Vol 455|11 September 2008|doi:10.1038/nature07244

LETTERS

A Mott insulator of fermionic atoms in an optical lattice

Robert Jördens[1]*, Niels Strohmaier[1]*, Kenneth Günter[1,2], Henning Moritz[1] & Tilman Esslinger[1]

Strong interactions between electrons in a solid material can lead to surprising properties. A prime example is the Mott insulator, in which suppression of conductivity occurs as a result of interactions rather than a filled Bloch band[1]. Proximity to the Mott insulating phase in fermionic systems is the origin of many intriguing phenomena in condensed matter physics[2], most notably high-temperature superconductivity[3]. The Hubbard model[4], which encompasses the essential physics of the Mott insulator, also applies to quantum gases trapped in an optical lattice[5,6]. It is therefore now possible to access this regime with tools developed in atomic physics. However, an atomic Mott insulator has so far been realized only with a gas of bosons[7], which lack the rich and peculiar nature of fermions. Here we report the formation of a Mott insulator of a repulsively interacting two-component Fermi gas in an optical lattice. It is identified 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 an increase in atom number, and the appearance of a gapped mode in the excitation spectrum. Direct control of the interaction strength allows us to compare the Mott insulating regime 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; that is, 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 a half-filled band the particles get localized, and an incompressible state with one fermion per site forms. Because no symmetry is broken, the transition between the metallic and the Mott insulating regime at finite temperature shows a crossover rather than a phase transition.

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

In comparison with real materials, a fermionic quantum gas trapped in an optical lattice is a much purer realization of the Hubbard model[5,6,9–11]. It offers a new approach to understanding the physics of strongly correlated systems. In an optical lattice three mutually perpendicular standing laser waves create a periodic potential for the atoms. The kinetics of the atoms is determined by their tunnelling rate between neighbouring lattice sites, and the interaction is due to interatomic 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 transition from superfluid to Mott insulator by using bosonic atoms trapped in an optical lattice[7]. Yet it is the fermionic character combined with repulsive interactions that provides the intimate link to fundamental questions in strongly correlated electron systems. Whereas experimental studies of fermionic quantum gases in three-dimensional optical lattices have so far been scarce and focused on non-interacting and attractively interacting cases[12–16], we investigate the repulsive Fermi–Hubbard model and its distinctive feature, 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 (Fig. 1).

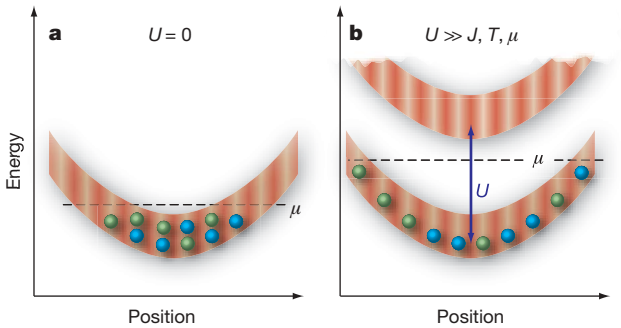

Figure 1 | Energy spectrum of a Fermi gas in an optical lattice with an underlying confining potential. a, In the non-interacting case the curvature of the lowest Bloch band reflects the harmonic confinement. At zero temperature all states up to the chemical potential μ are filled with atoms of both 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 parameterized 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.

[1]Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland. [2]Laboratoire Kastler Brossel, École Normale Supérieure, 24 rue Lhomond, 75005 Paris, France.
*These authors contributed equally to this work.

An important quantity with which to characterize the state of the system is the fraction D of atoms residing on lattice sites that 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 N of atoms in the trap.

A very different behaviour can be predicted for a gas with increasingly strong repulsive interactions. 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 (Fig. 1). Because 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 has reached a level at which 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 in comparison with the temperature, to keep the number of thermally excited doubly occupied sites small. Thermally excited holes in the centre are suppressed by the chemical potential μ.

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, where F is the total angular momentum. Feshbach resonances allow us to tune the s-wave scattering length between $a = (240 \pm 4)a_0$ and $(810 \pm 40)a_0$ as well as to prepare non-interacting samples. Here a_0 is the Bohr radius. 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 E_r and 12E_r. Here h is Planck's constant, m is the atomic mass and $\lambda = 1{,}064$ nm is the wavelength of the lattice beams. The system is described by the Hubbard Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle, \sigma} \left(\hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} + \text{h.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_i \varepsilon_i \hat{n}_i .$$

The onsite interaction energy is given by U and the tunnelling matrix element between nearest neighbours $\langle ij \rangle$ by J. The quotient $U/(6J)$ that characterizes 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 and h.c. is the Hermitian conjugate. 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.

To characterize the state of the Fermi gas in the optical lattice we have developed a technique to reliably measure the fraction D of atoms residing on doubly occupied sites down to values of 1%. 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 double occupancy as a function of total atom number is plotted in Fig. 2a, where the non-interacting situation is compared with 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, μ, where a Mott insulator is expected. The double occupancy is strongly reduced to values systematically below

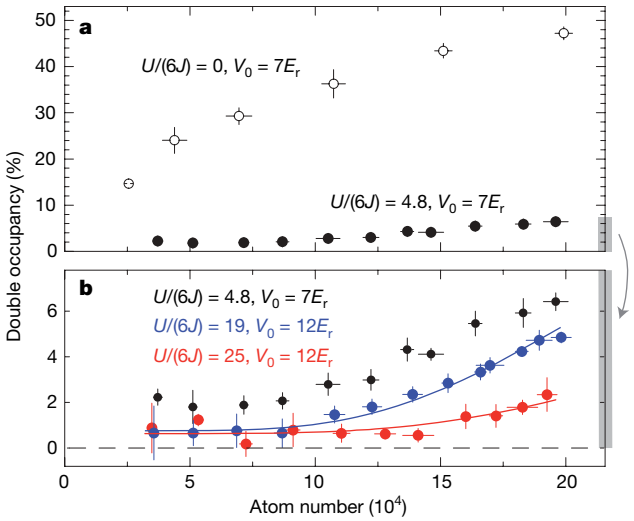

Figure 2 | Double occupancy in the non-interacting and Mott insulating regimes. a, A significant increase in the double occupancy with atom number is observed in the non-interacting regime (open circles), whereas on entering the Mott insulating regime the double occupancy is suppressed (filled circles). The corresponding onsite interaction strengths are $U/h = 0 \pm 80$ Hz and 5.0 ± 0.6 kHz, respectively. **b**, In the Mott insulating regime the double occupancy is strongly suppressed. It starts to increase for large atom numbers, indicating the formation of a metallic region in the trap centre. The blue and red lines represent the theoretical expectation for D in the atomic limit (see the text and Methods). Values and error bars are the means and s.d. of four to eight 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.

2% for small atom numbers. This is direct evidence for the suppression of fluctuations in the occupation number and for the localization of the atoms.

To experimentally investigate the compressibility on entering the Mott insulating regime we determine how the double occupancy changes with increasing atom number; that is, we extract the slope $\partial D/\partial N$ from curves such as those shown in Fig. 2. This slope is a good measure of the compressibility $\kappa = \partial n/\partial \mu$ in those regions of the cloud where the filling n is near unity or larger, because n increases with D. We estimate the filling in the trap centre for the non-interacting case from the measured double occupancy[20]. It significantly exceeds one atom per site; for example, $\langle \hat{n} \rangle = 1.4$ 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 shown in Fig. 3 for a wide range of interaction strengths. The data show 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 $U/h > 5$ 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[21] 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). We find good agreement between theory (black line in Fig. 3) and experimental data for $U \gg 6J$, where the above assumption is acceptable. For the calculation we have assumed a temperature of $T = 0.28T_F$, which is deduced from the entropy in the dipole trap as discussed in Methods. For zero temperature the slope $\partial D/\partial N$ would vanish as soon as U becomes larger than the chemical potential μ, which is $h \times 2.7$ 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

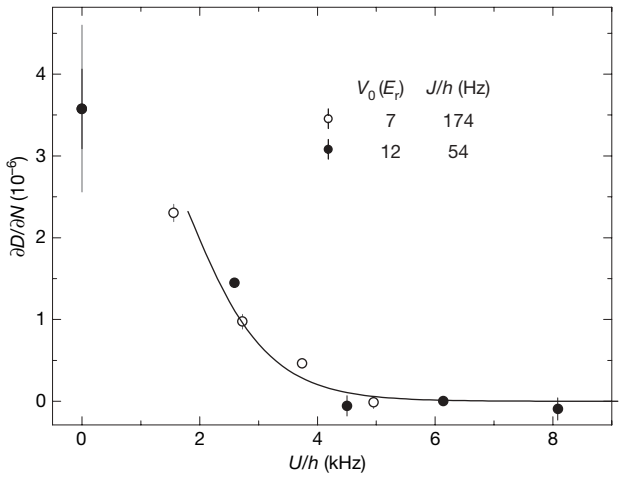

Figure 3 | The transition to an incompressible sample. On changing U, two regimes can be distinguished by the slope $\partial D/\partial N$. For vanishing interaction the large initial slope signals the filling of the Bloch band. Increasing U reduces the change in double occupancy. For $U/h \gtrsim 5$ 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 that shown in Fig. 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 $T = 0.28T_F$.

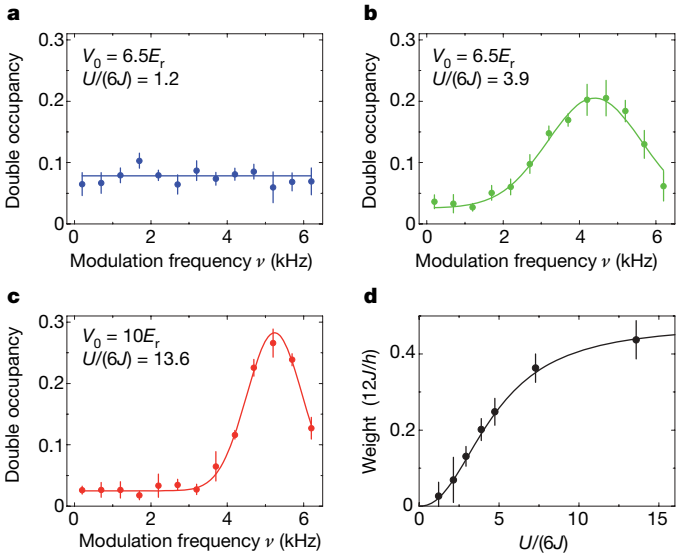

Figure 4 | Emergence of a gapped mode. **a**–**c**, With increasing interaction (blue (**a**), green (**b**), red (**c**)) the response to modulation of the lattice depth shows the appearance of a gapped mode. The weight of this peak grows with $U/(6J)$ and saturates. All modulation spectra were obtained with $(32 \pm 2) \times 10^3$ atoms. **d**, The weight of the peaks defined as

$$\sum_i \Delta\nu \left\{ D(\nu_i) - \frac{1}{2}[D(200\ \text{Hz}) + D(700\ \text{Hz})] \right\}$$

is shown. Here $D(\nu_i)$ is the measured double occupancy at frequencies ν_i, which are evenly spaced in steps of $\Delta\nu = 500$ Hz. It is plotted in units of $12J/h$. The first four data points are taken for a lattice depth of $6.5E_r$, the next at $7E_r$, $8E_r$ and $10E_r$, from left to right, respectively. The lines serve as a guide to the eye. Values and error bars are the mean and s.d. of four to eight identical measurements.

compressibility extending beyond $U/h = 2.7$ kHz, which can be attributed to thermal excitations. For the largest attained interaction $U/h = 8.1$ kHz, the thermal excitations are characterized by $T = 0.11U/k = 0.28T_F$, corresponding to 3% vacancies in the trap centre according to the theoretical analysis presented in Methods (k is Boltzmann's constant). The vanishing slope $\partial D/\partial N$ at this filling implies incompressibility of the core. The obtained ratio T/U is comparable to estimates for the bosonic Mott insulator[22].

In the strongly repulsive regime, the measured compressibility should vanish if $\mu < U$. For atom numbers corresponding to higher chemical potentials a metallic phase will appear in the trap centre and the double occupancy will increase. We observe this characteristic behaviour[23], which is a consequence of the presence of a Mott insulator (Fig. 2b). The behaviour agrees well with that expected from the Hubbard model in the atomic limit (lines in Fig. 2b). The free parameters in the theory curves, 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 accuracy is limited by 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.

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 because of the width of the energy bands experienced by particles and holes[24]. 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[25–27]: 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 (Fig. 4). 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 divided by $12\ J/h$ as a measure for its width increases with interaction strength and starts to saturate at large values of $U/(6J)$ (see Fig. 4d).

The approach to the physics of the repulsive Fermi–Hubbard model that we have presented is completely different and complementary to that encountered in solid state systems, and it provides a new avenue to one of the predominant concepts in condensed matter physics. In this first experiment we have found clear evidence for the formation of a Mott insulator of fermionic atoms in the optical lattice. We could set limits for the deviation from unity filling in the Mott insulator by directly measuring the residual double occupancy and by deducing the number of holes from a realistic estimate of the temperature. The temperature is found to be small compared with the onsite interaction energy and the Fermi temperature. In addition, we have obtained good quantitative agreement with the Hubbard model in the atomic limit for a wide range of parameters. In further investigations of, for example, the energy spectra, the high resolution achieved may give direct insights into the width of Hubbard bands[24], the lifetime of excitations and the level of antiferromagnetic ordering[11,26] in the system.

METHODS SUMMARY

In the atomic limit $U \gg 6J$ of the Hubbard model we assume full localization 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 Z_i for site i is then

$$Z_i = \Sigma_n z^n \exp(-\beta E_{i,n}) = 1 + 2z\exp(-\beta\varepsilon_i) + z^2\exp(-2\beta\varepsilon_i - \beta U)$$

where $\beta = 1/kT$ is the inverse temperature, $z = \exp(\beta\mu)$ is the fugacity, μ is the chemical potential, $E_{i,n}$ is the energy of n particles on site i, and ε_i is the energy offset due to the harmonic confinement. For the probability of finding a double occupancy $\langle d\rangle_i$ or a vacancy $\langle v\rangle_i$ one obtains $\langle d\rangle_i = z^2\exp(-2\beta\varepsilon_i - \beta U)/Z_i$ and $\langle v\rangle_i = 1/Z_i$. Double occupancy D and total particle number N of the system are

obtained by summing over all sites; for example, $D = \Sigma_i 2\langle d\rangle_i / N$, where the equation for N is first solved numerically with respect to z. The entropy is

$$S = \frac{\partial}{\partial T}\left(kT \sum\nolimits_i \ln Z_i\right)$$

We calculate the temperature in the lattice by assuming that this entropy is the same as the entropy determined from temperature measurements in the dipole trap. The fits in Fig. 2b involve U as determined by modulation spectroscopy ($U/h = 4.7 \pm 0.1$ and 6.1 ± 0.1 kHz) because band structure calculations disagree with the measured value by up to 30% for the largest scattering lengths.

Full Methods and any associated references are available in the online version of the paper at www.nature.com/nature.

Received 15 April; accepted 9 July 2008.

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Acknowledgements We thank J. Blatter, S. Huber, M. Köhl, C. Kollath, L. Pollet, N. Prokof'ev, M. Rigol, M. Sigrist, M. Troyer and W. Zwerger for discussions. Funding was provided by the Swiss National Science Foundation (SNF), the EU projects Optical Lattices and Quantum Information (OLAQUI) and Scalable Quantum Computing with Light and Atoms (SCALA) and the Quantum Science and Technology (QSIT) project of ETH Zurich.

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METHODS

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. Initially, a balanced spin mixture of atoms in the $|m_F\rangle = |-9/2\rangle$ and $|-7/2\rangle$ states is prepared and evaporatively cooled at a magnetic bias field of 203.06 G. Using this mixture we realize non-interacting samples with a scattering length of $a = (0 \pm 10)a_0$. Repulsive interactions are obtained by transferring the atoms in the $|-7/2\rangle$ state to the $|-5/2\rangle$ state during the evaporation, thus cooling and preparing a spin mixture of atoms in the $|-9/2\rangle$ and $|-5/2\rangle$ states, close to a Feshbach resonance at 224.21 G (ref. 28). After tuning the scattering length to the desired value, we load the atoms into the lowest Bloch band of the optical lattice by increasing the intensity of three retroreflected laser beams within 200 ms with the use of a spline ramp. The beams have circular profiles with $1/e^2$ radii of (160, 180, 160) μm 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% in U with respect to the single-band model.

Radiofrequency 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 G, where a molecular state for a $|-9/2\rangle$, $|-7/2\rangle$ pair with binding energy $h \times 99 \pm 1$ 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 G, dissociating any molecules, and the lattice potential is ramped down 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.

Imaging. After 6 ms of time-of-flight all three clouds are imaged simultaneously. As a result of 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 from the two-dimensional column densities by simultaneously fitting the sum of three quartic terms $A \cdot \max(1 - (x/w_x)^4, 0) \cdot \max(1 - (y/w_y)^4, 0)$ with identical widths $w_{x,y}$ and mutual distances. 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. The fraction D of atoms residing on doubly occupied sites is defined as $D = 2N_{m_{F'}}/N$, where $N = N_{-9/2} + N_{-7/2} + N_{-5/2}$ and $m_{F'} = -5/2$ $(-7/2)$ for samples initially containing atoms in the $|-7/2\rangle$ ($|-5/2\rangle$) state. The relative uncertainty in D is 10%, validated against measurements of the adiabatic molecule formation efficiency[13,16]. We estimate the relative systematic error for the total atom number N to be less than 20%. The $|-9/2\rangle$, $|-5/2\rangle$ mixture shows an offset of 0.5% in D as a result of $|-7/2\rangle$ atoms remaining from the initial spin transfer during evaporation.

Temperature. The temperature is measured in the harmonic dipole trap before ramping up the lattice and after a subsequent reversed ramp back into the dipole trap. The highest temperatures measured before and after ramping are $T_i = 0.15T_F$ and $T_f = 0.24T_F$, respectively. Because we expect non-adiabatic heating to occur during the lattice ramp up as well as during ramp down, we use the mean value of $0.195T_F$ as a realistic estimate. With this we calculate a temperature of $T = 0.28T_F$ in the Mott insulating regime ($a = 810a_0$, $V_0 = 12E_r$, $N = 10^5$), corresponding to 3.3% holes and a compressibility as low as $\partial n/\partial\mu = 0.09/\mu$ in the centre. For the temperatures in the dipole trap before and after the lattice ramp we would obtain 0.3% holes for T_i and 11.5% for T_f. The reported temperatures represent upper limits, because we have achieved temperatures down to $0.08T_F$ in the dipole trap before loading. Owing to inelastic collisions we lose at most (4.8 ± 0.6)% of the atoms during the preparation of the Mott insulating state for the parameters above, where the losses are expected to be highest. The inelastic decay time for atoms on doubly occupied sites exceeds 850 ms, which is significantly longer than the relevant experimental timescale.

28. Regal, C. A. & Jin, D. S. Measurement of positive and negative scattering lengths in a Fermi gas of atoms. *Phys. Rev. Lett.* **90**, 230404 (2003).