A Mott insulator of fermionic atoms in an optical lattice

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In a solid material strong interactions between the electrons can lead to surprising properties. A prime example is the Mott insulator, where the suppression of conductivity is a result of interactions and not the consequence of a filled Bloch band[1]. The proximity to the Mott insulating phase in fermionic systems is the origin for many intriguing phenomena in condensed matter physics[2], most notably high-temperature superconductivity[3]. Therefore it is highly desirable to use the novel experimental tools developed in atomic physics to access this regime. Indeed, the Hubbard model[4], which encompasses the essential physics of the Mott insulator, can be realised with quantum gases trapped in an optical lattice[5,6]. However, the Mott insulating regime has so far been reached only with a gas of bosons[7], lacking the rich and peculiar nature of fermions. Here we report on the formation of a Mott insulator of a repulsively interacting two-component Fermi gas in an optical lattice. It is signalled by three features: a drastic suppression of doubly occupied lattice sites, a strong reduction of the compressibility inferred from the response of double occupancy to atom number increase, and the appearance of a gapped mode in the excitation spectrum. Direct control of the interaction strength allows us to compare the Mott insulating and the non-interacting regime without changing tunnel-coupling or confinement. Our results pave the way for further studies of the Mott insulator, including spin ordering and ultimately the question of d-wave superfluidity[6,8].

The physics of a Mott insulator is well captured by the celebrated Hubbard model which is widely used to describe strongly interacting electrons in a solid. It assumes a single static energy band for the electrons and local interactions, i. e. spin-up and spin-down fermions are moving on a lattice and interact when occupying the same lattice site. The consequence of strong repulsive interactions is that even fermions in different spin states tend to avoid each other. In the case of a half filled band the particles get localised and an incompressible state with one fermion per site forms. Since no symmetry is broken, the transition between the metallic and the Mott insulating regime at finite temperature exhibits a crossover rather than a phase transition.

The Hubbard model ignores various complexities of materials[2] but it has been highly successful to study the nature of the Mott insulating regime, including magnetic phenomena[2] and high-temperature superconductivity[3]. Yet, despite its simplicity, it turned out that the fermionic Hubbard model is in many cases computationally intractable and important puzzles remain to be solved. In particular, the question whether the ground state of the lightly doped 2D Hubbard model supports d-wave superconductivity is as yet unanswered.

Compared to real materials, a fermionic quantum gas trapped in an optical lattice is a much purer realisation of the Hubbard model[5,6,9,10,11]. It offers a new approach to understand the physics of strongly correlated systems. In an optical lattice three mutually perpendicular standing laser waves create a periodic potential for the atoms. Cooled to sufficiently low temperatures the atoms can be loaded into the lowest energy band of the potential. The kinetics of the atoms is determined by their tunnelling rate between neighbouring lattice sites and the interaction is due to inter-atomic collisions occurring when two atoms are on the same site. In a gas of fermions in different spin states this collisional interaction can be widely tuned through a Feshbach resonance without encountering significant atom losses[10].

A landmark result has been the observation of the superfluid to Mott insulator transition using bosonic atoms trapped in an optical lattice[7]. Yet it is the fermionic character combined with repulsive interactions which provides the intimate link to fundamental questions in strongly correlated electron systems. While so far experimental studies of fermionic quantum gases in three-dimensional optical lattices have been scarce and focused on non-interacting and attractively interacting cases[12,13,14,15,16], we investigate the repulsive Fermi-Hubbard model and its paradigm, the Mott insulator.

In optical lattice experiments the presence of an underlying harmonic trapping potential has an important influence on the observable physics. Let us first consider a zero temperature Fermi gas prepared in an equal mixture of two non-interacting spin components. All available single particle quantum states will be filled up to the Fermi energy and, for a sufficiently large number of trapped atoms, a band insulating region with two atoms per site appears in the trap centre, surrounded by a metallic shell with decreasing filling, see figure 1. An important quantity to characterise the state of the system is the fraction D of atoms residing on lattice sites which are occupied by two atoms, one from each component. For the non-interacting case this double occupancy should increase in a continuous fashion with the number

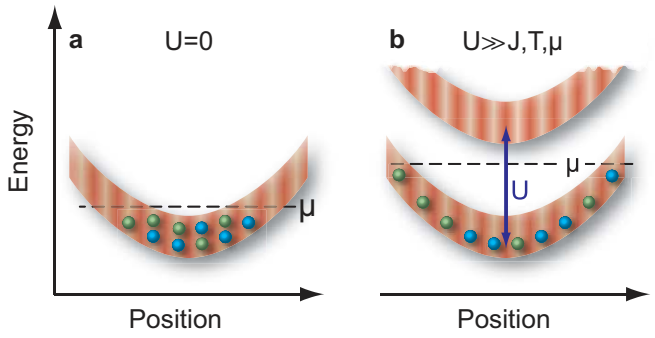

FIG. 1: **Energy spectrum of a Fermi gas in an optical lattice with an underlying confining potential.** In the non-interacting case (a) the curvature of the lowest Bloch band reflects the harmonic confinement. At zero temperature all states up to the chemical potential μ are filled with atoms of both spin states (green and blue). (b) In the Mott insulating limit the energy cost for creating doubly occupied sites greatly exceeds the temperature T and the kinetic energy parametrised by J, giving rise to a gap of order U. The energy spectrum of single particle excitations is then depicted by two Hubbard bands. Doubly occupied sites correspond to atoms in the upper Hubbard band.

N of atoms in the trap.

A very different scenario can be anticipated for a gas with increasingly strong repulsive interactions. Atoms in different spin states now repel each other and a Mott insulator will appear[17,18], at first in those regions of the trap where the local filling is approximately one atom per site. For very strong repulsion the entire centre of the trap contains a Mott insulating phase and double occupancy is suppressed, see figure 1. Since the Mott insulating region is incompressible[18,19], the suppression of double occupancy should be robust against a tightening of the trapping potential, or equivalently, against an increase in the number of trapped atoms. However, once the chemical potential μ reaches a level where double occupation of sites becomes favourable, a metallic phase appears in the centre and the double occupancy increases accordingly. The energy spectrum in the Mott insulating phase is gapped, with a finite energy cost required to bring two atoms onto the same lattice site. This energy has to be large compared to the temperature in order to keep the thermal depletion of the Mott insulator small.

Our experiment is performed with a quantum degenerate gas of fermionic ^{40}K atoms, prepared in a balanced mixture of two magnetic sublevels of the $F = 9/2$ hyperfine manifold (F: total angular momentum). Strong repulsive interactions with an s-wave scattering length ranging between $a = 240 \pm 4\,a_0$ and $810 \pm 40\,a_0$ are obtained by preparing the sample in the $|m_F\rangle = |-9/2\rangle$ and $|-5/2\rangle$ states, close to a Feshbach resonance at 224.21 Gauss[20], where a_0 is the Bohr radius. For comparison, the regime of vanishing interactions with $a = 0 \pm 10\,a_0$ is accessed by making use of a Feshbach resonance at 202.10 Gauss acting between the magnetic sublevels $|-9/2\rangle$ and $|-7/2\rangle$.

The two-component Fermi gas is subjected to the potential of a three-dimensional optical lattice of simple cubic symmetry. In terms of the recoil energy $E_R = h^2/(2m\lambda^2)$ the lattice potential depth V_0 is chosen between 6.5 and $12E_R$. Here h is Planck's constant, m the atomic mass and $\lambda = 1064\,\mathrm{nm}$ the wavelength of the lattice beams. The system is described by the Hubbard Hamiltonian:

$$\hat{H} = -J \sum_{\langle ij\rangle,\sigma} (\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + \mathrm{h.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_i \epsilon_i \hat{n}_i.$$

The onsite interaction energy is given by U and the tunnelling matrix element between nearest neighbours $\langle ij\rangle$ by J. The quotient $U/(6J)$ which characterises the ratio between interaction and kinetic energy can be tuned from zero to a maximum value of 30. The fermionic creation operator for an atom on the lattice site i is given by $\hat{c}^\dagger_{i\sigma}$, where $\sigma \in \{\uparrow,\downarrow\}$ denotes the magnetic sublevel. The particle number operator is $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$, and ϵ_i is the energy offset experienced by an atom on lattice site i due to the harmonic confining potential.

In order to characterise the state of the Fermi gas in the optical lattice we have developed a technique to measure the fraction D of atoms residing on doubly occupied sites with a precision of down to 1%. This gives us access to the compressibility of the gas and enables us to probe the excitation spectrum[21,22]. The experimental procedure is as follows. The depth of the optical lattice is rapidly increased to $30E_R$ to inhibit further tunnelling. In the next step, we shift the energy of atoms on doubly occupied sites by approaching a Feshbach resonance. This enables us to specifically address only atoms on doubly occupied sites by using a radio frequency pulse to transfer one of the spin components to a third, previously unpopulated magnetic sublevel. The fraction of transferred atoms is obtained from absorption images and allows us to deduce the double occupancy. The images are taken after spatially separating the three spin components by time of flight expansion in a magnetic gradient field.

The double occupancy as a function of total atom number is plotted in figure 2, where the non-interacting situation is compared to the case of strong repulsive interactions. The former shows the expected rapid increase of double occupancy with atom number. A strikingly different behaviour is observed in the strongly repulsive regime with $U \gg J, T, \mu$, where a Mott insulator is expected. The double occupancy is strongly reduced to values systematically below 2% for small atom numbers. This is direct evidence for the suppression of fluctuations in the occupation number and for the localisation of the atoms.

In order to experimentally investigate the compressibility on entering the Mott insulating regime we determine how the double occupancy changes with increasing atom number, i.e. we extract the slope $\partial D/\partial N$ from curves such as shown in figure 2. This slope is a good measure of the compressibility $\kappa = \partial n/\partial\mu$ in those regions

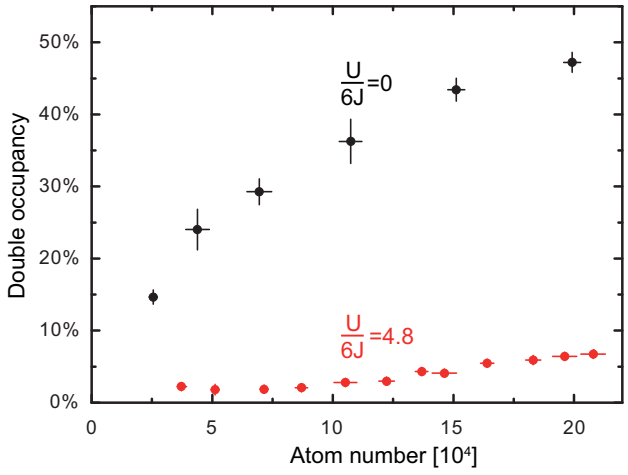

FIG. 2: **Double occupancy in the non-interacting and Mott insulating regime.** A significant increase of the double occupancy with atom number is observed in the non-interacting regime (black circles) whereas in the Mott insulating regime the double occupancy is suppressed (red circles). Both curves correspond to the same lattice depth of $V_0 = 7E_R$ with $J/h = 174\,\mathrm{Hz}$ and only differ in the onsite interaction strength: $U/h = 0 \pm 80\,\mathrm{Hz}$ and $U/h = 5.4 \pm 0.6\,\mathrm{kHz}$. Values and error bars are the statistical mean and standard deviation of 4 to 8 identical measurements. The systematic relative errors for the atom number, double occupancy, and lattice depth are estimated to be 20%, 10%, and 10% respectively, with corresponding relative errors in J of up to 30%. These systematic errors apply to all further measurements.

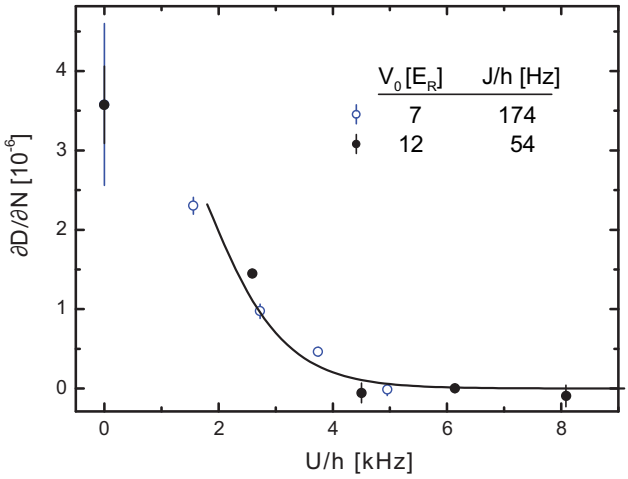

FIG. 3: **The transition to an incompressible sample.** Upon changing U, two regimes can be distinguished by the slope $\partial D/\partial N$. For vanishing interaction the large initial slope signals the filling of the Bloch band. Increasing U reduces the double occupancy. For $U/h \gtrsim 5\,\mathrm{kHz}$ a change in atom number can no longer change the double occupancy. The compressibility $\partial D/\partial N$ is obtained from a least squares fit of $D(N) = (\partial D/\partial N)N + D_0$ to data such as shown in figure 2, with atom numbers in the interval from 25×10^3 to 8×10^4. Error bars denote the confidence interval of the fit. The expected slope in the atomic limit is illustrated with a black line for a lattice depth of $12E_R$ and $T = 0.28\,T_F$.

of the cloud where the filling n is near unity or larger, since n increases with D. We estimate the filling in the trap centre for the non-interacting case from the measured double occupancy[23]. It significantly exceeds one atom per site, e. g. $\langle \hat{n} \rangle = 1.4$ for $N = 5 \times 10^4$, $V_0 = 7E_R$ and a temperature T of 30% of the Fermi temperature T_F.

The slope $\partial D/\partial N$ is displayed in figure 3 for a wide range of interaction strengths. The data shows that we access two regimes: For small onsite interaction energies U the slope $\partial D/\partial N$ is positive and the system is compressible. Yet for $U/h > 5\,\mathrm{kHz}$ the measured compressibility vanishes. This indicates that we have entered the Mott insulating regime. It implies a large central region with a filling reduced to one atom per site, surrounded by a metallic region with lower filling.

Further insight is gained by comparing our measurements with the theoretical values of $\partial D/\partial N$ calculated in the atomic limit[24] of the Hubbard model, including confinement and finite temperature. In this limit the kinetic energy is neglected by setting the tunnelling matrix element J to zero (see also methods summary). We find good agreement between theory (black line in figure 3) and experimental data for $U \gg 6J$, where the above assumption is acceptable. For the calculation we have assumed a temperature of $T = 0.28\,T_F$, which is deduced in the following way. We measure the temperature of the gas in the harmonic dipole trap, calculate its entropy[23] and find the temperature at which the atomic limit of the Hubbard model yields the same entropy. For the temperature in the optical dipole trap we use the mean value between the temperature measured before loading the lattice and after reversing the loading procedure, i. e. going back to the optical dipole trap after preparing the Mott insulating state. In each case the highest measured temperatures are taken for various $U/(6J)$, which are $0.15\,T_F$ and $0.24\,T_F$, respectively. For zero temperature the slope $\partial D/\partial N$ would vanish as soon as U becomes larger than the chemical potential μ, which is $h \times 2.7\,\mathrm{kHz}$ for $N = 8 \times 10^4$ atoms and a lattice potential of $V_0 = 12E_R$. Both our measurements and the model at finite temperature show a finite compressibility extending beyond $U/h = 2.7\,\mathrm{kHz}$, which can be attributed to thermal excitations. For the largest attained interaction $U/h = 8.1\,\mathrm{kHz}$ the thermal depletion is characterised by $T = 0.11\,U/k = 0.28\,T_F$ and corresponds to 3% vacancies in the trap center according to theory (k is Boltzmann's constant). The vanishing slope $\partial D/\partial N$ at this filling directly implies incompressibility of the core. The obtained ratio T/U is comparable to estimates for the bosonic Mott insulator[25].

In the strongly repulsive regime, the compressibility should vanish if $\mu < U$. For atom numbers correspond-

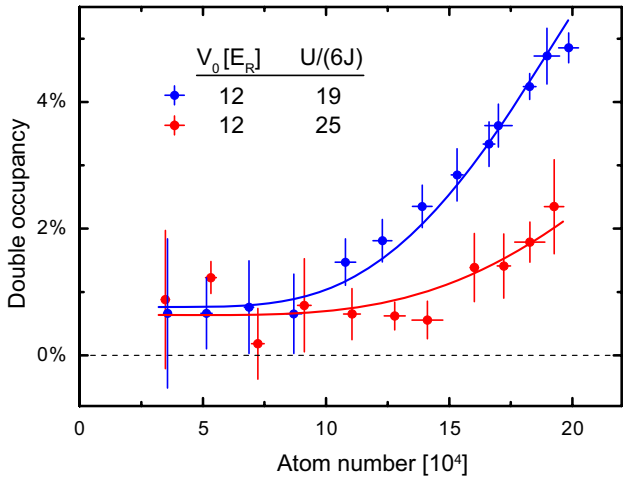

FIG. 4: **Appearance of double occupancy in the strongly interacting regime.** The double occupancy for low atom numbers is nearly constant and starts to increase only for large atom numbers. The blue and black lines represent the theoretical expectation for D in the atomic limit (see methods). The free parameters in the theory, the temperature and a constant offset in D, are determined by a least squares fit to the data. The fits yield temperatures of $0.2 \pm 0.1\,T_F$. However, the reliability is restricted due to the high sensitivity to the energy gap and the harmonic confinement. The constant offset in D accounts for the finite double occupancy in the ground state caused by second order tunnelling processes as well as a systematic offset of 0.5% stemming from technical imperfections in the initial preparation of the spin mixture. Data and errors as in figure 2.

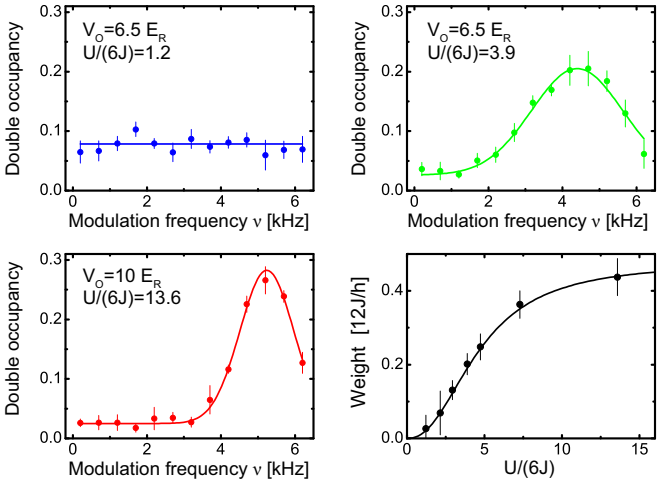

FIG. 5: **Emergence of a gapped mode.** With increasing interactions (blue, green, red) the response to modulation of the lattice depth shows the appearance of a gapped mode. The weight of this peak grows with $U/(6J)$ and saturates. All modulation spectra were obtained with $(32 \pm 2) \times 10^3$ atoms. The weight of the peak is $\sum_i \Delta\nu \left[D(\nu_i) - \frac{1}{2}(D(200\,\mathrm{Hz}) + D(700\,\mathrm{Hz}))\right]$, $\Delta\nu = 500\,\mathrm{Hz}$, and is plotted in units of $12J/h$. The lines serve as a guide to the eye. Data and errors as in figure 2.

ing to higher chemical potentials a metallic phase will appear in the trap centre and the double occupancy will increase. We observe this characteristic behaviour which is a consequence of the presence of a Mott insulator[26], see figure 4. The behaviour agrees well with that expected from the Hubbard model in the atomic limit (lines in figure 4).

An important feature of a Mott insulator is the energy gap in the excitation spectrum. The lowest lying excitations are particle-hole excitations centred at an energy U. The actual gap in the energy spectrum is reduced with respect to this value due to the width of the energy bands experienced by particles and holes[27]. A suitable technique for probing this excitation spectrum is to measure the response of the quantum gas in the optical lattice to a modulation of the lattice depth[21,22,28]: we apply 50 cycles of sinusoidal intensity modulation of all three lattice beams with an amplitude of 10%. The response is quantified by recording the double occupancy as a function of modulation frequency. With increasing interactions we observe the emergence of a gapped mode in the excitation spectrum (figure 5). For small values of $U/(6J)$, the double occupancy is not affected by the modulation of the lattice depth but for large values of $U/(6J)$ a distinct peak appears for modulation frequencies ν near U/h. Furthermore, the area under the excitation curve increases with interaction strength and starts to saturate at large values of $U/(6J)$, see figure 5d.

The presented approach to the physics of the repulsive Fermi-Hubbard model is completely different and complementary to that encountered in solid-state systems, and provides a new avenue to one of the predominant concepts in condensed matter physics. In this first experiment we could establish clear evidence for the formation of a Mott insulator of fermionic atoms in the optical lattice. We have observed that double occupancy is robustly suppressed in the Mott insulating regime and found good quantitative agreement between our measurements and the Hubbard model in the atomic limit, for a wide range of parameters. A realistic estimate for the temperature yields values small compared to the onsite interaction energy and Fermi temperature resulting in a correspondingly small thermal depletion of the Mott insulator. Our evidence is on an equal footing with the data collected for bosonic atoms in an optical lattice, where signatures of a shell structure[29,30] are widely considered to be the strongest substantiation of the insulating regime. Indeed, using a slicing technique a shell with suppressed double occupancy could be identified in a bosonic experiment[29], yet no statement on the uniformity of the density could be made. Evidently, a direct observation of regions with constant density remains a challenge for future bosonic and fermionic experiments. In further investigations of e.g. the energy spectra, the high resolution achieved may give direct insights into the width of Hubbard bands[27], the lifetime of excitations and

the level of anti-ferromagnetic ordering[11,21] in the system.

A. Methods summary.

In the atomic limit $U \gg 6J$ of the Hubbard model we assume full localisation of the fermions and thus neglect the kinetic energy. Each site is treated in the grand canonical ensemble with three possible occupation numbers $n \in \{0,1,2\}$. The partition function for site i is then $\mathcal{Z}_i = \sum_n z^n \exp(-\beta E_{i,n}) = 1 + 2z\exp(-\beta\epsilon_i) + z^2\exp(-2\beta\epsilon_i - \beta U)$ where $\beta = 1/kT$ is the inverse temperature, $z = \exp\beta\mu$ the fugacity, μ the chemical potential, $E_{i,n}$ the energy of n particles on site i, and ϵ_i the energy offset due to the harmonic confinement. For the double occupancy one obtains $\langle d\rangle_i = \langle n_D\rangle_i/\langle n\rangle_i$, $\langle n_D\rangle_i = 2z^2\exp(-2\beta\epsilon_i - \beta U)/\mathcal{Z}_i$. Double occupancy D and total particle number N of the system are obtained by summing over all sites, e. g. $D = \sum_i \langle n_D\rangle_i/N$, where the equation for N is first solved numerically with respect to z. The entropy is $S = \frac{\partial}{\partial T}(kT\sum_i \ln \mathcal{Z}_i)$. The fits in figure 3 involve U as determined by modulation spectroscopy ($U/h = 4.7 \pm 0.1\,\mathrm{kHz}$ and $6.1 \pm 0.1\,\mathrm{kHz}$) since band structure calculations disagree with the measured value by up to 30% for the largest scattering lengths. Corrections in J are expected to decrease the temperature as determined by the fit.

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I. METHODS

A. Preparation.

After sympathetic cooling with ^{87}Rb, 2×10^6 fermionic ^{40}K atoms are transferred into a dipole trap operating at a wavelength of 826 nm, and the spin mixture is cooled by forced evaporation. The final trapping frequencies of the dipole trap are $2\pi\times(34,23,122)\pm1$Hz.

To load the atoms into the lowest Bloch band of the optical lattice we increase the intensity of three retroreflected laser beams within 200 ms using a spline ramp. The beams have circular profiles with $1/e^2$ radii of $(160,180,160)\,\mu$m at the position of the atoms. For a given scattering length and lattice depth J and U are inferred from the Wannier functions including the interaction induced coupling to the second Bloch band. The latter leads to corrections of up to 15% with respect to the single band model.

B. Radio-frequency spectroscopy.

By increasing the depth of the optical lattice to $30E_R$ in 0.5 ms tunnelling is suppressed. The magnetic field is tuned to 201.28 Gauss, where a molecular state for a $|-9/2\rangle$, $|-7/2\rangle$ pair with binding energy $E_b/h = 99\pm1$ kHz and a weakly interacting state for a $|-9/2\rangle$, $|-5/2\rangle$ pair exist[13]. A radio-frequency π-pulse dissociates (associates) pairs and changes the spin state of those $|-7/2\rangle$ ($|-5/2\rangle$) atoms that share a site with a $|-9/2\rangle$ atom. Finally the magnetic field is increased to 202.80 Gauss dissociating any molecules and the lattice potential is ramped down linearly in 10 ms. All confining potentials are switched off and the homogeneous magnetic bias field is replaced by a magnetic gradient field in the same direction applied for 2 ms, thus spatially separating the spin states.

C. Imaging.

After 6 ms of time-of-flight all three clouds are imaged simultaneously. Due to a reproducible change of the imaging beam profile between the atomic absorption image and the subsequent reference image without atoms, residual structures are present in the density profiles. These are reduced by repeating the entire experiment without loading atoms and subtracting the obtained residual density distribution from the atomic density distribution. The number of atoms N_{m_F} per spin component m_F is determined by simultaneously fitting three quartic profiles with identical width, height and mutual distance to the 2D column densities. This permits accurate detection of atom numbers down to 200 atoms per spin state. We have validated the absolute accuracy of the fits against integration of the density and estimate the relative systematic error for the total atom number N to be less than 20%. The fraction D of atoms residing on doubly occupied sites is defined as $D = 2N_{m_F\prime}/N$ where $N = N_{-9/2}+N_{-7/2}+N_{-5/2}$ and $m_F\prime = -5/2$ $(-7/2)$ for samples initially containing atoms in the $|-7/2\rangle$ ($|-5/2\rangle$) states, respectively. The relative uncertainty in D is 10%, validated against measurements of the adiabatic molecule formation efficiency[13,16]. The $|-9/2\rangle$, $|-5/2\rangle$ mixture shows an offset of 0.5% in D due to $|-7/2\rangle$ atoms remaining from the initial spin transfer during evaporation.