Trapping and Cooling Fermionic Atoms into Mott and Néel States

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We perform a theoretical study of a fermionic gas with two hyperfine states confined to an optical lattice. We derive a generic state diagram as a function of interaction strength, particle number, and confining potential. We discuss the central density, the double occupancy, and their derivatives as probes for the Mott state, connecting our findings to the recent experiment of Jördens *et al.* [Nature (London) **455**, 204 (2008)]. Using entropic arguments we compare two different strategies to reach the antiferromagnetic state in the presence of a trapping potential.

Remarkable experimental progress has been made in handling and controlling quantum degenerate atomic gases. The confinement of these gases within optical lattices, and the use of Feshbach resonances allow for the investigation of strongly correlated quantum phases [1]. An outstanding example is the experimental study of the superfluid to Mott-insulator transition in bosonic gases [2]. A Mott-insulating state is characterized by the suppression of density fluctuations. Very recently, the observation of an incompressible Mott state has been reported in a fermionic gas using two hyperfine states of ^{40}K [3]. A future major step will be the observation of the antiferromagnetic ordering of the two hyperfine components in the lattice. However, whereas an incompressible Mott state is reached when the temperature is low enough as compared to the Mott gap, stabilizing a magnetically ordered state requires cooling down to a lower temperature scale set by the superexchange intersite coupling.

In this article, we address theoretically several issues which have immediate relevance to those experimental efforts. We establish a state diagram of cold fermions subject to an optical lattice and a trapping potential, as a function of the number of atoms and coupling strength. We discuss how to detect different states, by considering observables such as the fraction of doubly occupied sites, the local occupancy, and the compressibility at the center of the trap. Finally, we outline two possible strategies for adiabatically cooling the system into a long-range ordered antiferromagnet.

A quantum degenerate mixture of two hyperfine states of fermionic atoms can be described by a Hubbard-type Hamiltonian [4,5]:

$$H = -J \sum_{\langle j,j' \rangle, \sigma} (c^\dagger_{j,\sigma} c_{j',\sigma} + \text{H.c.}) + U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} - \mu_0 \sum_{j,\sigma} \hat{n}_{j,\sigma}$$
$$+ V_t \sum_{j,\sigma} (r_j/d)^2 \hat{n}_{j,\sigma}. \tag{1}$$

Here, $\sigma = \uparrow, \downarrow$ labels the two hyperfine states, j the sites of a three-dimensional (3D) cubic lattice, and $\langle j, j' \rangle$ neighbor-

ing sites. r_j is the distance between j and the center, d the lattice spacing, and μ_0 the chemical potential. We consider a mixture with equal number $N/2$ of $\uparrow$ and $\downarrow$ atoms. Experimentally the interaction parameter U and the hopping parameter J can be tuned independently changing the optical lattice height and using a Feshbach resonance. Note that the description by a one-band model is only valid for large enough lattice depth, small enough scattering length, and low temperatures, i.e., situations in which the higher bands and more complicated interaction or hopping terms can be neglected [4,6].

One important effect of the confining potential is to allow for the spatial coexistence of different quantum states [7,8]. For a 1D tube of fermionic atoms, a Mott-insulating phase next to a liquid phase was pointed out [9,10]. More recently, the stability of antiferromagnetically ordered regions has been investigated in a 2D system [11]. Helmes *et al.* [12] studied the coexistence of the liquid and insulating phases, in 3D, calculating, in particular, the density and momentum profiles and the local spectral function. In Fig. 1, we display a state diagram which summarizes the different possible shapes of the density profiles as a function of coupling strength and atom number at the temperature $k_B T/(6J) = 0.1$. All calculations in this Letter were obtained using a local density approximation (LDA), in combination with dynamical mean field theory (DMFT) [13,14] to simulate the homogeneous system in the paramagnetic state.

To compare different trapping energies and particle numbers, we use the scaled number of atoms $\rho = N(V_t/6J)^{3/2}$ (see Ref. [9] for 1D). Within LDA and the continuum limit, ρ entirely determines the shape of the density profile at a fixed interaction strength and temperature, allowing for a straightforward comparison to experimental setups. The state diagram in Fig. 1 displays four distinct regimes, labeled by (L), (Mc), (Ms), and (B). (L): For small interaction or small density, the whole system is in a (Fermi-) liquid phase. There, the density profile depends strongly on the trapping potential. (Mc): Above a
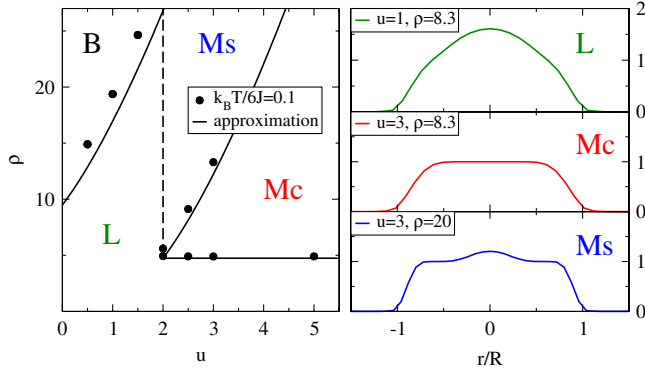
FIG. 1 (color online). Left panel: State diagram for fermionic atoms as a function of interaction strength $u \equiv U/(6J)$ and scaled particle number $\rho \equiv N(V_t/6J)^{3/2}$. Symbols show results of DMFT calculations. The boundaries of the region (Mc) with a Mott insulator in the center of the trap are defined from the constraint $|n_0 - 1| < 0.005$ on the central density. Lines are an analytical continuum approximation at $T = 0$. Right panel: typical density profiles for regions (L), (Mc), and (Ms), with the radius R set by $n(R) = 0.1$.

critical interaction strength $u \equiv U/(6J) \gtrsim 2$ and a characteristic density $\rho \gtrsim 5$ a Mott central plateau with $n \approx 1$ forms. A liquid phase surrounds this plateau. (Ms): When the particle number is further increased the pressure exerted by the trapping potential overwhelms the incompressibility of the Mott state. This leads to a state with a central occupancy larger than 1 particle per site surrounded by a Mott-insulating shell. (B): For even larger particle numbers a band-insulating plateau with $n = 2$ forms, surrounded by liquid and possibly Mott-insulating shells.

To detect the occurring quantum phases we investigated mainly two observables: the occupancy at the center of the trap n_0 and the fraction of atoms residing on doubly occupied sites $D = \frac{2}{N}\sum_j \langle n_{j\uparrow}n_{j\downarrow}\rangle$. D was measured by molecule formation in the experiments of Ref. [3]. The experimental observation of the density in a small central region is more involved. However, a lot of effort is currently devoted to the development of probes with good spatial resolution. To make contact with current experiments, we assume the slow experimental loading process [3] into the optical lattice to be adiabatic, and perform calculations at a fixed value of the entropy per particle, s [15]. The latter is related to the initial temperature of the noninteracting fermion gas in the absence of the lattice by $T_i/T_F = s/\pi^2 + O[(T_i/T_F)^3]$.

The first panel of Fig. 2 displays n_0 and D as a function of particle number at a fixed initial temperature $T_i/T_F = 1.0/\pi^2$. As we detail later on, a plateau in n_0 vs ρ provides a good indicator of the formation of an incompressible Mott-insulating region in the center of the trap. The three sets in Fig. 2 (first panel) correspond to different regimes of coupling. For weak interactions ($u \lesssim 1.5$), no plateau is present: n_0 smoothly increases and saturates at $n_0 \approx 2$ corresponding to the regimes (L) and (B). At intermediate coupling $u \gtrsim 2.5$, a Mott plateau starts forming ($\rho \approx 5$),
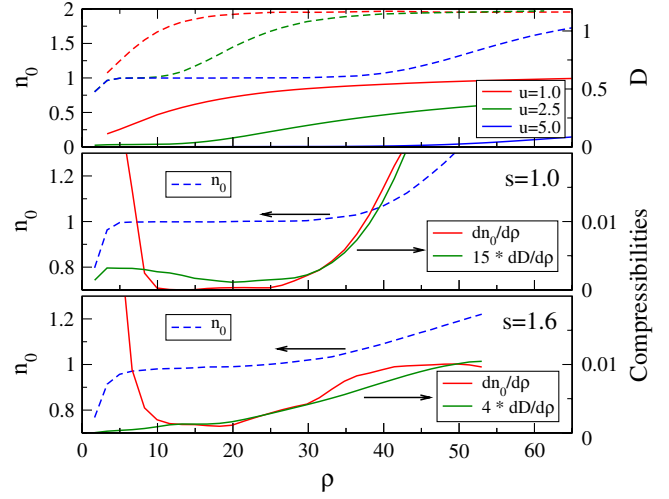

FIG. 2 (color online). First panel: Occupancy n_0 at the center of the trap and fraction D of atoms residing on doubly occupied sites versus the scaled particle number ρ at constant initial temperature $T_i/T_F = s/\pi^2 = 1.0/\pi^2$. The central occupancy n_0 and the "compressibilities" $\partial n_0/\partial\rho$ and $\partial D/\partial\rho$, for $u = 5$, at two different initial temperatures $T_i/T_F = 1.0/\pi^2$, $1.6/\pi^2$ are shown in the second and the third panel, respectively.

corresponding to regime (Mc). n_0 eventually deviates from unity as ρ is further increased into regime (Ms). With increasing coupling (cf. $u \gtrsim 5$), the central plateau broadens. From Fig. 2 (first panel), it is also clear that there is a qualitative correlation between the existence of a Mott central plateau and the behavior of D. At weak coupling, D just increases smoothly as ρ is increased. At stronger coupling, D remains very small for the low values of ρ, and starts raising approximately at the transition from the central incompressible regime (Mc) into regime (Ms).

We now make this correlation between D and n_0 more quantitative plotting in the lower panels of Fig. 2 the derivatives $\partial n_0/\partial\rho$ and $\partial D/\partial\rho$, for $u = 5$, at two different initial temperatures $T_i/T_F = 1.0/\pi^2$, $1.6/\pi^2$. In the LDA approximation, $\partial n_0/\partial\rho$ is directly proportional to the local compressibility at the center of the trap $\kappa_0 = \partial n_0/\partial\mu_0$, through: $\rho\partial n_0/\partial\rho = \kappa_0/\langle\kappa\rangle$. In this expression, $\langle\kappa\rangle$ is an average of the compressibility over the whole trap. The average $\langle\kappa\rangle$ is a nonsingular quantity since it always has sizable contributions from the liquid wings of the density profile. Hence, $\partial n_0/\partial\rho$ is a direct measure of the local incompressibility and its vanishing signals the Mott state. Indeed, it is seen from Fig. 2 (second panel) that, for the lowest temperature studied $T_i/T_F = 1.0/\pi^2$, this derivative is very small ($\lesssim 10^{-4}$) inside the (Mc) regime, and increases dramatically as one departs from a Mott insulator in the trap center. For the higher temperature $T_i/T_F = 1.6/\pi^2$ (Fig. 2, third panel), $\partial n_0/\partial\rho$ is only of order 10^{-3} in the rather narrow (Mc) regime, and increases less steeply as ρ is increased. In both cases, it is apparent from Fig. 2 that, remarkably, the dependence of $\partial D/\partial\rho$ on ρ is very similar to that of the "compressibility" $\partial n_0/\partial\rho$, for values of ρ in the (Mc) and (Ms) regimes. The reason for

this observation is that, despite being a global quantity over the whole trap, the double occupancy fraction remains very small in the boundary regions due to the low density. Therefore it is dominated by the central regions with occupancies $n \gtrsim 1$. Hence $\partial D/\partial \rho$ is small in regime (Mc) and increases sharply when the incompressibility at trap center is broken. At smaller values of ρ, these quantities are obviously very different: D is very small due to the low filling whereas $\partial n_0/\partial \rho$ is finite due to the liquid character of the state. Thus, we conclude that D and $\partial D/\partial \rho$ are rather good indicators of when the Mott state ceases to exist at trap center. This validates the use of these quantities as a diagnostic for a Mott-insulator region, as done in Ref. [3]. A closely related observation was made by Scarola *et al.* [16], who further supported it by showing that the compressibility $\partial n/\partial \mu$ is essentially identical to $\partial(D/N)/\partial \mu$ in the homogeneous system for $n \gtrsim 1$.

Comparing directly to the experimental results shown in Fig. 2 of Ref. [3], we find good agreement between the upturn of $D(\rho)$ in the experimental data for $U/6J = 4.8$ approximately at $\rho = 20$ and our theoretical results for $U/6J = 5$ (cf. Fig, 2). However, in this regime of coupling, the estimated lowest temperature in the experiments ($T_i/T_F \simeq 0.15$), while being at the onset of the incompressible Mott regime, still implies a sizable contribution of thermal excitations within the Mott gap (Fig. 2 third panel). In contrast, at lower temperature (second panel) a much flatter plateau and lower value of the compressibility are obtained. Obviously, a Mott plateau forms at even higher temperature for stronger interactions, but then equilibration times may become an issue.

A crucial point in experiments is to estimate the temperature of the interacting fermionic system in the presence of an optical lattice. For a confined noninteracting gas the double occupancy fraction has been used experimentally [17] as a thermometer since $D(T)$ *decreases* as the temperature is increased [18,19]. We find that the decrease of D with temperature persists throughout the weak and intermediate interaction regimes ($u \lesssim 1.5$, Fig. 3, lower panel). As in the noninteracting gas, the transfer of atoms from the trap center (cf. Fig. 3, upper panel) towards the trap boundaries, due to thermal fluctuations, causes this effect. It leads to a decrease of D which overwhelms the increase found in the high-T or large-U regime for the homogeneous system. Also, the Pomeranchuk effect [6,20] at low-T and intermediate U reinforces this trend. In contrast, for stronger interactions, D hardly changes with temperature ($u \lesssim 2.5$, Fig. 3) and ceases to be useful for thermometry because the density profile becomes almost frozen as the incompressible Mott state is approached.

One major step after observing the Mott regime will be the realization of the antiferromagnetically (AF) ordered phase, which occurs at a still lower temperature T_N (Néel temperature). We now discuss two possible strategies to reach this phase. (a) A first possibility is to work at intermediate coupling ($u \simeq 2.5$), for which T_N is the largest. (For possible ways of increasing T_N further, see [21]). The
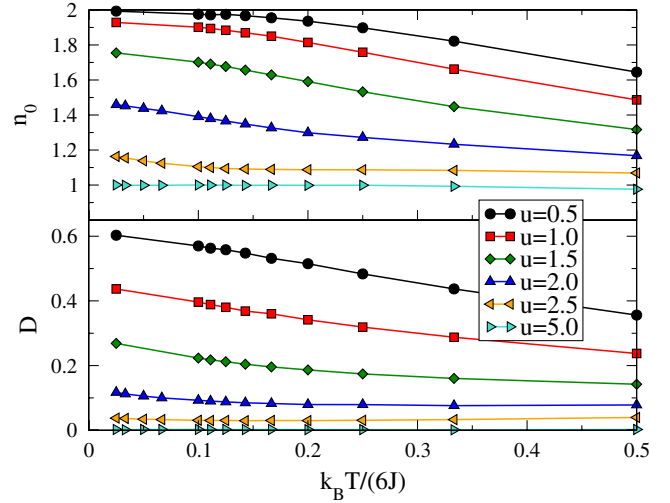

FIG. 3 (color online). Upper panel: Central occupancy n_0 versus temperature for different interaction strengths. Lower panel: double occupancy D versus temperature. ($\rho \approx 13.3$).

drawback of this strategy is that a sizable Mott-insulating region can only be stabilized within a narrow range of particle numbers [cf. Fig. 1]. (b) The second possibility is to work at stronger coupling (e.g., $u \simeq 5$) so that a Mott region can be stabilized over a much wider range of particle numbers (Fig. 1). Since $T_N \propto J^2/U$ at large U, this requires cooling the gas down to very low temperatures. However, assuming an adiabatic evolution, the entropy per particle at which the ordering takes place, $s(T_N)$, is the key quantity to focus on, rather than the absolute temperature T_N. In Ref. [6], it was pointed out that, for the homogeneous half-filled system, $s_h(T_N)$ reaches a *finite* value in the strong-coupling limit, even though T_N is very small in this limit. Here, we compare the initial temperatures T_i/T_F needed to reach the AF ordered state for the two strategies (a) and (b), in the presence of the trapping potential [22].

Once an incompressible Mott region is formed in the center of the trap, the entropy is the sum of two contributions: one from the liquid wings of the density profile, and one from the central Mott region. The entropy of the Fermi-liquid fraction is linearly increasing with temperature, below some characteristic coherence temperature (which is larger at low density and smaller for densities close to 1 particle per site). By contrast, the entropy in the Mott state remains almost constant upon cooling.

At intermediate coupling (a), the contribution of the liquid wings dominates over that of the central Mott region in the whole temperature range above T_N (Fig. 4, left panel). This is because the fraction of atoms in the central region is rather small ($\sim 30\%$) and T_N in this regime is high enough such that part of the wings have not yet reached Fermi-liquid coherence. Hence, strategy (a) can benefit from the high entropic contributions of the liquid wings. The lowest temperature displayed in Fig. 4 is close to T_N at $u = 2.5$. The entropy per particle which must be reached is
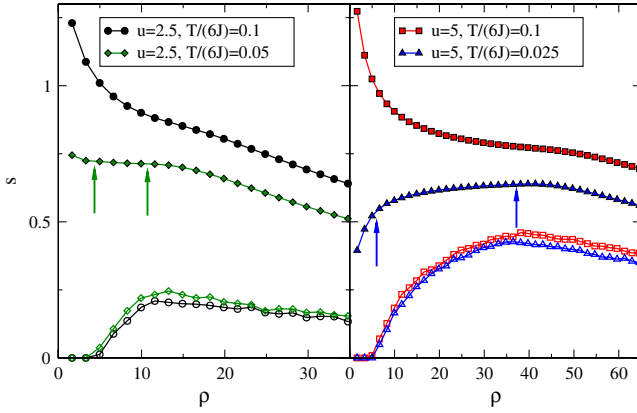
FIG. 4 (color online).   Entropy per particle s of the total system (solid symbols) and the Mott region (open symbols) versus characteristic density ρ. The lowest T is chosen slightly above the Néel temperature and the arrows delimit the density range where a central Mott plateau is formed.

of order $s \simeq 0.67$ (taking $\rho \simeq 5$–10 where a Mott central region is stabilized). This corresponds to an initial temperature $T_i/T_F \simeq 0.07$.

For stronger interaction (b), the density profile is dominated by a wide Mott-insulating region, for a large range of particle numbers. The entropy of this region gives a major contribution to the total entropy already at relatively large temperatures ($\sim 50\%$ at $k_B T/6J = 0.1$ as shown in Fig. 4, right panel) and it does not change much upon cooling. In contrast, the contribution of the liquid wings decreases strongly and eventually becomes very small (30% at $k_B T/6J = 0.025$). In this regime, DMFT yields a value of the entropy per particle of order 0.6 near T_N, comparable to strategy (a) above. However, DMFT overestimates the entropy of the Mott state. We propose a lower bound on the entropy at T_N by neglecting the contribution of the liquid wings, and considering only that of the Mott region. This leads to the estimate $s = s_h(T_N)N_c/N$. Using a typical value $N_c/N = \frac{2}{3}$ for the fraction of atoms in the central Mott region, and the entropy per particle of the homogeneous Mott state at T_N, $s_h(T_N) \approx \ln2/2$ (as estimated from fluctuation effects in the Heisenberg model [6], see also [23]), we obtain $s \simeq 0.2$. This corresponds to an initial cooling down to $T_i/T_F \simeq 0.02$ to reach AF ordering. We view this estimate as a pessimistic lower bound.

To summarize we established a state diagram of cold fermions in an optical lattice and a trapping potential. We further showed how to detect the Mott-insulating state using the central density, the fraction of doubly occupied sites, and their derivatives. The latter were shown to be related to the compressibility at the center of the trap. We found that the double occupancy is well suited for thermometry in the lattice at weak and intermediate coupling, but not at strong coupling. Finally, we compared two strategies for adiabatically cooling into a long-range ordered antiferromagnet. The intermediate coupling route (a) is somewhat more favorable from the cooling point of

view. By contrast the stronger coupling route (b) is more favorable in terms of the number of atoms and extension of the Mott plateau, while the corresponding ordering temperatures may still be reachable.

Note added in proofs.—After the completion of this work also Schneider [24] reported the observation of an incompressible Mott state.

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