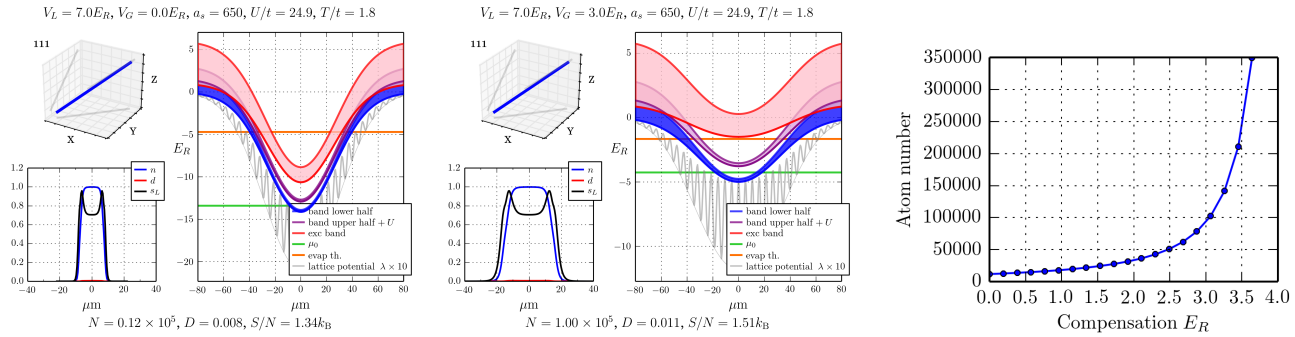
Plugging in these values we obtain $\mu \approx 18t$ or $T/\mu \approx 1.8/18 = 0.1$. When the temperature is so low, one can safely assume that $\mu \approx E_F$, so this system would have $T/T_F = 0.06$ at an overall entropy per particle of $S/N = 1.94k_{\rm B}$. If the sample was obtained by ramping up the lattice adiabatically starting from a harmonic trap, then the initial entropy in the harmonic trap should also be $1.94k_{\rm B}$. In the harmonic trap this corresponds to $T/T_F = S/(\pi^2 N) \approx 0.2$.

We conclude from these rough estimates that as the sample gets loaded into the lattice it gets adiabatically cooled, its value of T/T_F is reduced. This is in contrast with the result obtained in [8] where it was concluded that loading a gas adiabatically from a harmonic trap to a deep optical lattice would adiabatically heat the gas. In this case we are considering interactions and not neglecting the width of the lowest band. Our observation that the gas is adiabatically cooled as it is loaded into the lattice are consistent with the results from [5].

(NOTE: I NEED TO ASK THEREZA ABOUT THESE REMARKS TO CHECK THAT I AM NOT MAKING A MISTAKE.

The main question is whether it is ok to take $\mu = E_F$ since μ is in the Mott gap. Should one take

[7] The $6t$ here is half the bandwidth. Note that in typical treatments the chemical potential is always measured from the center of the lowest band, so the $6t$ will be omitted. In that case the chemical potential associated with half-filling Will be $U/2$. Some treatments even shift the zero of energy by $U/2$ so that half filling occurs nominally at μ=0 regardless of U.



(a) $w_L = 47\,\mu$m and $w_C = 40\,\mu$m without compensation.

(b) $w_L = 47\,\mu$m and $w_C = 40\,\mu$m with $3.05\,E_R$ compensation.

(c) Atom number as a function of compensation illustrates the concept of enlarging the Mott state.

Figure 12: Illustrating the idea of enlarging the Mott state.

$E_F = 12t$ in that case, since the top of the band is the largest energy state that could potentially be occupied??)

3.2.2 Enlarging the Mott state

In this section we consider our experimental setup ($w_{\mathrm{L}} = 47\,\mu$m, $w_{\mathrm{C}} = 40\,\mu$m) and we vary the amount of compensation. What we find is that if no compensation is used, then the number of atoms has to be very small in order to achieve half-filling at the center. On the other hand, when using compensation one can still hold a large number of atoms and maintain half-filling. This leads to the concept of enlarging the Mott state (or Néel state if your temperature is low enough) which can be a very dramatic effect as was shown in the paper by Mathy, Huse and Hulet [4].

The effect of enlarging the Mott state is shown in Fig. 12, where we show the relationship between atom number and compensation when the filling is set to $n = 1$ at the center of the cloud. This figure also shows the profile plots for no compensation and a compensation of $3.05\,E_R$, in order to illustrate how the Mott plateau in the density profile is enlarged for larger compensation.

From what was discussed in §3.2.1 we see that it is also possible to reach an large Mott plateau for $N = 350,000$ and without compensation beams: you just need to have larger lattice beam waists. As we saw there, the advantage of realizing the large Mott plateau with small lattice beam waists and compensating beams is that this system has a larger entropy capacity than the large-beam-waist-uncompensated counterpart.

In addition to this entropy capacity advantage, the small-beam-waist-compensated setup offers the possibility of evaporative cooling since the chemical potential comes much closer to the energy threshold for an atom escaping along one of the lattice beams. We will address this point in the following section.

4 Evaporative cooling in a lattice

If we refer back to Fig. 10 we can see that on the energy landscape plot we used an orange line to indicate the evaporation threshold, that is the energy necessary for an atom to escape along one of the lattice beams. Comparing the two cases one sees that the small beam waist compensated case has a global chemical potential (green line) that is much closer to the evaporation threshold.

When evaporative cooling a thermal gas of atoms, one considers the parameter $\eta = U_{\rm trap}/k_{\rm B}T$, where $U_{\rm trap}$ is the energy threshold for a particle leaving the trap (i.e. the trap depth) and T is the temperature of the gas. The evaporation rate is suppressed by a factor $\exp(-\eta)$ where typically $\eta \sim 10$ and, as the gas cools down, the trap depth is reduced to force further evaporation [9].

For a deeply degenerate Fermi gas, $T \ll T_F$, the evaporation rate is given by [9].

$$\Gamma_{\rm evap} \propto \gamma_{\rm coll} \frac{T}{T_F} \exp\left[-\frac{U_{\rm trap} - k_{\rm B}T_F}{k_{\rm B}T}\right] \tag{32}$$

where $\gamma_{\rm coll}$ is the classical collision rate evaluated at the Fermi surface. This can also be written as

$$\Gamma_{\rm evap} \propto \gamma_{\rm coll} \frac{T}{T_F} \exp\left[\frac{1}{T/T_F}\right] \exp\left[-\frac{1}{T/T_F}\left(\frac{U_{\rm trap}}{k_{\rm B}T_F}\right)\right] \tag{33}$$

We define $\eta_F \equiv U_{\rm trap}/k_{\rm B}T_F$ and observe that

$$\Gamma_{\rm evap} \propto \gamma_{\rm coll} \frac{T}{T_F} \exp\left[-\frac{\eta_F - 1}{T/T_F}\right] \tag{34}$$

For the deeply degenerate gas, the η factor which determines the exponential suppression of the evaporation due to the trap depth is effectively

$$\eta = \frac{\eta_F - 1}{T/T_F} \tag{35}$$

Notice that the evaporation rate is additionally suppressed by a factor T/T_F due to Pauli blocking of one of the final states of a collision, which occurs for $T \ll T_F$ [9].

We start by considering a red-detuned lattice with no extra confinement or compensation. We set $n = 1$ at the center of the sample and vary the waist of the lattice beams. From our knowledge of the potentials we can determine $U_{\rm trap}$, which in this case is the energy required for an atom to escape along one of the lattice beams. At a temperature of $T = 1.8t$ we can make the approximation $k_{\rm B}T_F \approx \mu$, where μ is the global chemical potential. Figure 13 shows η_F as a function of lattice beam waist, and also shows the number of atoms required to achieve half-filling.

In our experiment we can produce cold samples with ∼350,000 atoms. As can be seen in Fig. 13 (and also was already shown in Fig. 10a), using a beam waist of $146\,\mu$m would produce the confinement necessary to reach half-filling at the center with $N = 350,000$. The flip side of this is that, for that beam waist η_F would be ≈ 8.5, which for $T/T_F = 0.1$ means that the rate of evaporation would be suppressed by

$$\frac{T}{T_F} \exp\left[-\frac{\eta_F - 1}{T/T_F}\right] \equiv \xi_{\rm evap} \approx 10^{-34} \tag{36}$$

Going back to our current setup, which has $w_L = 47\,\mu$m and $w_C = 40\,\mu$m, with 350,000 atoms; we can achieve half filling if we use $3.64E_R$ of compensation. This yields $\eta_F \approx 2.95$. This is a lot better than the large-beam-waist-uncompensated case, however the suppression factor for the rate of evaporative cooling is still very small. For our current setup it would be

$$\xi_{\rm evap} = 3.4 \times 10^{-10} \tag{37}$$

Under typical evaporation conditions $\eta = 10$, and for a non-degenerate sample we have

$$\xi_{\rm evap} = e^{-10} = 4.5 \times 10^{-5} \tag{38}$$

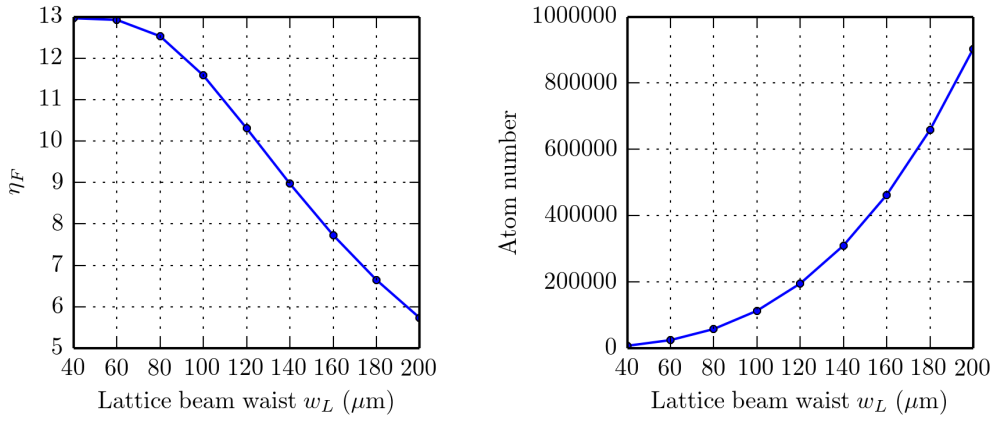


Figure 13: η_F, an indicator of the exponential suppression of evaporation is shown as a function of lattice beam waist for a red-detuned lattice without any extra confinement or compensation. To determine η_F the number of atoms is adjusted such that filling is $n = 1$ at the center. The required number is shown on the right.

We conclude that our current setup would have an evaporation rate **five orders of magnitude smaller** compared to the typical evaporative cooling rate for a thermal gas (given the same rate of elastic collisions γ_{coll}). In addition, in order to get a more realistic estimate we would need to incorporate the implications of the chemical potential being in a gapped region of the spectrum (for half-filling the chemical potential is at the center of the Mott gap) which should further reduce the evaporation rate.

We now explore the entire parameter space, where we allow the lattice and compensation beam waists to vary. We set the chemical potential so that $n = 1$ at the center of the sample, we do this because half-filling is a prerequisite to achieve Mott or Néel states. We attempt to find a compensation such that $N = 350,000$ atoms. For some values of the beam waists that is not possible because it would lead to either spilling atoms from the trap[8] or to the creation of a negative curvature in the confinement at the center of our sample[9].

The results of the exploration of the beam waist parameter space are shown in Fig. 14. The main points that stand out are

- An optimal value of η_F is achieved for $w_L \approx w_C$.
- At $w_L \approx w_C$, smaller beam waists give better entropy capacity
- The atom number can only reach 350,000 if $w_C < w_L$, such as in our current setup. Otherwise the atom number is limited, being smaller for larger w_C.

To get another look at the results, on Fig. 15 we plot η_F, S/N, and N as a function of w_C for three different values of w_L. The evaporation factor is optimized for nearly equal beam waists and the entropy capacity also peaks up around there. Given this observation, we now set $w_L = w_C$ and vary both together to see if it is favorable to make smaller or larger beam waists. This is shown in Fig. 16. The main observations are:

- For beam waists up to $\approx 68\,\mu$m one can keep getting lower η_F by making the beam waists larger. This trend would continue if we had an unlimited number of atoms, however beyond $\approx 68\,\mu$m the number of atoms required to fill the trap goes above our cap of 350,000 atoms.

[8] In cases when $w_C > w_L$.
[9] In cases when $w_C < w_L$. We also refer to this as making a donut

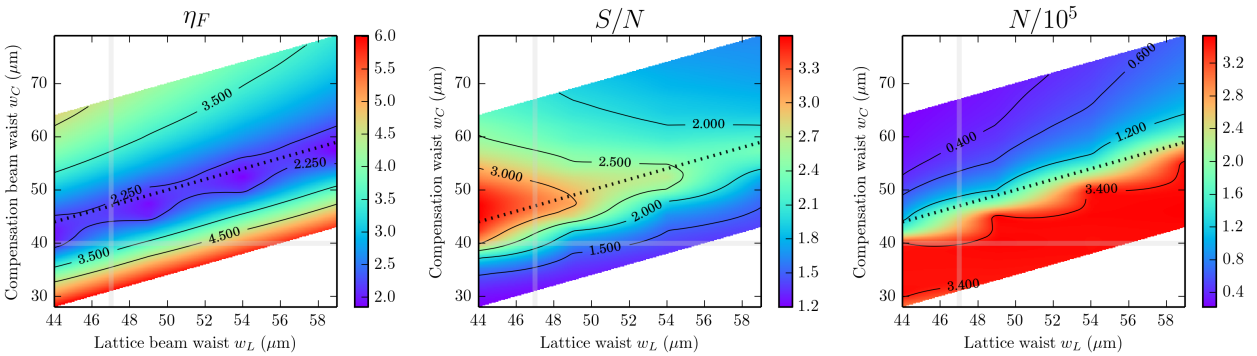


Figure 14: η_F and S/N and N are plotted for various lattice and compensation beam waists. The filling is set to $n = 1$ at the center. The compensation depth is adjusted so that $N = 350,000$ if it is possible, otherwise it is set to maximize the atom number without spilling any atoms form the trap or creating a Mexican hat at the center of the potential. The dotted line in the plots corresponds to $w_L = w_C$. The current values of our experimental setup are shown as gray lines, such that the intersection between these two gray lines represents our current conditions.

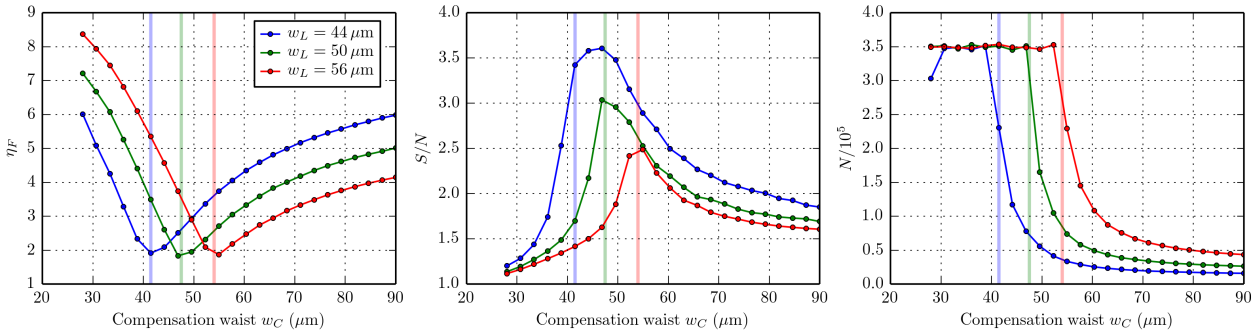


Figure 15: η_F, S/N, and N as a function of w_C for various values of w_L.

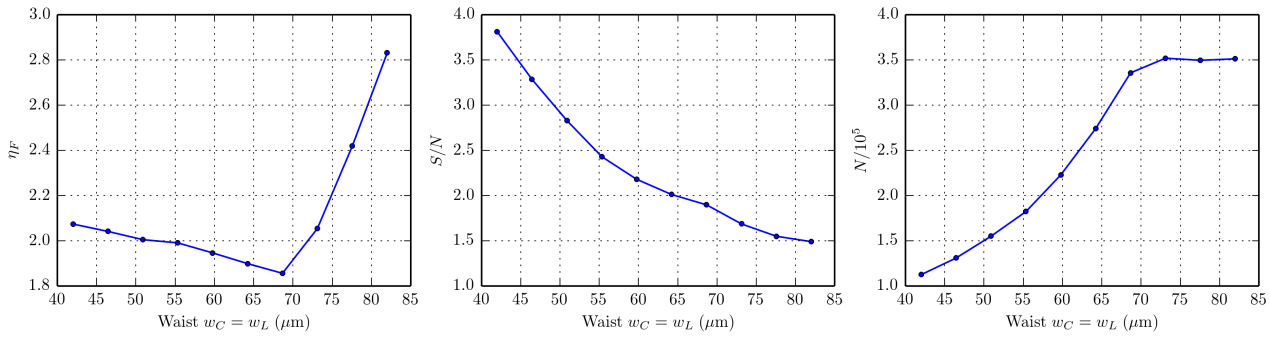


Figure 16: η_F and S/N as a function of beam waist for $w_L = w_C$. Results are shown for various atom numbers.

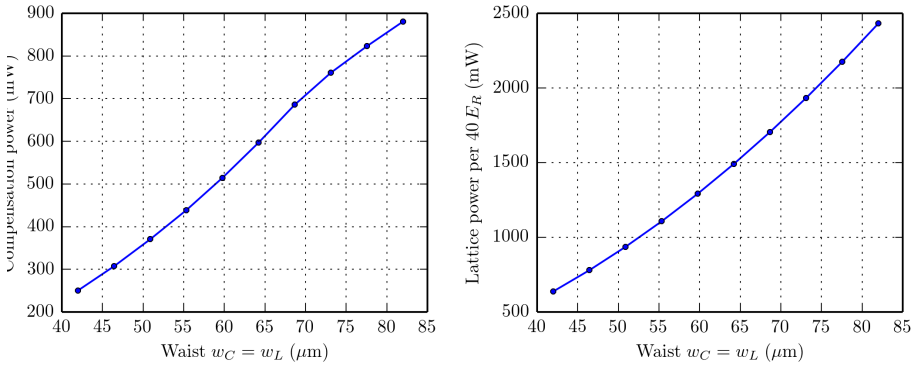


Figure 17: Compensation power required to compensate a $7\,E_R$ lattice and lattice powered required to achieve a $40\,E_R$ lattice depth.

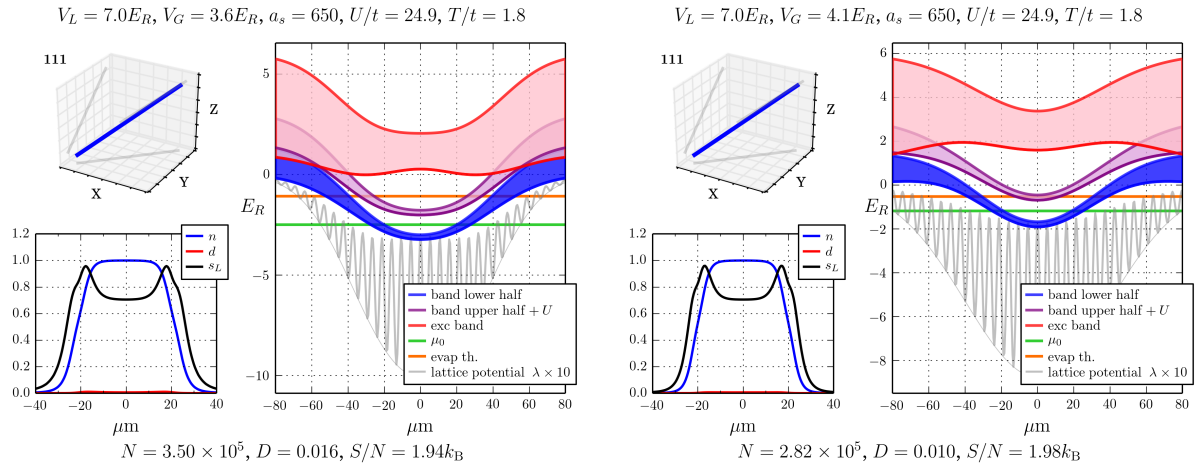
- For larger beam waists the entropy capacity is always lower, so the choice of beam waist will be a compromise between η_F and the entropy capacity.

The results shown in Figs. 16, 15 show that it is desirable to have equal lattice and compensation beam waists. The choice of their value is a compromise between the achievable η_F and the entropy capacity, given by S/N. Another important experimental constraint is the available of power at the lattice and compensation wavelengths, which is a bigger issue for larger beam waists. In that case larger power is necessary to achieve the required potential depths. The compensation power needed to compensate a $7\,E_R$ lattice and the lattice power needed to make a $40\,E_R$ deep lattice[10] are shown in Fig. 17. With this in mind and our available powers we can safely realize any choice of beam waists below $65\,\mu$m.

To fully exploit the atom number that we can produce in our experiment our opinion is to go to the larger lattice beam waists, so we recommend values of $w_L = w_C = 65\,\mu$m. These proposed parameters would change the evaporation factor and entropy capacity and number capacity of our setup according to the following table:

	$w_L\,(\mu\text{m})$	$w_C\,(\mu\text{m})$	η_F	ξ_{evap}	S/N
Current setup	47	40	2.95	3.4×10^{-10}	1.94
Proposed change	65	65	1.52	1.36×10^{-5}	1.99

[10] If we want to freeze out tunneling in the lattice we required depths as large as $40\,E_R$ where the tunneling rate goes down to 3 Hz. We currently "lock" the lattice at $20\,E_R$ for our Bragg scattering measurements. At $20\,E_R$ the tunneling rate is 72 Hz. This is good enough for Bragg scattering, but not good enough for measurements that take longer, such as associating through the narrow Feshbach resonance to measure double occupancies.



(a) $w_L = 47\,\mu$m and $w_C = 40\,\mu$m. Compensation is chosen so that unit filling is achieved at the center for an atom number of 350,000.

(b) $w_L = 65\,\mu$m and $w_C = 65\,\mu$m. Atom number maxes out at 284,000 atoms.

Figure 18: Full trap profiles of band structure and thermodynamic quantities for our current setup and the proposed setup with equal beam waists.

We see that for the optimal beam waist ratio a value of $\xi_{\text{evap}} \sim 10^{-5}$ may be reached that could lead to reasonable rates of evaporation in the lattice. A comparison of our current setup and this proposed scenario is shown in Fig. 18.

5 Conclusions

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