3 Sample inhomogeneity

The Quantum Monte Carlo (QMC) calculations done by the theorists in our collaboration are for systems with uniform filling, and at a fixed value of the interaction strength U/t. Our sample is far from these uniform conditions. Since it is a trapped finite sample, the filling (density) goes all the way down to zero. Typically, optical lattices are realized with laser beams that have large beam waists, so the parameters U and t have a negligible variation over the size of the sample. In our experiment we used a beam waist ($\approx 45\,\mu$m) which is comparable to the size of the sample ($1/e$ radius of $\approx 20\,\mu$m). For this reason we have a strong variation of U and t over the size of the sample. In our system, as you move from the center to the outside of the atom cloud the lattice gets shallower, which results in reduced U and increased t. The Hubbard interaction strength U/t thus suffers from both numerator and denominator which results in a significant variation of U/t over the cloud.

The motivation for reducing U and increasing t in length scales comparable with the sample is such that there may be entropy redistribution to the edges of the cloud. Near the edges the system has a larger entropy capacity due to the lower filling there. Additionally, since towards the edge the lattice is shallower, elastic collisions may lead to evaporation of the particles which may resulting in cooling of the system.

To incorporate the effects of inhomogeneity in the comparison between QMC and our measurements we will divide our sample into five bins, each with equal number of particles and then get the values of the filling n and the Hubbard parameters U and t for each of the bins. QMC calculations of the structure factor can be performed for each bin and then averaged before comparing with the experimental results.

To calculate the average value of the parameters in each bin we need knowledge of the density profile of our cloud, as well as knowledge of our optical lattice potential. The potential can be calculated from the calibrated beam waists and power of our optical lattice beams.

For the density profile we can perform in-situ phase-contrast images of the atom cloud. Alternatively, with our known atom number and the calculated potential we can use a thermodynamic model of the system to calculate the expected density distribution. The thermodynamic model we use is the high temperature series expansion up to second order in T/t, which can be calculated readily and is accurate down to about $T/t \approx 1.8$. To avoid complications with the repeatability in the realization of a certain density distribution we choose this second alternative. We feed into the model the atom number measured in the experiment. As a sanity check we can plot a particular realization of the density distribution and compare it with the calculation from the thermodynamic model. We can check if the peak density, double occupancy, and cloud size roughly agree with the model.

In Fig. 1 we show a plot of the in-situ density distribution measured using phase-contrast imaging in a $5.5\,E_R$ lattice with $3.0\,E_R$ of green compensation. It can be seen that the distribution is not spherically symmetric and that it is some irregularities. The $1/e$ sizes are 14 μm and 23 μm. The number of atoms in the cloud is 330,000. The density at the peak is estimated from the number and the cloud sizes to be 6.45e12 cm^{-3} which corresponds to 0.97 atoms per site. The image shown was taken at a scattering length of 380 a_0.

If we put 330,000 atoms into the model we obtain the results shown in Fig. 2 for various values of the green compensation. The peak density and double occupancy depend sensitively on the green compensation. In order to calculate the density profiles that will be used to estimate the effect of inhomogeneity on the spin structure factor we have to pick a value for the green compensation. The value that we use in the experiment is $3\,E_R$, but our observations of the peak density and the double occupancy as a function of scattering length do not match the model at $3\,E_R$ compensation. Our measurement of the double occupancy in the $5.5\,E_R$ lattice is shown in Fig. 3 and it resembles the curve with a compensation of $2.7\,E_R$ in the model. Our measurement of the density as a function of scattering

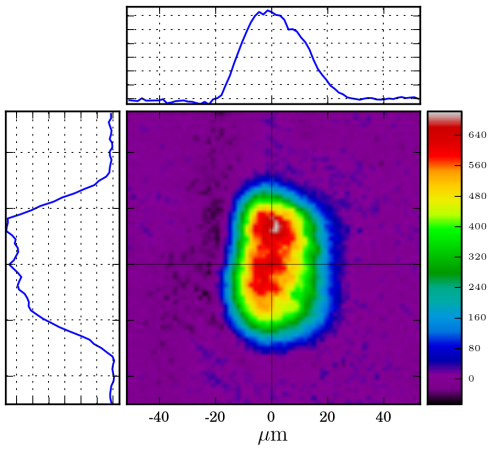

Figure 1: In-situ column density distribution in a $5.5\,E_R$ lattice with $3\,E_R$ of green compensation.

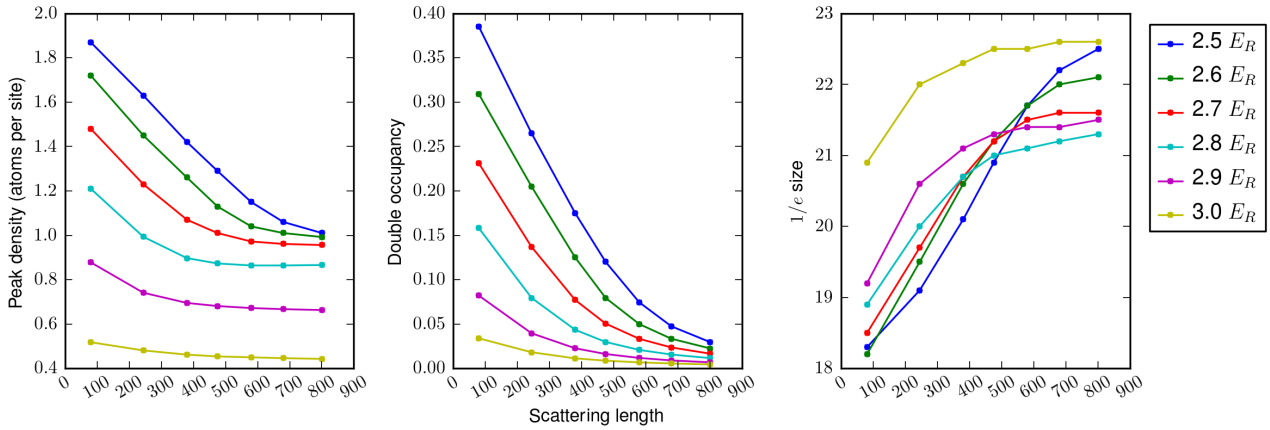

Figure 2: System parameters as a function of scattering length for various values of the green compensation. The model used is the high temperature series expansion.

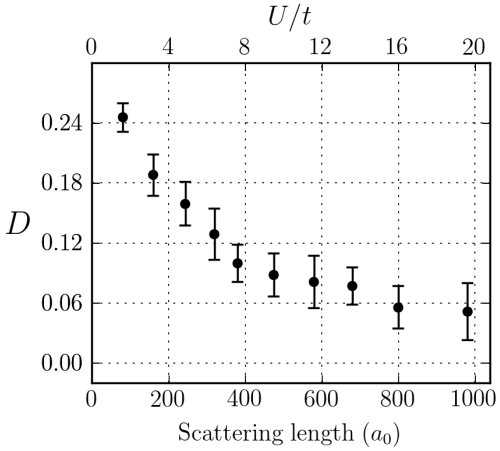

Figure 3: Double occupancy in the $5.5\,E_R$ lattice.

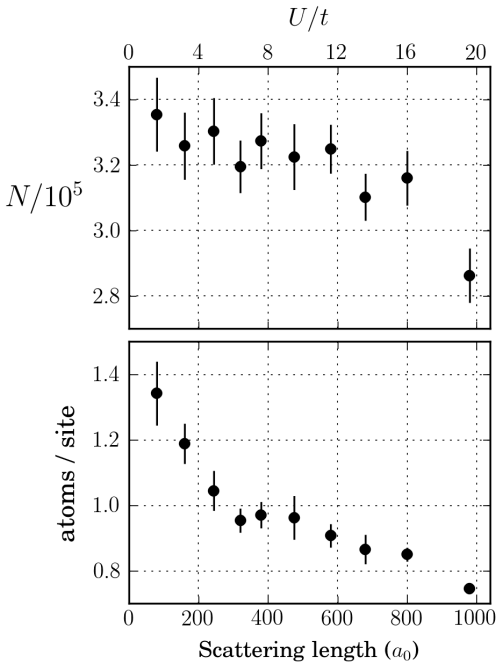

Figure 4: Peak density and atom number in the $5.5\,E_R$ lattice. The plateau in the density is characteristic of the insulating state. As the scattering length is increased three-body losses become important as it is seen in both the atom number losses and decrease in the peak density.

length is shown in Fig. 4 along with the measurement of the atom number. Both the density and double occupancy measurements are consistent with a compensation of $2.7\,E_R$ in the model. Discrepancies between our measurements and the model is most likely due to calibration errors and our inexact knowledge of the potential, however since the temperature used for the model is $T/t = 1.8$ it is possible that the discrepancy is also due to a lower temperature in our system than the one this model can handle. In what follows we will use $2.7\,E_R$ in the model to stay consistent with our observations.

With all the parameters that go into the model in hand, we can go ahead and calculate density distributions. We then split those density distributions into bins with an equal number of atoms and calculate the filling n, and the Hubbard parameters U and t for each bin. An example of this calculation for a scattering length of 580 a_0, which corresponds to U/t at the center equal to 11.9 is shown in Fig. 5.

In the averaging of the bins to calculate the structure factor we will assume that the entire system is isothermal at some temperature T, this corresponds to a reduced temperature T/t at the center of the sample. In a given bin, b, the reduced temperature (which will be relevant for the QMC in the bin) is given by

$$\frac{T}{t_b} = \left(\frac{T}{t}\right)\frac{t}{t_b}$$

where t is the tunneling at the center of the sample and t_b is the average tunneling in b^{th} bin.

Table 1 shows an example of the binning results for a value of $U/t = 11.86$ at the center of the sample. The table shows first the values of the parameters at the center of the sample, and then for each bin the columns show respectively n_b, t/t_b, and U_b/t_b. These three values are what is needed to perform the QMC calculation in each bin.

Below, in Table 2, we produce seven tables like Table 1 for the seven different values of U/t at the center that correspond to our structure factor data in the $5.5\,E_R$ lattice. We add a column labeled u, which corresponds to the ratio of U_b/t_b to U/t at the center.

$V_L = 5.50$, $V_G = 2.70$, $a_s = 580$, $U/t = 11.8$, $T/t = 1.8$, $N = 3.28 \times 10^5$

Sample is divided in 5 bins, all containing the same number of atoms (see panel 2).
Average Fermi-Hubbard parameters n, U, t, and U/t are calculated in each bin (see panels 1, 3, 4, 5)

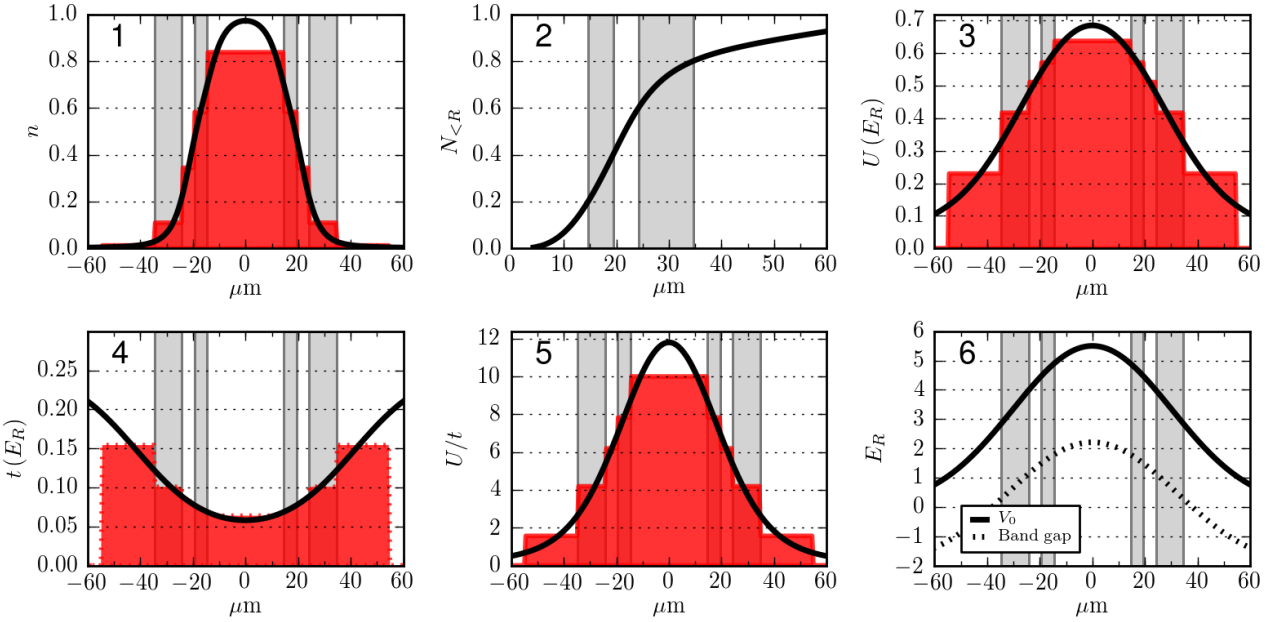

Figure 5: Binned filling and Hubbard parameters are shown in panels 1, 3, 4, and 5. The average value in each bin is shown as the shaded red area. The cumulative number up to a certain radius is shown in panel 2, this illustrates how all the bins have the same number of atoms. The lattice depth and band gap as a function of radius are shown in panel 6.

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.687 Er
U/t = 11.860 Er

At bins:
bin#      nb      t/tb       Ub/tb
------------------------------
000     0.84      0.91        9.97
001     0.58      0.79        7.82
002     0.34      0.70        6.19
003     0.11      0.57        4.13
004     0.01      0.38        1.49
```

Table 1: Binning for $U/t = 11.86$

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.095 Er
U/t = 1.636 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   1.18   0.93   1.42   0.87
001   0.79   0.83   1.17   0.71
002   0.45   0.74   0.95   0.58
003   0.14   0.62   0.67   0.41
004   0.02   0.41   0.27   0.17
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.288 Er
U/t = 4.976 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.99   0.91   4.25   0.86
001   0.66   0.81   3.41   0.69
002   0.39   0.72   2.75   0.55
003   0.12   0.60   1.90   0.39
004   0.02   0.40   0.73   0.16
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.450 Er
U/t = 7.771 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.89   0.91   6.54   0.84
001   0.61   0.80   5.19   0.67
002   0.37   0.71   4.17   0.54
003   0.12   0.59   2.83   0.37
004   0.01   0.39   1.05   0.14
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.563 Er
U/t = 9.713 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.85   0.91   8.17   0.84
001   0.60   0.80   6.48   0.67
002   0.36   0.71   5.14   0.53
003   0.11   0.58   3.42   0.36
004   0.01   0.38   1.27   0.14
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.687 Er
U/t = 11.860 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.84   0.91   9.97   0.84
001   0.58   0.79   7.82   0.66
002   0.34   0.70   6.19   0.52
003   0.11   0.57   4.13   0.35
004   0.01   0.38   1.49   0.13
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.806 Er
U/t = 13.905 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.83   0.91  11.69   0.84
001   0.58   0.79   9.17   0.66
002   0.35   0.70   7.25   0.52
003   0.11   0.57   4.84   0.35
004   0.01   0.38   1.75   0.13
```

```
------------------------------
At center:
  t = 0.058 Er
  U = 0.948 Er
U/t = 16.359 Er

At bins:
bin#    nb   t/tb   Ub/tb     u
------------------------------
000   0.83   0.91  13.78   0.84
001   0.57   0.79  10.80   0.66
002   0.33   0.70   8.43   0.52
003   0.10   0.57   5.51   0.34
004   0.01   0.37   1.98   0.13
```

Table 2: Binning for various values of U/t

bin#	nb	t/tb	u
000	0.92	0.91	0.85
001	0.63	0.80	0.67
002	0.37	0.71	0.54
003	0.12	0.59	0.37
004	0.01	0.39	0.14

Table 3: Binning for general case. To estimate the trap averaged structure factor at a temperature $T/t \equiv x$ and with an interaction given by $U/t \equiv y$, a QMC calculation will be performed for each bin using filling n_b, temperature $x(t/t_b)$ and interaction strength yu.

We point out that the n, t/t_b and u columns do not differ much across the different values of U/t at the center. To simplify the matter, and since this treatment is only a crude estimation we create a single table, Table 3, which averages the binnings for the seven values of U/t at the center. In this way we obtain a binning with which we can represent the inhomogeneity of our sample in a general case.

3.1 Raw data for S_π/S_θ and S_π

Below we show the raw data for the best estimate of S_π/S_θ which uses the simultaneous measurement of both cameras with a calibrated normalization. This is panel 3 on the figure with the data.

U/t	Spi/Sth	error
1.6	1.21	0.065
5.0	1.32	0.099
7.8	1.34	0.098
9.7	1.48	0.108
11.9	1.64	0.110
13.9	1.35	0.140
16.4	1.24	0.136

Below we show $S_{\boldsymbol{\pi}}$ determined from $S_{\boldsymbol{\pi}}/S_{\boldsymbol{\theta}}$ and $S_{\boldsymbol{\theta}}$, this is panel 5 on the figure with the data .

U/t	Spi	error
1.6	0.735	0.055
5.0	0.923	0.078
7.8	1.021	0.087
9.7	1.141	0.099
11.9	1.199	0.099
13.9	1.168	0.138
16.4	1.031	0.123

Below we show $S_{\boldsymbol{\pi}}$ determined using only the camera at $\boldsymbol{\pi}$, this is panel 2 on the figure with the data.

U/t	Spi	error
1.6	0.639	0.049
5.0	0.882	0.078
7.8	0.963	0.094
9.7	1.162	0.124
11.9	1.331	0.096
13.9	1.240	0.172
16.4	1.069	0.125