Maximizing the Néel temperature of fermions in a simple-cubic optical lattice

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(Dated: June 5, 2008)

For a simple-cubic optical lattice with lattice spacing $d$, occupied by two species of fermionic atoms of mass $m$ that interact repulsively, we ask what conditions maximize the Néel temperature $T_N$ in the Mott insulating phase at density one atom per site, with equal numbers of the two species. This maximum, $k_B T_N^{(\text{max})} \approx 0.15 \hbar^2/(m d^2)$, occurs near the edge of the regime where the system is well-approximated by the usual Hubbard model. The correction to the Hubbard-model approximation that produces a “direct” ferromagnetic interaction between atoms in nearest-neighbor Wannier orbitals is the leading term that limits how high $T_N$ can be made.

PACS numbers:

One of the next notable milestones in the production of new strongly-correlated many-body states with ultracold atoms is expected to be the antiferromagnetic Néel phase of two hyperfine species of fermionic atoms in an optical lattice [1, 2]. Important progress towards this goal includes the recent realization of the Mott insulating phase with fermions [3], and the demonstration of controllable superexchange interactions in an optical lattice, albeit with bosonic atoms [4]. When the optical lattice is sufficiently deep and the repulsive $s$-wave interaction between the atoms is sufficiently weak, the Néel temperature $T_N$ for the case of one atom per lattice site can be estimated by modeling the system as a one-band Hubbard model, and one can analyze the possibility of reaching this phase by adiabatically ramping up the interactions and the optical lattice [1, 5, 6, 7, 8]. The most accessible conditions for first producing this ordered phase in an experiment will most likely be some compromise between the highest $T_N$ and the highest entropy at the transition $S(T_N)$. If the parameters of the system, namely the intensity $V_0$ of the optical lattice and the $s$-wave scattering length $a_s$, can be tuned in a perfectly adiabatic manner, then to access the Néel phase only requires achieving sufficiently low entropy [5, 6, 7]. But in the more likely event that there is always some “background” heating, so things are not perfectly adiabatic, the phase will be more accessible when it occurs at higher absolute temperature. Thus in this paper we study how the Néel temperature $T_N$ depends on the two tunable parameters $V_0$ and $a_s$ as one leaves the region where the standard Hubbard model is a good approximation to this system. Away from the Hubbard regime, theoretical studies have suggested that one may be able to access a wealth of phases governed by quantum spin hamiltonians [1, 9, 10].

According to quantum Monte Carlo simulations [11] of the simple-cubic fermionic Hubbard model, for a given nearest-neighbor hopping matrix element $t$ the highest $k_B T_N \approx t/3$ occurs at interaction $U \approx 8 t$, while for a given $U$ the maximal $k_B T_N \approx U/20$ occurs at $t \approx 0.15 U$. Thus to increase $T_N$ one wants to move to larger $t$, which means a weaker optical lattice (smaller $V_0$), and to larger $U$, which means larger $a_s$. This necessarily moves the system away from the regime where it is well-approximated by the usual Hubbard model. The mapping from the real system to the Hubbard model uses the single-atom Wannier orbitals as the basis states [1, 5, 12]. The standard one-band Hubbard model includes only the lowest-energy Wannier orbital at each lattice site and only the on-site interaction between two atoms of different hyperfine states occupying the same Wannier orbital.

We find that it is the corrections due to including the interactions between Wannier orbitals on nearest-neighbor lattice sites that are the leading effects that stop and reverse the increase of $T_N$ as $t$ and $U$ are increased by decreasing $V_0$ and increasing $a_s$. In particular, these interactions produce a “direct” ferromagnetic exchange interaction favoring neighboring sites to be occupied by the same species. These ferromagnetic interactions are of the opposite sign from the antiferromagnetic superexchange interactions that cause the Néel ordering, and thus they suppress $T_N$. Within the approximations that we make (discussed in detail below) the maximal $k_B T_N^{(\text{max})} \approx 0.03 E_r$ occurs near $V_0 \approx 3 E_r$ and $a_s \approx 0.15 d$, where $E_r = (\pi \hbar)^2/(2 m d^2)$ is the recoil energy and $d$ is the lattice spacing. For example, $E_r \approx 1.4 \mu$K for $^4$Li with $d = 532$ nm, which puts the maximum Néel temperature near 40 nK, which seems to be well within the reach of current experimental cooling techniques.

This regime of large repulsive $a_s$ is attained by approaching a Feshbach resonance from the repulsive side. But the atoms must scatter repulsively without “falling” in to the weakly-bound molecular state. Ref. [13] studied the Mott insulator with $^{40}$K at $a_s \approx 0.08 d$ and did not mention any problem with excessive molecule formation. It is not clear whether this can be increased to the $a_s \approx 0.15 d$ that maximizes $T_N$ [13]. It is also not clear whether the optical lattice increases or decreases molecule formation. The lattice breaks momentum conservation, thus possibly opening up channels for molecule formation, while in the Mott insulator the atoms are kept apart in different wells of the optical lattice, which, naively, reduces the opportunities for molecule formation.

The system we consider is made up of fermionic atoms in a simple-cubic optical lattice with a single-atom potential of the standard form [2]:

$$ V_1(x, y, z) = V_0(\sin^2 \frac{\pi x}{d} + \sin^2 \frac{\pi y}{d} + \sin^2 \frac{\pi z}{d}) \, . $$

This is a separable potential, so the energy eigenstates of a single atom in this potential can be chosen to be the product

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This is a separable potential, so the energy eigenstates of a single atom in this potential can be chosen to be the product
of one-dimensional (1D) eigenstates along each direction. We solve for these 1D bands and thus obtain the properly normalized wavefunctions $w_\alpha(x)$ of the maximally-localized 1D Wannier orbitals for each band $\alpha$. The 3D Wannier orbitals are then $\phi_{n_x n_y n_z}(x, y, z) = w_{n_x}(x)w_{n_y}(y)w_{n_z}(z)$.

We will be focusing on the Mott insulating regime with density exactly one atom per lattice site and low temperature, where the atoms are primarily in the lowest band, $n_x = n_y = n_z = 0$. The nearest-neighbor hopping matrix element $t_0$ in this band is a strongly decreasing function of $V_0$, the lattice strength, behaving as $t_0 \approx 4\pi^{-1/2}E_r^{1/4}V^{3/4}e^{-2\sqrt{V/E_r}}$ for large $V_0$.[3] The wavefunction $w_0(x)$ of the lowest Wannier orbital at a given lattice site is positive and has its maximum amplitude at $x = 0$, the center of the well of the optical lattice at that site, while its amplitude is negative and of smaller magnitude in the nearest-neighbor wells of the lattice. The ratio of these amplitudes is one small parameter that is important in the approximations we use below.

We are interested in the antiferromagnetic Mott insulating phase in the regime where the on-site repulsive interaction $U$ is stronger than the hopping $t$. We do not treat the limit of weak interaction, where the system is a paramagnetic Fermi liquid. We assume the atoms equally populate two different hyperfine states; as is standard, we will call these two states $|\uparrow\rangle$ and $|\downarrow\rangle$. There is presumably also a paramagnetic Fermi liquid ground state in the lower left corner of this phase diagram, but our approximations are not well-suited to estimating where this phase is.

We approximate this 2-atom interaction as the standard regularized contact potential[14]

$$V_2(\vec{r}_1 - \vec{r}_2) = \frac{4\pi \hbar^2 a_s}{m} \delta(\vec{r}_1 - \vec{r}_2) \frac{\partial}{\partial \vec{r}}$$

where $r$ distance between the two particles. The expectation value of this interaction energy for two atoms of opposite spin occupying the same lowest Wannier orbital is our first estimate of the strength of the on-site interaction $U_0 a_{\uparrow\downarrow}$ in the corresponding one-band Hubbard model:

$$U_0 = \frac{4\pi \hbar^2 a_s}{m} \left[ \int dx w_0^3(x) \right]^2.$$

In the Hubbard model, when adjacent sites $i$ and $j$ are each singly-occupied by atoms with the same spin, then the hopping between those two sites is Pauli-blocked. When these adjacent sites are each singly-occupied by opposite spins, then virtual hopping between these sites, treated in second-order perturbation theory, allows them to lower their energy and thus generates an antiferromagnetic superexchange interaction $J_s(\vec{S}_i \cdot \vec{S}_j - \frac{1}{2})$ with $J_s = 4t^2/U$.

The leading corrections to the Hubbard model approximation to this system in the regime we are interested in are due to the interactions between atoms of opposite spin occupying lowest Wannier orbitals on nearest-neighbor sites $i$ and $j$. There are 2 contributions: First, and apparently most important in limiting how large $T_N$ can be made, is the “direct” interaction[3]

$$U_{nn} = \frac{4\pi \hbar^2 a_s}{m} \left[ \int dx w_0^3(x) \right] \int dy w_0^2(y) w_0^2(y + d)$$

between atoms of opposite spin in adjacent orbitals. This term is due to the overlap of the probability distributions of adjacent Wannier orbitals. It raises the energy of the Néel state. It thus produces a direct ferromagnetic exchange interaction $J_f(\vec{S}_i \cdot \vec{S}_j - \frac{1}{2})$ with $J_f = -2U_{nn} < 0$ that partially cancels the antiferromagnetic superexchange $J_s$ that occurs in the Hubbard model. It is primarily this ferromagnetic interaction that stops and reverses the increase in $T_N$ as one moves towards stronger interaction and a weaker lattice while staying near the optimal values of $U/t$. At the global maximum of $T_N$, indicated in Fig. 1, we find $J_f \simeq -J_s/4$.

For large enough $a_s$ this direct ferromagnetic exchange is stronger than the superexchange and thus we have a ground-state phase transition to a ferromagnetic phase, as indicated in Fig. 1, and discussed more below. [Very near this $|J_f| = J_s$ line, effects due to weaker further-neighbor interaction might produce some other magnetically-ordered phases.]

The “direct” nearest-neighbor interaction (4) also reduces the effective $U$ that enters in the superexchange interaction, so at this level of approximation our simple-cubic Hubbard model has interaction $U = U_0 - 6U_{nn}$, since it is the change

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**Phase diagram**

![Phase diagram](image1)

**FIG. 1:** Approximate phase diagram for filling one fermion per lattice site. The line marked $|J_f| = J_s$ is our approximation to the ground-state phase boundary separating the antiferromagnetic phase at smaller $a_s$ from the ferromagnetic phase at larger $a_s$. The ferromagnetic phase is mostly a fully-polarized band insulator, but there is a small sliver of polarized Fermi liquid at small $V_0$ between the lines marked $|J_f| = J_s$ and “FM to FI”. The line marked “Optimal $T_N$” indicates where $T_N$ as a function of $V_0$ is maximized for each given $a_s$. The dot on that line is our estimate of the parameters that produce the overall maximum of $T_N/E_r$, and at that point $J_f \simeq -J_s/4$ (see text). The $U = 14t$ line is near where the entropy is maximized at $T_N$[5] and $T_N$ on this line is maximized at the dot. The $t_0 = t_I$ line signals when the interaction correction to the hopping becomes strong. There is presumably also a paramagnetic Fermi liquid ground state in the lower left corner of this phase diagram, but our approximations are not well-suited to estimating where this phase is.
of the interaction energy due to moving the atom that enters in the energy denominator in the superexchange process.

Also, the interaction generates an additional hopping term of the same sign as $t_0$: 

$$t_I = -\frac{4\pi^2a_s^2}{m} \left( \int dx w_0^4(x) \right)^2 \int dy w_0^3(y) w_0(y + d)$$

that is operative when the two sites are each singly-occupied by opposite spins. The resulting effective hopping that enters in the superexchange process at this level of approximation is thus $t = t_0 + t_I$.

Thus once we include these leading effects due to the nearest-neighbor interaction, the effective Hamiltonian in the vicinity of the ground state of the half-filled Mott insulator has hopping $t = t_0 + t_I$, an effective on-site interaction $U = U_0 - 6U_{nn}$, and an additional ferromagnetic nearest-neighbor exchange interaction $J_f = -2U_{nn}$ when both sites are singly-occupied. To estimate the Néel temperature of our system we propose the following approximation: For the Hubbard model without $J_f$, we have estimates of its Néel temperature $T_N^{(H)}(t, U)$ from quantum Monte Carlo simulations [11]. This Néel ordering is due to the antiferromagnetic superexchange interaction $J_s = 4t^2/U$ between neighboring singly-occupied sites. When we include $J_f < 0$ this reduces this magnetic interaction, and we will approximate the resulting reduction of $T_N$ as being simply in proportion to the reduction of the total nearest-neighbor exchange interaction:

$$T_N(V_0, a_s) \approx (1 + \frac{J_f}{J_s})T_N^{(H)}(t, U).$$

In Fig. 1 we show the lattice strength $V_0/E_r$ that maximizes this approximation to $T_N$ for each value of the interaction $a_s/d$. The highest $T_N$ occurs near $a_s/d = 0.15$, but the system at this value of $a_s$ is may be too close to the Feshbach resonance and thus not stable against formation of molecules. The highest achievable $T_N$ thus may be somewhere along this line at a lower value of $a_s$ and thus a stronger lattice $V_0$. We note that a recent experiment [3] has studied $a_s/d \approx 0.08$ for $^{40}$K, albeit at a temperature well above $T_N$, without noting any strong instability towards molecule formation. We also show on Fig. 1 the line along which $U = 14t$, since this is near where the critical entropy $S(T_N)$ is maximal [5], so if the system can be adjusted adiabatically this is where the Néel phase is most accessible.

In Fig. 2 we show $k_B T_N/E_r$ as a function of $a_s/d$ at the value of $V_0$ that maximizes our estimate of $T_N$, as well as at the value of $V_0$ that gives $U = 14t$ and thus is near the maximum of $S(T_N)$. Note that in Fig. 2 the horizontal scale for $a_s/d$ is logarithmic, so $T_N$ drops rather weakly as $a_s$ is reduced, meaning that the possible limitation in how large $a_s$ can be made will not “cost” a lot in terms of the resulting reduction of $T_N$.

The approximations we are making are clearly beginning to break down in the vicinity of the parameter values that maximize $T_N$. Thus, although we expect that these approximations give reasonably reliable rough estimates of the maximal values of $T_N$, there are many higher-order effects that we are ignoring that may alter these estimates by a little (our calculations suggest on the $\sim 10\%$ level). At the maximum of $T_N$, $|J_f|$ is about $25\%$ of $J_s$. The correction to $J_s$ due to $t_I$ is also of roughly this size, but its dependence on $a_s$ is much weaker, which is why $J_f$ is the important factor in causing the maximum in $T_N$.

FIG. 2: Our estimates of the optimal Néel temperature, $T_N$, as a function of $a_s/d$. For each value of $a_s$, $T_N$ is maximized by varying the lattice depth $V_0$. We also plot $T_N$ at the line $U = 14t$, which is near where the critical entropy is maximized [5].

FIG. 3: The strongest higher-order process contributing to the energy of the antiferromagnetic Mott insulator at the maxima of $T_N$ shown in Fig. 1. It consists of (1) a nearest-neighbor hop in the lowest (S) band, (2) an on-site “pair hopping” of both fermions up to the next (P) band, (3) on-site pair hopping back to the S band, and (4) a nearest-neighbor hop back to the original configuration. At both maxima of $T_N$, this process corrects $J_s$ by about 10%.

The approximations we have used are those appropriate for the Mott insulator, and are based on the inequalities on energy scales $\varepsilon_0 > U > t$, where $\varepsilon_0$ is the expectation value of the single-particle energy in a lowest Wannier orbital. We have analyzed in perturbation theory many corrections beyond those included above. We find that at the maximum of $T_N$ (both the global maximum and the maximum along the $U = 14t$ line) the strongest next correction is the fourth-
order process illustrated in Fig. 3, it alters $J_s$ by about 10%. Since our perturbatively-based approximations are breaking down near this regime of interest where $T_N$ is maximized, it would be nice to have a more systematic approach that can obtain more precise and reliable estimates of the phase diagram in this regime. For example, quantum Monte Carlo simulations might be possible for temperatures near $T_N$, although of course the famous fermionic “minus signs” may prevent this from being feasible in the near term.

The ferromagnetic phase of this model at strong repulsion is mostly a band insulator, with a band gap between the spin-polarized bands. But in the weaker lattice regime there should also be a partially-polarized Fermi liquid ground state near the phase boundary to the Néel state. The transition from the fully-polarized band insulator to the partially-polarized ferromagnet occurs when the spin-polarized bands overlap, so the system can lower its energy by flipping spins. A single spin flip makes a hole and a doubly-occupied site that can be accurately treated in some form of quantum Monte Carlo simulations. Of course this is a system of many fermions, so it is not clear whether this weak lattice regime can be accurately treated in some form of quantum Monte Carlo simulations.

We thank Randy Hulet for many discussions, and Meera Parish for helpful suggestions. This work was supported under ARO Award W911NF-07-1-0464 with funds from the DARPA OLE Program.

### Conclusion
We have shown that to maximize the Néel temperature one must leave the region of parameter space where the Hubbard model approximation for fermionic atoms in an optical lattice is well-controlled. We have found that the nearest-neighbor direct ferromagnetic exchange is the most important correction to the Hubbard model that limits the maximal $T_N$. There are also higher-order corrections to the Hubbard model: virtual hopping into higher bands and other higher-order processes. For the parameters that maximize $T_N$, these higher-order terms are smaller than the nearest-neighbor terms we include, although not by a large margin of “safety”.

The relative contribution of the higher-order corrections in the vicinity of the optimal $T_N$ drops exponentially as one goes to smaller interaction $a_s$ and thus a stronger optical lattice. Thus our results are accurate in the large $V_0$ (strong lattice) limit, and should qualitatively capture the phase diagram for weaker lattices. For quantitatively more accurate results in the weak lattice regime, one needs to resort to more systematic quantum calculations. Of course this is a system of many fermions, so it is not clear whether this weak lattice regime can be accurately treated in some form of quantum Monte Carlo simulations.

**Table I: The values of the various energies at the two $T_N$ maxima.**

| $\varepsilon_0 (E_r)$ | 4.2 | 5.5 |
| $U_0 (E_r)$ | 0.9 | 1.3 |
| $t_0 (E_r)$ | 0.11 | 0.07 |
| $\epsilon_J (E_r)$ | 0.02 | 0.02 |
| $J_J (E_r)$ | 0.08 | 0.03 |
| $J_s$ correction ($E_r$) | 0.007 | 0.004 |

We focus on the ground state $\{\uparrow\uparrow\}$, although these ferromagnetic phases at high $a_s$ are very likely to be inaccessible in experiments with cold fermionic atoms in optical lattices. Also, the present approximations are probably not very reliable in this regime of large $a_s/d$.

There is also a paramagnetic Fermi liquid phase at weak enough lattice and at weak enough interaction, as well as possibly an antiferromagnetic Fermi liquid near it. These phases occur well away from the regimes we have focussed on here, and the present approximations are not well suited to estimating the location of the corresponding phase transitions, so we leave that part of the phase diagram as “terra incognita” for now. The quantum phase transition between the Néel state and the paramagnet should occur in parameter regimes that are accessible to the experiments, although it may not be possible to see its effects at accessible temperatures, since $T_N$ decreases strongly as this regime is approached.

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