A Mott insulator of fermionic atoms in an optical lattice

Robert Jördens,¹ Niels Strohmaier,¹ Kenneth Günter,¹,² Henning Moritz,¹ and Tilman Esslinger¹

¹Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland
²Laboratoire Kastler Brossel, École Normale Supérieure, 24 Rue Lhomond, 75005 Paris, France

(Dated: September 11, 2008)

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. The proximity to the Mott insulating phase in fermionic systems is the origin for many intriguing phenomena in condensed matter physics, most notably high-temperature superconductivity. Therefore it is highly desirable to use the novel experimental tools developed in atomic physics to access this regime. Indeed, the Hubbard model, which encompasses the essential physics of the Mott insulator, also applies to quantum gases trapped in an optical lattice. However, the Mott insulating regime has so far been reached only with a gas of bosons, 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.

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 this collisional interaction can be widely tuned through a Feshbach resonance without encountering significant atom losses.

A landmark result has been the observation of the superfluid to Mott insulator transition using bosonic atoms trapped in an optical lattice. Yet it is the fermionic character combined with repulsive interactions which 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 been scarce and focused on non-interacting and attractively interacting cases, 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 \( N \) of atoms in the trap.

A very different scenario can be anticipated for a gas with increasingly strong repulsive interactions. A Mott insulator will appear, at first in those regions of the
The two-component Fermi gas is subjected to the potential all states up to the chemical potential $\mu$ are filled with atoms of both spin states (green and blue). 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.

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). Feshbach resonances allow us to tune the $s$-wave scattering length between $a = 240 \pm 4a_0$ and $810 \pm 40a_0$ 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 $E_R = \hbar^2/(2m\lambda^2)$ the lattice potential depth $V_0$ is chosen between 6.5 and $12E_R$. Here $\hbar$ is Planck’s constant, $m$ the atomic mass and $\lambda = 1064 \text{ nm}$ the wavelength of the lattice beams. The system is described by the Hubbard Hamiltonian:

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

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 $\hat{c}_{i\sigma}$, 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 $\epsilon_i$ 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%. 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 figure 2a, 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 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. 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 $U/\hbar > 5 \text{ kHz}$ the measured compress-
FIG. 2: Double occupancy in the non-interacting and Mott insulating regime. a, A significant increase of the double occupancy with atom number is observed in the non-interacting regime (empty 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 $U/h = 5.0 \pm 0.6$ kHz. 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 text and methods summary). Values and error bars are the mean and s. d. 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.

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 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 $T = 0.28T_F$, which is deduced from the entropy in the dipole trap as discussed in the methods section. For zero temperature the slope $\partial D/\partial N$ would vanish as soon as $U$ becomes larger than the chemical potential $\mu$, 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 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 characterised by $T = 0.11U/k = 0.28T_F$, corresponding to 3% vacancies in the trap centre according to the theoretical analysis presented in the methods section ($k$ 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[22] which is a consequence of the presence of a Mott insulator, see figure 2b. The behaviour agrees well with that expected from the Hubbard model in the atomic limit (lines in figure 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 $0.2 \pm 0.1T_F$. However, the accuracy is limited 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.

An important feature of a Mott insulator is the energy...
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 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 to 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 e.g. the energy spectra, the high resolution achieved may give direct insights into the width of Hubbard bands\cite{22} the lifetime of excitations and the level of anti-ferromagnetic ordering\cite{11,20} in the system.

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 $Z_i = \sum_n z^n \exp(-\beta E_{i,n}) = 1 + 2z \exp(-\beta \epsilon_i) + z^2 \exp(-2\beta \epsilon_i - \beta U)$ where $\beta = 1/kT$ is the inverse temperature, $z = \exp(\beta \mu)$ the chemical potential, $E_{i,n}$ the energy of $n$ particles on site $i$, and $\epsilon_i$ the energy offset due to the harmonic confinement. For the probability to find a double occupancy $\langle d|_i$ or a vacancy $\langle v|_i$ one obtains $\langle d|_i = z^2 \exp(-2\beta \epsilon_i - \beta U)/Z_i$ and $\langle v|_i = 1/Z_i$. Double occupancy $D$ and total particle number $N$ of the system are obtained by summing over all sites, e.g. $D = \sum_i \langle d|_i/N$, where the equation for $N$ is first solved numerically with respect to $z$. The entropy is $S = kT \sum_i \ln Z_i$. 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 (see methods). The fits in figure 2b involve $U$ as determined by modulation spectroscopy ($U/h = 4.7 \pm 0.1$ kHz and $6.1 \pm 0.1$ kHz) since band structure calculations disagree with the measured value by up to 30% for the largest scattering lengths.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Emergence of a gapped mode. With increasing interaction (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 shown in the bottom right panel is $\sum \Delta \nu \left[ D(\nu) - \frac{1}{2} (D(200 \text{ Hz}) + D(700 \text{ Hz})) \right]$, where $D(\nu)$ is the measured double occupancy at frequencies $\nu$ which are evenly spaced in steps of $\Delta \nu = 500 \text{ Hz}$. It is plotted in units of $12J/h$. The first four data points are taken for a lattice depth of $6.5ER$, the next at $7, 8$ and $10ER$, 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 4 to 8 identical measurements.}
\end{figure}

\begin{itemize}
\item These authors contributed equally to this work.
\item Mott, N. F. \textit{Metal Insulator Transitions} (Taylor and Francis, London, 1990).
\item Imada, M., Fujimori, A. & Tokura, Y. \textit{Metal-insulator transitions. Rev. Mod. Phys.} \textbf{70}, 1039-1263 (1998).
\item Lee, P. A., Nagaosa, N. & Wen, X.-G. Doping a Mott insulator: physics of high-temperature superconductivity. \textit{Rev. Mod. Phys.} \textbf{78}, 17-85 (2006).
\end{itemize}
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 E.U. projects Optical Lattices and Quantum Information (OLAQUI) and Scalable Quantum Computing with Light and Atoms (SCALA) and the Quantum Science and Technology (QST) project of ETH Zurich.

Author Information. Correspondence should be addressed to H. M. (mailto: moritz@phys.ethz.ch).
Methods

Preparation. After sympathetic cooling with $^{87}$Rb, $2 \times 10^6$ 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 Gauss. Using this mixture we realise 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 $|-9/2\rangle$ and $|-5/2\rangle$ states, close to a Feshbach resonance at 224.21 Gauss. 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 using 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% with respect to the single band model.

Radio-frequency spectroscopy. By increasing the depth of the optical lattice to $30 E_R$ 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 $h \times 99 \pm 1$ kHz and a weakly interacting state for a $|-9/2\rangle$, $|-5/2\rangle$ pair exists. 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 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. 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 from the 2D 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 $m_F t = -5/2$ ($-7/2$) 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. 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 $D$ due to $|-7/2\rangle$ 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 $T_1 = 0.15 T_F$ and $T_1 = 0.24 T_F$, respectively. Since we expect non-adiabatic heating to occur during the lattice ramp up as well as during ramp down, we use the mean value of 0.195 $T_F$ as a realistic estimate. With this, we calculate a temperature of $T = 0.28 T_F$ in the Mott insulating regime $(a = 810 a_0, V_0 = 12 E_R, N = 10^5)$, 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 $T_1$ and 11.5% for $T_F$. The reported temperatures represent upper limits, since we have achieved temperatures down to 0.08 $T_F$ in the dipole trap prior to loading. Due 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.