Preparing a highly degenerate Fermi gas in an optical lattice

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We propose a method to prepare a sample of fermionic atoms in a three-dimensional (3D) optical lattice at unprecedentedly low temperatures and uniform filling factors. The process involves adiabatic loading of atoms into multiple energy bands of an optical lattice followed by a filtering stage whereby atoms from all but the ground band are removed. Of critical importance is the use of a non-harmonic trapping potential, taken here to be the radial profile of a high-order Laguerre-Gaussian laser beam, to provide external confinement for the atoms. For realistic experimental parameters, this procedure should produce samples with temperatures \( \sim 10^{-3} \) of the Fermi temperature. This would allow the investigation of the low-temperature phase diagram of the Fermi-Hubbard model as well as the initialization of a high-fidelity quantum register.

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Investigations of degenerate Fermi gases loaded into optical lattices have indicated that these systems are ideal for creating a robust quantum register for quantum computing applications [1, 2] as well as providing a testing ground for paradigm models of condensed matter physics. Models currently under investigation include studying Fermi surfaces and band insulator states [3], fermionic superfluidity in a lattice [4], and transport properties of interacting fermions in one and three dimensional optical lattices [3, 4]. These seminal experiments demonstrate the high precision and versatility available in simulating solid state systems with fermions in optical lattices.

Theoretical studies of such systems have predicted that a number of exotic phases emerge at low temperatures, including quantum magnetic ordering and possibly d-wave superfluidity [4, 8]. However, temperatures low enough to observe exotic phases such as these are difficult to achieve when optical lattices are loaded with a harmonic external confining potential. It has been theoretically predicted [3] and experimentally observed [3] that fermions adiabatically loaded into an optical lattice with harmonic external confinement experience heating for all but very high initial temperatures and filling factors (number of atoms per lattice site) [10].

Alternative methods to prepare fermionic atoms in optical lattices at low temperatures and/or high uniform filling factors include: cooling by adiabatic loading into a three-dimensional (3D) homogeneous trapping potential with high filling factor [11], defect filtering in a state dependent optical lattice [1], adiabatic loading [2] and filtering [12] of high entropy atoms from a 1D lattice with harmonic confinement.

In this Letter, we propose a method to prepare a highly degenerate Fermi gas in a 3D optical lattice using a box-like potential for external confinement and taking advantage of the Pauli exclusion principle to selectively remove atoms from multiply-occupied lattice sites. Specifically, we assume that the radial profile of a blue-detuned, high-order Laguerre-Gaussian (LG) laser beam provides confinement along each cartesian axis. The atoms are prepared via a two step process: (1) adiabatically loading atoms initially confined in the LG trap into a superimposed optical lattice, followed by (2) irreversibly filtering atoms from all but the ground energy band. Amplitude modulation of the lattice potential can selectively transfer these atoms to high-lying bands via a two-photon transition where they then tunnel out of the region. Dramatic cooling results when the Fermi energy (prior to filtering) lies within the second band.
Blakie demonstrated that this energy band structure can be exploited to dramatically increase the degeneracy of the sample for a homogeneous system [11]. For a dense atomic gas, with a filling factor greater than unity, application of the lattice increases the Fermi energy, since it lies within the first excited band, and compresses the Fermi surface resulting in a dramatic reduction in the degeneracy temperature $T/T_F$, where $T_F$ is the Fermi temperature.

This band structure also permits state-selective operations to manipulate and probe the energy distribution of the sample. One such method involves modulating the depth of the optical lattice to selectively excite atoms from the $n$ to $n + 2$ energy band with no change in the crystal momentum $q$ [13]. In contrast to non-interacting Bose systems, where a single $q$ can be macroscopically occupied, a Fermi system necessarily begins to fill all the bottom band and $\Delta q = 0$ transitions must be excited for all occupied values of $q$. In Fig. 2(b), we show band excitation energies as a function of lattice depth for $n = 1 \rightarrow 3$ and $n = 2 \rightarrow 4$ transitions spanning all $q$ within a Brillouin zone. By loading the sample into an optical lattice with a depth of $V_0 = 5E_R$ (where $E_R = \hbar^2 k^2/2m$ is the recoil energy and $k$ is the wavenumber of the laser light), we find that these transitions are well resolved. It is therefore possible to apply a filtering process which selectively removes atoms from all but the ground energy band. Using adiabatic rapid passage, population may be selectively transferred from $n = 2 \rightarrow 4$ by sweeping the amplitude modulation frequency from below to above all $2 \rightarrow 4$ transition frequencies while remaining below the lowest $1 \rightarrow 3$ transition frequency. Then, lowering the height of the trapping potential allows atoms in the third and higher energy bands to tunnel out of the system.

In order to experimentally approximate the homogeneous lattice potential described above, we consider the addition of a box-like external potential produced by a blue-detuned, $\ell^{th}$-order, LG laser beam with a radial profile

$$V_{LG}(r) = V_{peak} \left( \frac{2e \ell^2 \ell}{w_0^4 \ell} \right) e^{-2r^2/w_0^2}$$

at the beam waist $w_0$. For a given charge $\ell$, the peak value $V_{peak}$ of the potential occurs at $r_{max} = w_0 \sqrt{\ell/2}$ and the width of this peak decreases with decreasing $w_0$. Therefore, for a given trap size $r_{max}$, the LG profile more closely approximates a box potential when $w_0$ is reduced and $\ell$ is correspondingly increased. Trapping of ultracold gases has been demonstrated in single or crossed beam configurations of LG beams up to $\ell = 16$ [14, 15, 16].

Along a given cartesian axis, we take the single particle Hamiltonian to be

$$H(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{LG}(x)$$

$$+ V_0 \cos^2(kx + \phi_x) + \frac{1}{2}m\omega^2x^2,$$

where the third term represents a lattice potential of depth $V_0$ and phase offset $\phi_x$. We also include a harmonic term that arises if red-detuned Gaussian beams are used to produce the lattice potential; in this case $\omega \propto \sqrt{V_0}$. The 1D eigenvalues and eigenfunctions for a given depth of the optical lattice are calculated by numerically diagonalizing the Hamiltonian (Eq. 2) using the method described in [17]. For sufficiently shallow lattice depths, the low energy eigenstates are delocalized and closely approximate Bloch states in the first band of a homogeneous system. However, higher energy states are either localized at the edges of the trap (i.e. near $x = r_{max}$) or delocalized and correspond to Bloch states in higher bands. While a band structure picture is not strictly valid for this inhomogeneous system, we classify the set of eigenfunctions without nodes to constitute the first band, $\epsilon_{1\text{band},n}$.

We extend this model to three dimensions by assuming a separable Hamiltonian $H_{3D} = H(x) + H(y) + H(z)$. For simplicity, we assume equal lattice depths in each direction. The 3D spectrum ($E_m$) for a given depth of the optical lattice is then generated by calculating all possible combinations of the sum $E_m = \epsilon_i + \epsilon_j + \epsilon_k$ for all values of the 1D eigenenergies ($\epsilon_p$) in each spatial direction. The 3D energy spectrum for energy states in the first band of the optical lattice is calculated in a similar manner ($E_{1\text{band},m} = \epsilon_{1\text{band},i} + \epsilon_{1\text{band},j} + \epsilon_{1\text{band},k}$).

In calculating thermodynamic quantities during the proposed cooling method, we assume constant thermal equilibrium before and after the selective removal of atoms from high-lying bands. Equilibrium is maintained by elastic collisions in a 50/50 mixture of spin-1/2 fermions and changes in the trapping potential are adiabatic with respect to the rethermalization time scale.

**FIG. 2:** (color online) (a) Band structure for a $5E_R$ deep lattice. (b) Atoms can be selectively excited from the $n$ to $n + 2$ energy band by modulating the amplitude of the optical lattice light. The excitation energy between bands 1 and 3 (blue) and 2 and 4 (red) for fermions in all crystal momenta states are shown. As the depth of the optical lattice approaches $35E_R$, the excitation energy bands separate, and higher energy states tunnel out of the system. In Fig. 2(b), we show band excitation energies as a function of lattice depth for all values of $\ell$. The 1D eigenvalues and eigenfunctions for a given depth of the optical lattice are calculated by numerically diagonalizing the Hamiltonian (Eq. 2) using the method described in [17]. For sufficiently shallow lattice depths, the low energy eigenstates are delocalized and closely approximate Bloch states in the first band of a homogeneous system. However, higher energy states are either localized at the edges of the trap (i.e. near $x = r_{max}$) or delocalized and correspond to Bloch states in higher bands. While a band structure picture is not strictly valid for this inhomogeneous system, we classify the set of eigenfunctions without nodes to constitute the first band, $\epsilon_{1\text{band},n}$.
However, we also assume that the interactions are weak enough to not significantly modify the single-particle energy spectrum, $E_m$. We therefore use $E_m$ when calculating the following quantities:

\[ N = 2 \sum_{m} \frac{1}{1 + \exp[(E_m - \mu) / k_B T]} \]

\[ E = 2 \sum_{m} \frac{E_m}{1 + \exp[(E_m - \mu) / k_B T]} \]

\[ S = \frac{k_B}{2} \sum_{m} \ln[1 + \exp((E_m - \mu) / k_B T)] + \frac{E}{k_B T} - \frac{\mu}{k_B T} N, \]

where $T$ is the temperature, $\mu$ is the chemical potential of an atom in either spin state, $N$ is the total number of atoms, $E$ is the total energy in the system, and $S$ is the total entropy. The degeneracy temperature is given by $T / T_F$ where $k_B T_F = E_N$, the energy of the $N^{th}$ eigenstate of the multi-band, 3D spectrum. After filtering, the thermodynamic quantities in Eq. 3 are calculated for atoms only in the first band using $E_{1, \text{band}, m}$.

Our proposed method for cooling the atoms is comprised of (1) an adiabatic increase in the lattice depth starting from zero, (2) a non-adiabatic selective filtering of atoms and (3) an optional adiabatic change to a final lattice depth. To calculate changes in thermodynamic quantities during these stages we use the following procedures. For adiabatic changes of the potential we (1) calculate $S$ for a given $N$ and initial temperature $T_i$ using the energy spectrum for the initial potential and (2) numerically solve for $\mu_i$ and the final temperature $T_f$ in Eq. 3 using the spectrum for the final potential, assuming $N$ and $S$ are conserved. In contrast, for the selective filtering stage we (1) start from a thermalized sample of $N_f$ atoms at temperature $T_i$ for a given spectrum, (2) calculate, given this distribution, the energy $E_i$ and number $N_f$ for atoms restricted to the first band, and (3) solve for $\mu_i$ and the temperature $T_i$ in Eq. 3 using the multi-band energy spectrum assuming the sample equilibrates with total energy $E_i$ and number $N_i$.

We consider a 50/50 spin mixture of $^6$Li atoms initially trapped in a LG trapping potential with $\ell = 12$, $V_{\text{peak}} = 35 E_R$ and $r_{\text{max}} = 13.5 \mu m$. For reasonable lattice beam properties ($k = 2\pi/1064 \text{nm}$ and a waist of 200 $\mu m$) we find $\omega = 2\pi (586 \text{Hz})$ for the final lattice depth $V_{0, \ell} = 35 E_R$. The final degeneracy temperatures after adiabatic loading and filtering, along with the final atom number are shown in Fig. 3 for various initial degeneracy temperatures and sample sizes. In each case $\phi_x = \phi_y = \phi_z = 0$. This data shows that the thermodynamic properties of the system are highly dependent on the initial filling factor and can be separated into two distinct regions A and B. The vertical dashed line which separates the regions represents the number of atoms at which the Fermi energy enters the second band.

In region A, the Fermi energy before filtering lies below the second energy band. For very low filling factors, an increase in $T / T_F$ is observed for all initial temperatures. This increase in $T / T_F$ occurs because $T_F$ decreases more than $T$ as the lattice depth increases. Additionally, Fig. 3(b) demonstrates that we are not significantly filtering atoms for low initial temperatures. As the Fermi energy approaches the second energy band, we see a dramatic decrease in the final $T / T_F$. In this regime, where atoms are beginning to significantly occupy the localized energy states at the edge of the trapping potential, a dramatic increase of the Fermi energy is observed.

In region B, the density is such that the Fermi energy before filtering lies within the second band. In this region the adiabatic increase of the lattice depth results in a dramatic increase in $T_F$, a substantial reduction in the temperature $T$ [11], and allows for a significant reduction in entropy during the filtering stage. We find that significant cooling is achieved for initial temperatures in the vicinity of $T_i = 0.1 T_F$. Above this initial temperature cooling is less efficient. Below this initial tempera-

![FIG. 3: (color online) As a function of initial atom number we report (a) the final degeneracy temperature and (b) the final atom number after implementing the proposed cooling and filtering procedure for various initial temperatures between 0.005 and 0.3 $T_F$. The vertical dashed line represents the number of atoms for which the Fermi energy enters the second band. The trap and lattice parameters are as described in the text.](image-url)
ture, the final $T/T_F$ after filtering saturates. As can be seen in Fig. 3(b), $N_f$ is extremely insensitive to fluctuations in $N_i$ for low initial temperatures. For example, at $T_i = 0.05 T_F$, a variation of $\pm 10\%$ around $N_i = 1.6 \times 10^5$ yields a variation of only $+0.09\% / -0.2\%$ in $N_f$.

The cooling efficiency and number filtering were dependent on the choice of phases $\phi_x$, $\phi_y$, and $\phi_z$ due to the sensitive effect these phases had on the the location of localized edge state eigenenergies relative to the Fermi energy. To study this effect, we modeled the system allowing the phase in each direction to be independently selected from the set $\phi_i = (0, \pi/10, ..., \pi/2)$. We considered samples with an initial temperature $T_i = 0.05 T_F$ and an initial number $N_i = 1.6 \times 10^5$ atoms, parameters within the saturated regime for all choices of phase and close to optimal for cooling. From the set of all possible phase combinations, we find an average final temperature $T_f = 0.0031 T_F$ where $10\%$ of the ensemble achieved temperatures below $T_{10} = 0.0023 T_F$ and $90\%$ were below $T_{90} = 0.004 T_F$. From this same set, we find an average final number $N_f = 1.20 \times 10^5$, with $N_{10} = 1.18 \times 10^5$, and $N_{90} = 1.22 \times 10^5$. The filtering process further results in a substantial reduction in entropy. The initial entropy per atom $s_i = 0.28 k_B$ is reduced to an average final value of $s_f = 0.024 k_B$, with $s_{10} = 0.014 k_B$, and $s_{90} = 0.033 k_B$.

It is in general possible to prepare atoms at a low $T/T_F$ in a shallow lattice potential, if so desired, by adiabatically reducing the lattice depth after the filtering stage. Continuing the example from above, when the lattice depth is reduced to $5 E_R$ we find an average final temperature $T_f = 0.002 T_F$, $T_{10} = 0.0013 T_F$, and $T_{90} = 0.0028 T_F$.

We now consider the effects of the charge $\ell$ of the LG beam for samples with an initial $T_i = 0.05 T_F$, phase $\phi_x = \phi_y = \phi_z = 0$, final lattice depth of $35 E_R$, and various initial atom numbers. For each $\ell$-value, the waist of the LG beam is adjusted such that the number of states below the second energy band is held constant at $1.22 \times 10^5$. As shown in Fig. 4, the cooling efficiency of this procedure is highly dependent on the charge. Note that for $\ell = 1$, which harmonizes external confinement, the final degeneracy temperature $T_f/T_F$ never drops below its initial value of $T_i/T_F = 0.05$. For $\ell \geq 8$, the minimum degeneracy temperature saturates to $T_f/T_F \lesssim 0.003$. For higher values of $\ell$, the extent of the saturation regime grows. We believe that this saturation is caused by localized atoms at the edges of the LG potential rethermalizing into higher energy bands.

In this Letter we proposed a method for preparing a sample of highly degenerate fermions by adiabatic loading into a combined optical lattice and “box-like” trapping potential followed by selective removal of atoms from all but the ground energy band. Numerical calculations for sample sizes $\sim 10^5$ predict that temperatures $\sim 10^{-3} T_F$ can be prepared in this manner. This method is robust against initial number and temperature fluctuations for a sufficiently cold initial sample of atoms and yields samples with little variance in the final number. While the selective removal of atoms must occur in a deep lattice (in order to spectrally resolve the band excitations), subsequent reduction of the lattice depth, if desired, yields a modest amount of additional cooling. We expect that this method can be scaled to larger samples for which still lower degeneracy temperatures would be attained due to the diminished role localized edge states would play. Further, the “box-like” trapping potential offers an ideal spatial profile for simulating solid state physics with degenerate atoms in optical lattices as the relatively flat central region allows for a large number of delocalized states while the curvature at the edges of the traps removes the constraint of loading exact atom numbers to realize insulating states. Atoms prepared in this manner should be sufficiently cold to explore quantum spin phases of fermionic atoms which are currently inaccessible, and could provide a physical realization of an essentially perfect quantum register.

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