Compressibility of a fermionic Mott insulator of ultracold atoms

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We characterize the Mott insulating regime of a repulsively interacting Fermi gas of ultracold atoms in a three-dimensional optical lattice. We use in-situ imaging to extract the central density, and determine the local compressibility as a function of local density and interactions by making use of the variation of the chemical potential arising from the confining potential of the optical lattice. For strong interactions, we observe the emergence of a density plateau and a reduction of the compressibility at a density of one atom per site, consistent with the formation of a Mott insulator. Comparisons to numerical simulations of the Hubbard model set an upper limit for the compressibility at a density of one atom per site, consistent with the formation of a Mott insulator. Comparisons to numerical simulations of the Hubbard model set an upper limit for the compressibility at a density of one atom per site, consistent with the formation of a Mott insulator.

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The Hubbard model, which describes spin-1/2 fermions in a lattice with on-site interactions, is one of the fundamental models in quantum many-body physics. It is a notable example of how strongly correlated phases emerge from simple Hamiltonians: it exhibits a Mott insulating regime, antiferromagnetism, and is widely believed to support a d-wave superfluid state in two dimensions (2D), which could explain high-temperature superconductivity as observed in the cuprates [1]. Despite intense efforts, an exact solution of the Hubbard model in more than one dimension and for arbitrary filling has evaded theoretical and computational approaches to this day. Complementing these approaches, the last decade has seen the development of ultracold atoms in optical lattices [4]. Even though the temperatures required for pairing and superfluidity in the Hubbard model [5] have not yet been reached, the last decade has seen steady experimental progress. This includes the observation of Fermi surfaces in a band insulator [6], and the observation of the Mott insulating regime [7, 8]. For \( \mu = U/2 \), the average density of the system is \( n = 1 \) particle per lattice site (half-filling). As the temperature, \( T \), is reduced to \( T \ll U \), the system undergoes a smooth crossover to a Mott insulating regime, characterized by a suppression of the number of doubly occupied sites, a suppression of density fluctuations, and hence a reduction of the compressibility [9].

At even lower temperatures, below the Néel temperature \( T_N \) (\( \sim 4t^2/U \) for \( U \gg t \)), the system undergoes a phase transition to an antiferromagnetic (AFM) state. Recently, AFM spin correlations have been detected in 1D chains [10] [11] and in a 3D lattice [12], demonstrating close proximity to the AFM transition temperature and, in the latter work, also establishing Bragg scattering of light to measure spin correlations for thermometry [12] [13]. Although the AFM state has not yet been achieved, strongly interacting fermions exhibit a rich set of incompletely understood properties which begin to emerge at temperatures currently attainable, including pseudogap physics and a strange metallic phase. For reasonably large values of \( U/t \), the temperature scale of the Mott metal-insulator crossover is well above that of \( T_N \).

Realizations of the Hubbard model with ultracold atoms necessarily involve an overall confining potential and a finite number of particles. The presence of a trap,
which results in a spatially varying chemical potential, presents a challenge for the interpretation of bulk measurements of the system; on the other hand, it offers the possibility to characterize multiple regimes within a single cloud [14]. The local density approximation (LDA), which takes each site to be part of a uniform system with properly adjusted chemical potential, has been shown to agree well with numerical calculations of the inhomogeneous Hubbard Hamiltonian away from the quantum critical regime close to the Néel transition [15–17]. It predicts the appearance of a ‘wedding-cake’ density profile with incompressible plateaus at \( n = 1 \) and \( n = 2 \) particles per site, which correspond to the local formation of a Mott insulator and a band insulator, respectively [10].

Here we consider the local compressibility obtained from the LDA, by evaluating the conventional global compressibility on a uniform lattice with a matching density. If the trapping potential is well characterized, one can extract the local compressibility of the system from a measurement of the in-situ density profile, a procedure that has been previously demonstrated for a Fermi gas in a harmonic potential [13], and for lattice bosons [14]. The global compressibility in a sample of trapped lattice fermions with a Mott insulating domain has been studied previously by using the dependence of a bulk measurement of the double occupancy fraction on atom number [7, 19–20], and by studying the response of cloud radius to changes in external confinement [8]. In contrast, the measurements presented here use the local density and its first derivative to obtain the local compressibility. The local character allows differentiation between the incompressible Mott insulating core and the compressible surrounding metal.

The isothermal compressibility of a gas is defined as

\[
\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}. \tag{2}
\]

For atoms in a 3D lattice we consider the unitless quantity \((t/a^3)\kappa\), where \(a\) is the lattice spacing. In the limit of zero lattice depth, \( t \to -\frac{2\pi}{\hbar} \int_{-\pi/a}^{\pi/a} \frac{k^2}{2m} \exp[iaq] \, dq = (2/\pi^2)E_r\), where \( q \) is the quasimomentum, \( E_r = \frac{\hbar^2\pi^2}{2ma^2} \) is the recoil energy, and \( m \) is the mass of the particles. For a free gas with no interactions, the compressibility at zero temperature is given by \( \kappa_0 = \frac{1}{2\pi^2E_F} \), where \( E_F \) is the Fermi energy for each spin component. In this paper we consider the ratio \( \tilde{\kappa} \), defined as

\[
\tilde{\kappa} \equiv \frac{(t/a^3)\kappa}{(2E_r/(\pi^2a^3))\kappa_0} = \frac{(3\pi^2/2)^{2/3}}{2} \frac{\partial \tilde{n}^{2/3}}{\partial (\mu/t)}, \tag{3}
\]

where \( \tilde{n} = a^3n \).

In Fig. 1 we show theoretical results for \( \tilde{\kappa} \) at various values of \( T/t \) and \( U/t \), obtained using determinant quantum Monte Carlo (DQMC) [21–22], a numerical linked-cluster expansion (NLCE) [23–25] up to the eighth order in the site expansion, and a high temperature series expansion (HTSE) up to second order in \( T/t \) [24]. These three methods complement each other, and provide results over a wide range of interactions and temperatures. While NLCE can reach lower temperatures than DQMC at large \( U/t \), the opposite is true at weak coupling. Figure 1 shows that the theoretical compressibility diminishes at half-filling and larger \( U/t \) as the system enters the Mott insulating regime, and at \( n = 2 \), where a band insulator forms.

In our experiment, we produce a two-spin component degenerate Fermi gas of \(^6\text{Li} \) atoms in the \( |F = 1/2; m_F = \pm 1/2 \rangle \) and \( |F = 1/2; m_F = -1/2 \rangle \) hyperfine states, which we label \(|\uparrow\rangle \) and \(|\downarrow\rangle \), respectively. The apparatus has been described previously [12, 27]. Briefly, the spin mixture is evaporated into a harmonic dimple trap and then loaded into a simple cubic optical lattice. We control the total number of atoms, \( N \), by adjusting the final depth of the dimple trap. The temperature of the atoms in the dimple is measured by fitting the density distribution after time of flight. We obtain \( T/T_F = 0.04 \pm 0.02 \), independent of \( N \) within the range of atom numbers considered for this paper.

The optical lattice is formed by three retroreflected red-detuned (1064 nm) Gaussian laser beams of depth \( V_0 = 7E_r \). The lattice depth is calibrated via lattice phase modulation spectroscopy, up to a systematic uncertainty of \( \pm 5\% \). Due to the Gaussian beam profiles, the lattice depth decreases with distance from the center, which results in increasing \( t \) and decreasing \( U/t \). The lattice depth varies along the 111 body diagonals as \( V(r) = V_0 \exp[-4r^2/(3a_L^2)] \), where \( V_0 \) is the lattice depth at the center, \( r \) is the distance from the center.
and $w_L$ is the waist ($1/e^2$ radius) of the lattice beams. We make use of the broad Feshbach resonance in $^6$Li at 832 G \cite{28,29} to set the on-site interaction strength, $U$.

The lattice confinement is compensated by the addition of three blue-detuned (532 nm) Gaussian beams which overlap each of the lattice beams but are not themselves retroreflected \cite{12,30}. The overall confinement in the lattice, which sets the density of the cloud, is adjusted by changing the intensity of the compensation beams. We create samples which appear spherically symmetric with slight adjustment of the intensity of the three independent compensation beams. The average value of the compensation depth is set at 3.8 $E_r$, with a systematic ±10% relative error resulting from the calibration of $w_L$ and the compensation beam waists, $w_C$. The beam waists along each axis are calibrated by measuring the frequency of radial breathing mode oscillations \cite{31}. We find, up to a ±5% systematic uncertainty, the lattice beam waists to be $w_L = (47; 47; 44) \mu$m and the compensation beam waists to be $w_C = (42; 41; 40) \mu$m.

We measure the in-situ column density distribution of the atoms using polarization phase-contrast imaging \cite{32}. This technique can be used to image dense clouds, in contrast to absorption imaging which is limited to small optical densities due to saturation. The imaging light was detuned by -150 MHz from state $|\uparrow\rangle$ (-74 MHz from $|\downarrow\rangle$), keeping the phase shift across the cloud below $\pi/5$ to avoid significant dispersive distortions of the image.

Figure 2 shows azimuthal averages of the column density and density profiles; the latter are obtained from the former using the inverse Abel transform (which assumes spherical symmetry). The figure shows profiles for three different values of $U_0/t_0$ (where $U_0$ and $t_0$ denote the values of the Hubbard parameters at the center of the trap), compared with profiles calculated for our trap potential using the LDA. For the numerical calculations we set $T$ and the global chemical potential, $\mu_0$: local values of $U/t$, $T/t$, and $\mu/t$ are then calculated using the known trap potential. The local values of the calculated density are obtained by interpolation, from NLCE and DQMC results for a homogeneous system calculated in a $(U/t, T/t, \mu/t)$ grid. For $U/t \leq 8$, DQMC is to be used to obtain results down to temperatures $T \gtrsim T_N$ at arbitrary $\mu/t$. At large coupling, NLCE is used to obtain results down to $T/t = 0.4$. Because $T/t$ diminishes with $r$, the lowest value of $T/t_0$ calculated for the trap is limited to $T/t_0 = 0.6$.

We obtain the central density of the cloud by fitting the measured column density with the integral, $\int \tilde{n}(\rho, z) \, dz$, of a flat-topped Gaussian function

$$\tilde{n}(\rho, z) = \begin{cases} \tilde{n}_0 & \text{if } \rho^2 + z^2 < r_0^2 \\ \tilde{n}_0 \exp \left[ \frac{-(\rho^2 + z^2)}{\sigma^2} \right] & \text{otherwise} \end{cases},$$

where $\rho$ is the distance from the imaging axis, and the fit parameters are the central density, $\tilde{n}_0$, flat-top radius, $r_0$, and Gaussian $1/e$ radius of the cloud’s wings, $\sigma$.

The dependence of $\tilde{n}_0$ on atom number reflects changes in the compressibility of the cloud. In Fig. 3 we show $\tilde{n}_0$ for various interaction strengths. The symbols show the average for a set of 5 to 10 independent realizations, with error bars indicating the standard deviation. The shaded regions are the results of numerical calculations for our trap at $T/t_0 = 0.6$ (solid, green) and 2.4 (crosshatched, gray), with the width of each region corresponding to a ±14% systematic uncertainty in the value of $U_0/t_0$, arising from the ±5% uncertainty in $V_0$. The uncertainty in the calculated density becomes relatively insensitive to uncertainties in $U_0/t_0$ for the two larger values of $U_0/t_0$, which are deep in the Mott regime. For $T/t_0 = 0.6$ the total entropy per particle, $S/(Nk_B)$, is between 0.5 and 1.0 for the ranges of $N$ and $U_0/t_0$ shown in the figure. A temperature of $T/t_0 = 2.4$ is chosen for comparison, as $S/(Nk_B)$ in this case is between 1.5 and 2.4, which is similar to the range of 1.6 and 2.2 reported from the analysis of a previous experiment \cite{33}. 

![Figure 2](image1.png)  
**FIG. 2.** (color online) (a) Azimuthally averaged column density (including both spin states) vs. distance from the imaging axis $\rho$, for different values of $U_0/t_0$. Data points represent the average of eight individual realizations, with error bars corresponding to the standard deviation. The lines in (a) are obtained by integrating the density, calculated for $N = 2 \times 10^5$ atoms at $T/t_0 = 0.6$, along the imaging axis. (b) Data points correspond to density profiles extracted from the column densities using the inverse Abel transform, where $r$ is the distance from the center of the trap. The lines in (b) show the density calculated for our trap along a body diagonal of the lattice.

![Figure 3](image2.png)  
**FIG. 3.** (color online) Central density, $\tilde{n}_0$ vs. atom number for various interaction strengths. The symbols show the average for a set of 5 to 10 independent realizations, with error bars indicating the standard deviation. The shaded regions are the results of numerical calculations for our trap at $T/t_0 = 0.6$ (solid, green) and 2.4 (crosshatched, gray), with the width of each region corresponding to a ±14% systematic uncertainty in the value of $U_0/t_0$, arising from the ±5% uncertainty in $V_0$. The uncertainty in the calculated density becomes relatively insensitive to uncertainties in $U_0/t_0$ for the two larger values of $U_0/t_0$, which are deep in the Mott regime. For $T/t_0 = 0.6$ the total entropy per particle, $S/(Nk_B)$, is between 0.5 and 1.0 for the ranges of $N$ and $U_0/t_0$ shown in the figure. A temperature of $T/t_0 = 2.4$ is chosen for comparison, as $S/(Nk_B)$ in this case is between 1.5 and 2.4, which is similar to the range of 1.6 and 2.2 reported from the analysis of a previous experiment \cite{33}. 

$$\tilde{n}(\rho, z) = \begin{cases} \tilde{n}_0 & \text{if } \rho^2 + z^2 < r_0^2 \\ \tilde{n}_0 \exp \left[ \frac{-(\rho^2 + z^2)}{\sigma^2} \right] & \text{otherwise} \end{cases},$$

where $\rho$ is the distance from the imaging axis, and the fit parameters are the central density, $\tilde{n}_0$, flat-top radius, $r_0$, and Gaussian $1/e$ radius of the cloud’s wings, $\sigma$. The dependence of $\tilde{n}_0$ on atom number reflects changes in the compressibility of the cloud. In Fig. 3 we show $\tilde{n}_0$ for various interaction strengths. The symbols show the average for a set of 5 to 10 independent realizations, with error bars indicating the standard deviation. The shaded regions are the results of numerical calculations for our trap at $T/t_0 = 0.6$ (solid, green) and 2.4 (crosshatched, gray), with the width of each region corresponding to a ±14% systematic uncertainty in the value of $U_0/t_0$, arising from the ±5% uncertainty in $V_0$. The uncertainty in the calculated density becomes relatively insensitive to uncertainties in $U_0/t_0$ for the two larger values of $U_0/t_0$, which are deep in the Mott regime. For $T/t_0 = 0.6$ the total entropy per particle, $S/(Nk_B)$, is between 0.5 and 1.0 for the ranges of $N$ and $U_0/t_0$ shown in the figure. A temperature of $T/t_0 = 2.4$ is chosen for comparison, as $S/(Nk_B)$ in this case is between 1.5 and 2.4, which is similar to the range of 1.6 and 2.2 reported from the analysis of a previous experiment \cite{33}.
Figs. 3 and 4, respectively, show that the system enters profiles calculated at two different temperatures. A de-Mott insulator, is observed for $U/t_0$ shows $\tilde{\kappa}$ of $\tilde{\kappa}$ successive noise in the determination of the radial derivative. Abel transform are noisy at small radii, so, to avoid excessive noise in the moment of the column density, and the inverse. $p$ depends on the trap parameters. For the data, the azimuthal average of the column density, and the inverse numerical calculations are consistent with our previous measurements; hence, we obtain an upper bound to a moderate coupling, $U/t_0$ is indicative of the Mott insulating regime. Its persistence down to a moderate coupling, $U/t_0 = 11.1$, is indicative of the temperature being at or below the tunneling energy scale in the system, as revealed by comparison with the numerical calculations; hence, we obtain an upper bound $T/t_0 \lesssim 1.0$.

We obtain the local compressibility, $\tilde{\kappa}$, from the derivative of the measured and calculated density profiles as

$$\tilde{\kappa} = \frac{(3\pi^2)^{2/3}}{2} \frac{\partial \tilde{n}^{2/3}}{\partial r} \left( \frac{\partial (\mu/t)}{\partial r} \right)^{-1},$$

(5)

where the derivative of the local chemical potential depends on the trap parameters. For the data, the azimuthal average of the column density, and the inverse relaxation of the radial derivative of $\tilde{n}^{2/3}$, we restrict our analysis to $r/a > 12$. Figure 4 shows $\tilde{\kappa}$ vs $\tilde{n}$ for the experimental data and for density profiles calculated at two different temperatures. A decrease of the compressibility near $\tilde{n}$, as expected for a Mott insulator, is observed for $U_0/t_0 = 11.1$ and 14.5.

The central density and local compressibility, shown in Figs. 3 and 4, respectively, show that the system enters the Mott insulating regime for values of $U_0/t_0 \gtrsim 11$. The temperatures determined by comparing the data with numerical calculations are consistent with our previous measurement in the same system, $T/t_0 = 0.62^{+0.05}_{-0.03}$, obtained by measuring AFM correlations using Bragg scattering of light [12, 34]. Local compressibility, like the global double occupancy, is best suited for $T/t_0 \gtrsim 1$, where the entropy resides mainly in the “charge” degree of freedom, while Bragg scattering is sensitive to lower temperatures, where the majority of the entropy is in the spin sector.

We have shown that the local compressibility of a two-component Fermi gas in an optical lattice may be extracted from in-situ measurements of the column density. We have compared our measurements with DQMC and NLCE calculations obtained within the LDA. The data presented here shows Mott-insulating behavior for interaction strengths as low as $U_0/t_0 = 11$, close to where $T_N$ is expected to be maximal, and where AFM correlations were observed to be maximal for this system [12].

Measurements of local compressibility in an optical lattice, along with recently developed methods for detecting magnetic order, can improve our understanding of the onset of Mott insulating behavior in the Hubbard model and answer open questions about its proximity to the AFM phase in different coupling regimes. Measurements of the compressibility away from half-filling can also have important implications for the nature and extent of the non-Fermi liquid state of the 2D Hubbard model at relatively high temperatures [38]. Finally, as has been recently shown [39, 40], sharp signatures of phase separation and stripe formation are evident in the compressibility, raising the possibility that this central property of cuprate superconductors and of the Hubbard model might be accessible to this diagnostic.

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