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

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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, $k_B T_N^{(\max)} \cong 0.15\,\hbar^2/(md^2)$, 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.

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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 $k_B T_N \cong t/3$ occurs at interaction $U \cong 8\,t$, while for a given U the maximal $k_B T_N \cong U/20$ occurs at $t \cong 0.15\,U$. 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 $k_B T_N^{(\max)} \cong 0.03 E_r$ occurs near $V_0 \cong 3E_r$ and $a_s \cong 0.15\,d$, where $E_r = (\pi\hbar)^2/(2md^2)$ is the recoil energy and d is the lattice spacing. For example, $E_r \cong 1.4\,\mu$K for ^{6}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. [3] studied the Mott insulator with ^{40}K at $a_s \cong 0.08\,d$ and did not mention any problem with excessive molecule formation. It is not clear whether this can be increased to the $a_s \cong 0.15\,d$ 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]:

$$V_1(x,y,z) = V_0(\sin^2\frac{\pi x}{d} + \sin^2\frac{\pi y}{d} + \sin^2\frac{\pi z}{d})\,. \qquad (1)$$

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 $w_n(x)$ of the maximally-localized 1D Wannier orbitals for each band n [12]. 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 [5]. 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 "up" and "down" and treat them as the two states of a spin-1/2 degree of freedom. The s-wave repulsive interaction is only between atoms of opposite spin. To lowest order in (a_s/d), we approximate this 2-atom interaction as the standard regularized contact potential[14]

$$V_2(\vec{r}_\uparrow - \vec{r}_\downarrow) = \frac{4\pi\hbar^2 a_s}{m}\delta(\vec{r}_\uparrow - \vec{r}_\downarrow)\frac{\partial}{\partial r}r \qquad (2)$$

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 $U_0 n_{i\uparrow}n_{i\downarrow}$ in the corresponding one-band Hubbard model:

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

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 $J_s(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4})$ 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 [4]

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

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 $J_f(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4})$ 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*

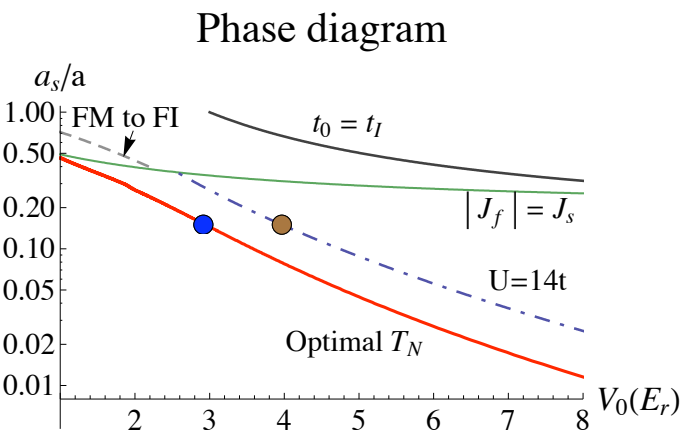

FIG. 1: Approximate phase diagram for filling one fermion per lattice site. The line marked $|J_f| = J_s$ is our approximation to the ground-state phase boundary separating the antiferromagnetic phase at smaller a_s from the ferromagnetic phase at larger a_s. The ferromagnetic phase is mostly a fully-polarized 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.

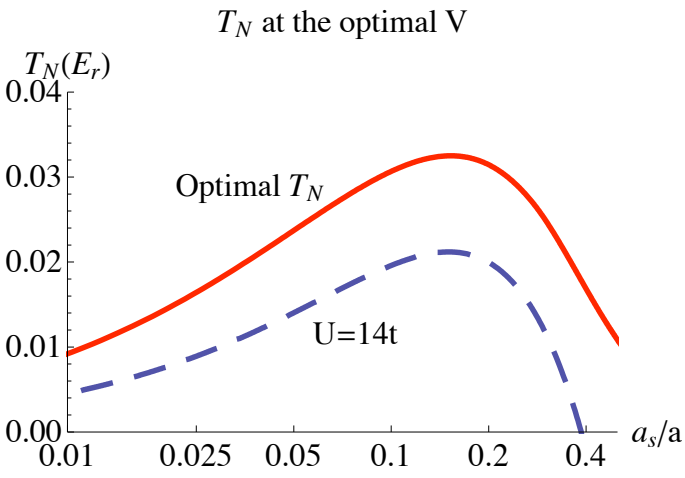

FIG. 2: Our estimates of the optimal Néel temperature, T_N, as a function of a_s/d. For each value of a_s, T_N is maximized by varying the lattice depth V_0. We also plot T_N at the line $U = 14t$, which is near where the critical entropy is maximized [5].

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: [5]

$$t_I = -\frac{4\pi\hbar^2 a_s}{m}[\int dx w_0^4(x)]^2 \int dy w_0^3(y) w_0(y+d) \quad (5)$$

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:

$$T_N(V_0, a_s) \cong (1 + \frac{J_f}{J_s}) T_N^{(H)}(t,U) \; . \quad (6)$$

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 $a_s/d \simeq 0.08$ 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 actor in causing the maximum in T_N.

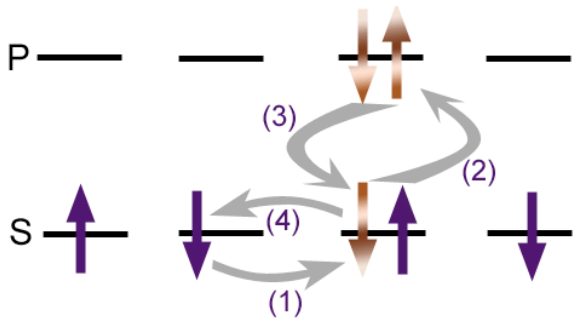

FIG. 3: The strongest higher-order process contributing to the energy of the antiferromagnetic Mott insulator at the maxima of T_N shown in Fig. 1. It consists of (1) a nearest-neighbor hop in the lowest (S) band, (2) an on-site "pair hopping" of both fermions up to the next (P) band, (3) on-site pair 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 ε_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-

TABLE I: The values of the various energies at the two T_N maxima. The "J_s correction" corresponds to the process detailed in fig. 3.

	Global maximum of T_N	Maximum of T_N at $U = 14t$
$\varepsilon_0\,(E_r)$	4.2	5.5
$U_0\,(E_r)$	0.9	1.3
$t_0\,(E_r)$	0.11	0.07
$t_I\,(E_r)$	0.02	0.02
$J_s\,(E_r)$	0.08	0.03
$J_f\,(E_r)$	-0.02	-0.008
J_s correction (E_r)	0.007	0.004

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 are each moving freely within the fully-polarized background state. At the level of approximation we have used in this paper, the hole moves freely with hopping t_0, so its lowest energy is $-6t_0$. The doubly-occupied state costs interaction energy $U_0 + 6U_{nn}$ and moves freely with effective hopping $t_2 = t_0 + 2t_I$ because its motion is the hopping of the flipped spin between sites that are both occupied by unflipped spins. The total energy of this particle-hole pair can be negative when $U_0 + 6U_{nn} < 12(t_0 + t_I) = 6(t_0 + t_2)$; this occurs below the line indicated in Fig. 1 as "FM to FI" (ferromagnetic metal to ferromagnetic insulator). We show this for completeness, 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.

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.

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