Mott transition of fermionic atoms in a three-dimensional optical trap

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We study theoretically the Mott metal-insulator transition for a system of fermionic atoms confined in a three-dimensional optical lattice and a harmonic trap. We describe an inhomogeneous system of several thousand sites using an adaptation of dynamical mean field theory solved efficiently with the numerical renormalization group method. Above a critical value of the on-site interaction, a Mott-insulating phase appears in the system. We investigate signatures of the Mott phase in the density profile and in time-of-flight experiments.

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Introduction: Ultracold atoms in optical lattices offer exciting possibilities to investigate many-particle effects and to realize and measure models of condensed matter physics like the Hubbard model with unprecedented control of the band structure and interaction strength.

One of the most dramatic effects of strong correlations is the Mott transition, where strong interactions drive a system insulating. While for bosonic atoms the Mott transition in an optical lattice has been realized a few years ago by Greiner et al.,\cite{Greiner02}, the corresponding experiment for fermionic systems turns out to be much more difficult, partially due to problems with cooling and due to the need to work with two fermionic species to model the spin degree of freedom. However, due to the enormous experimental progress, a realization of the Mott transition in fermionic systems is expected in the near future. For example, recently Köhl et al.\cite{Kohl08} succeeded to capture a single species of fermions in an optical lattice and to observe the Fermi surface. Also two species of fermions have been successfully trapped and cooled down in a series of experiments studying e.g. the BEC-BCS crossover\cite{Greiner03}.

For the interpretation of the experiments it is essential to investigate the effects of the smooth external confining potential holding the atoms in the trap. The resulting inhomogeneities can make it more difficult to interpret the experiments, but induce also new interesting effects, e.g. associated to the sharp surface between metallic and insulating regions. A frequently used approximation (e.g. in the present context by Ref.\cite{Buechler08}) is to describe the trapped atoms locally by a homogeneous system as in the local density approximation. However, in the presence of sharp domain walls between two phases, such an approximation is expected to fail and a more realistic treatment of the inhomogeneous system is necessary.

For one-dimensional (1D) systems, powerful numerical and analytical methods exists to study theoretically the Mott transition in fermionic systems. For example, in Refs.\cite{Kollath05,McGuire04} quantum Monte Carlo techniques were used to investigate the signatures of Mott phases in the presence of an external harmonic confinement potential for a 1D system. Rigol et al.\cite{Rigol08,Gring08} argued, that in one dimension the inhomogeneities resulting from the trapping potential essentially destroy the main signatures of Mott phases in time-of-flight experiments.

As exact numerical methods for fermions can only be applied to very small systems, one has to resort to approximations to calculate the properties of three dimensional lattices of realistic size. Here the method of choice is the so-called dynamical mean field theory (DMFT).\cite{Georges96,Kotliar06} Within DMFT, the only approximation is to neglect non-local contributions to the self-energy. This allows to map the N site lattice problems to N single-impurity Anderson models coupled by a self-consistency condition, see discussion below. DMFT is, for example, frequently used to describe complex bulk materials, e.g. by combining DMFT with band-structure calculations to obtain an ab-inito description of strongly correlated materials. In a few cases, DMFT has been employed to describe inhomogeneous systems\cite{Kollath05,Bohnet06,Leininger07} like the surface of Mott insulators\cite{Buechler08} or disordered materials\cite{Bohnet06}.

A main problem of DMFT is the need for an reliable and efficient method to solve the effective impurity problems. Previous applications of DMFT to inhomogeneous systems were using impurity solvers like a two-site approximation\cite{Bohnet06} or slave-boson mean-field theory\cite{Bohnet06}, implying severe further approximations, or started from simplified fermionic models such as the Falicov-Kimball model\cite{Falicov71}. We will show that one can also use efficiently one of the most accurate impurity solvers, the numerical renormalization group\cite{Wilson82,White92} (NRG), to obtain reliable results for traps containing several thousand atoms modeling a fermionic Hubbard model.

After introducing the model and our method (DMFT for inhomogeneous systems-NRG), we will show the resulting spectral functions and discuss how the transition from a metal to a Mott insulating phase can be seen in real-space and time-of-flight experiments. We investigate the role of temperature, filling and interaction strength.

Model and Method: We consider the fermionic Hub
where \( c_{i\sigma}^+ \) creates a fermion at site \( i \) with spin \( \sigma \), \( n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \) is the local density, \( J \) is the nearest-neighbor tunneling matrix element, and \( U \) the effective on-site interaction. The resulting Anderson impurity model is defined by the local self-energy \( \Sigma_i(\omega) \) (see below). From the \( \Sigma_i(\omega) \), one can construct the lattice Green’s function

\[
G_{\text{lat}}^{-1}(\omega)_{ij} = \delta_{ij} \left( \omega + \Sigma_i(\omega) - V_0 r_i^2 \right) - J_{ij},
\]

where \( J_{ij} = J \) if sites \( i \) and \( j \) are nearest neighbors and 0 otherwise. The bath of each impurity is then determined from the requirement that at each site the lattice Green’s function and the Green’s function of the impurity model coincide,

\[
G_{\text{lat}}(\omega)_{ii} = \left[ G_{\text{And},i}(\omega)^{-1} - \Sigma_i(\omega) \right]^{-1},
\]

thus establishing a self-consistency loop. The scheme described above scheme can be derived using as the only approximation that the self-energy is a local quantity. Both the non-local single particle quantum mechanics of fermions and all local effects of strong interactions are correctly described within DMFT.

A main difficulty of DMFT is, however, an accurate calculation of the self-energy of the Anderson impurity model. For this we use the NRG [18], see Ref. [16] for a description of the method. To obtain efficiently \( G_{\text{lat}} \) from an inversion of Eq. 2 it is essential to use the full symmetry of the cubic lattice.

In this paper we restrict ourselves to paramagnetic solutions which simplifies the rather challenging numerics considerably. Also experimentally, it is very difficult to reach the low temperatures below which magnetism is expected. Furthermore, we do not expect that magnetic order will change the density profiles or time-of-flight pictures considerably.

Results: Fig. 1 shows how the number of fermions per site evolves for increasing interactions \( U/J \), which push the fermions away from the center of the trap. For the chosen parameters, we obtain for \( U/D = 0, 1, 2 \) (\( D = 6J \) is half the bandwidth) a band insulator in the center of the trap and a metal further outside. For the homogeneous system the critical interaction is given by \( U_c/D = 2.52 \), but already for \( U/D = 2 \) the compressibility close to half-filling is strongly reduced as can be seen in a shoulder in the curve for \( \langle n_i \rangle \approx 1 \). For
When the Fermi energy starts to merge with one of the Hubbard bands with equal weight and projection, the Fermi function and we have normalized $n_k$ such that

$$\int n_k \frac{d^2k}{(2\pi)^2} = \int n^\text{tot}_k \frac{d^2k}{(2\pi)^2} = 1.$$  

FIG. 4: (color online) $n_k$ (left panel) and $n^\text{tot}_k$ (right panel) for $k = \pi/10(n_x, n_y, n_z)$, $n_{x,y,z} = -10, \ldots, 10$, plotted as a function of $\epsilon_k = -2J(\cos k_x + \cos k_y)$, respectively, for different values of $U$, $N$ and $T$ (upper, middle and lower panels, respectively). For a given value of $\epsilon_k$ a range of values of $n(\epsilon_k)$ exists. Nevertheless, each curve collapses to a single line in good approximation. Inset: $\Delta n = n_{0,0,0} - n_{\pi,\pi,\pi}$ (and $\Delta n^\text{tot} = n^\text{tot}_{0,0,0} - n^\text{tot}_{\pi,\pi,\pi}$) as a function of $U$. $\Delta n$ and $\Delta n^\text{tot}$ are largest for the predominantly metallic phases and smallest for phases with a large band- (small $U$) or Mott-insulating (large $U$) regions.

$U/D \geq 3$ the incompressibility of the Mott insulating state, $\partial n/\partial U = 0$, manifests itself in a plateau. The thickness of this Mott insulating ‘onion shell’ increases for increasing $U$ eliminating the metallic phase in the center for $U/D = 4.5$. The insets of Fig. 1 show how the Mott insulating region at $U/D = 4.5$ shrinks again when the number of fermions in the trap is reduced and how thermal excitations destroy the Mott plateau.

Our method allows to study the spatial dependence of the spectral functions. While this quantity is difficult to measure for atoms in a trap, it is a highly sensitive probe of the metal-insulator transition. Fig. 2 shows how the local spectral function evolves when moving from the center to the edge of the trap at $U/D = 4.5$. In the insulating regime, the spectral function $A(\omega)$ is characterized by the two Hubbard bands with equal weight and $A(\omega = 0)$ becomes very small (it never vanishes exactly as atoms from the metallic regions can tunnel into the insulator). As a function of the distance from the center, the Hubbard bands shift due to the harmonic potential.

In a time-of-flight experiment, the two-dimensional projection, $n^\text{tot}_k = \int n_k dk_z/(2\pi)$, of the three-dimensional momentum distribution

$$n_k = -\frac{1}{N} \sum_{i,j} \int \frac{d\omega}{\pi} f(\omega) e^{i(kr_i - r_j)} \text{Im} G_{ij}(\omega)$$

of the fermions can be measured. Here $f(\omega)$ is the Fermi function and we have normalized $n_k$ such that $\int n_k \frac{d^2k}{(2\pi)^2} = \int n^\text{tot}_k \frac{d^2k}{(2\pi)^2} = 1$.

FIG. 3: (color online) Momentum distribution $n^\text{tot}_k$ for $U/D = 0, 2, 3, 4.5$. Both in the predominantly band-insulating phase ($U/D = 0$) and Mott insulating phase ($U/D = 4.5$) the curves are considerably flatter than for $U/D = 2, 3$ where most fermions are in the metallic phase.
mentum varies smoothly within the trap, all jumps are smeared out. However, the slope of $n(c_k)$ or the difference $\Delta n^{tot} = n^{tot}_{0,0} - n^{tot}_{\pi,\pi}$ is still a good measure of how metallic or insulating the system is. The inset of Fig. 4 describes the evolution from a mainly band-insulating via a dominantly metallic to a Mott insulating regime when $U/D$ is increased. Similarly, the middle panel of Fig. 4 shows how $\Delta n^{tot}$ increases when at large $U/D$ the number of particles and therefore the size of the Mott insulating region is reduced (compare with upper inset of Fig. 1). For increasing temperature (lower panel of Fig. 4) the destruction of quantum coherence leads to a flattening of $n^{tot}_k$. Note that $n^{tot}_k$ is more sensitive to changes of $T$ compared to $\langle n_k \rangle$, see Fig. 1.

Conclusions: In this paper we investigated the signatures of the Mott transition of fermions in an optical trap using a local approximation to the self energy (space-resolved DMFT+NRG) which allows to treat several thousand atoms. The clearest signature of a Mott phase is a plateau in the density profile $n(r)$ of the atoms, see Fig. 4. These plateaus are, however, washed out if only the column density, $\int dz n(r)$, which can be measured directly, is considered (not shown). The Mott transition is more difficult to observe in a time-of-flight experiment. However, the insets of Fig. 4 show that a characteristic flattening of $n^{tot}_k$ can be seen when a large fraction of the trap becomes a band or Mott insulator.

Our calculations did not rely on a local density approximation (LDA) which allows us to investigate whether this widely used approximation is valid in the present context. It turns out that both density profiles and TOF experiments are rather well described by LDA. As discussed in the introduction, LDA is expected not to be valid close to a sharp domain boundary. Indeed, Fig. 5 shows that the LDA fails completely to describe the low-energy excitation spectrum at the boundary of the Mott insulating region. The coherence peak at the Fermi energy arises due to the penetration of the metallic phase into the Mott insulator via the Kondo effect.

For the future it will be interesting to investigate the effects of magnetism. In systems with a population imbalance we expect that the majority spin will accumulate in the Mott insulating regions. These effects will be studied in a forthcoming publication.

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