Achieving the Néel state in an optical lattice

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We theoretically study the possibility of reaching the antiferromagnetic phase of the Hubbard model by starting from a normal gas of trapped fermionic atoms and adiabatically ramping up an optical lattice. Requirements on the initial temperature and the number of atoms are determined for a three-dimensional square lattice by evaluating the Néel state entropy, taking into account fluctuations around the mean-field solution. We find that these fluctuations place important limitations on adiabatically reaching the Néel state.

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I. INTRODUCTION

An optical lattice is a regular periodic potential for neutral cold atoms [1] which enables the controlled experimental exploration of paradigmatic ideas and models from condensed-matter physics. This is because cold atomic gases generally allow for a great deal of experimental tunability. For example, Feshbach scattering resonances allow for the interaction strength to be experimentally varied over a considerable range [2,3]. Other quantities that may be altered include temperature, density, and strength and shape of the trapping potential. In particular, an optical-lattice potential plays the role of the ion-lattice potential encountered in electronic solid-state physics. The energy bands resulting from this periodic potential lead to a quenching of the kinetic energy of the atoms with respect to their interaction energy, enabling the exploration of strongly correlated phases that play a significant role in condensed-matter physics.

An important model that can be studied experimentally with cold atoms is the single-band Hubbard model, which consists of interacting fermions in the tight-binding approximation. The Hubbard Hamiltonian is realized by cold atoms in an optical lattice when the potential is strong enough so that only the lowest-energy band is populated [4]. For bosonic atoms one then commonly refers to this model as the Bose-Hubbard model. The theoretically predicted Mott-insulator-to-superfluid phase transition [5] for this model has indeed been observed experimentally [6].

The fermionic Hubbard model, referred to simply as the Hubbard model, is important in the context of high-temperature superconductivity [7,8] and has also been realized with cold atoms [9]. At half filling, corresponding to one particle per lattice site, the ground state of this model is antiferromagnetic, i.e., a Néel-ordered state, for strong enough on-site interactions. As the filling factor is reduced by doping, the system is conjectured to undergo a quantum phase transition to a *d*-wave superconducting state [10]. A theoretical proof of the existence of *d*-wave superconductivity in the Hubbard model is still lacking and would be a major step toward understanding the superconducting state of the cuprates. With the recent experimental advances in the field of ultracold atoms, an experimental exploration of this issue is within reach.

In view of this motivation, a significant problem is determining how the Néel state of the Hubbard model can be reached experimentally. In this paper, we study theoretically the process of adiabatically turning on the optical lattice [11,12], with the goal of determining the conditions required for an initially trapped balanced two-component Fermi gas with repulsive interactions to reach the Néel state in the lattice. Experimentally, the presence of antiferromagnetic order in this cold-atom experiment can be subsequently detected from shot-noise correlations in the density distribution [13,14].

Our results are summarized in Fig. 1. For initial temperatures lower than T_F, the Fermi temperature in the trap, the entropy per particle in the trap depends linearly on temperature as is shown by the dashed line. The optical lattice is then turned on adiabatically, and to determine the final temperature of the gas we need the entropy per atom in the lattice. For a sufficiently smooth trapping potential such that the tunneling does not become site-dependent, the only effect of the trap is to place a restriction on the total number of particles which we discuss later and, other than this, we may neglect the trap for calculations in the lattice. Since we con-
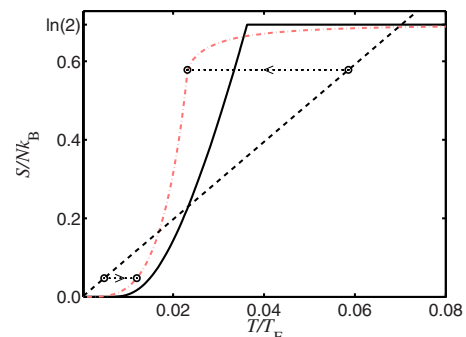

FIG. 1. (Color online) The entropy per particle in the harmonic trapping potential only (dashed line), in a lattice of depth $V_0 = 6.5 E_R$ (E_R is the recoil energy) from single-site mean-field theory (solid curve) and with fluctuations (dash-dotted curve), where T_F is the Fermi temperature in the trap. The horizontal dotted lines illustrate cooling and heating into the Néel state at constant entropy by starting in the harmonic trap and adiabatically turning on the lattice.
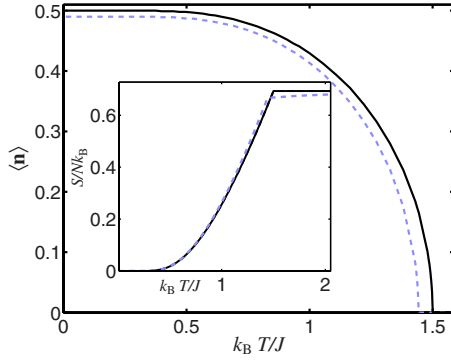
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FIG. 2. (Color online) The staggered magnetization $\langle \mathbf{n} \rangle$ of the single (solid curves) and two-site (dashed curves) mean-field theories, the latter of which shows depletion at $T=0$ and a lowering in T_c. The entropy of both theories is plotted in the inset. Above T_c we see that the entropy of the two-site theory is temperature dependent.

sider balanced gases here, we will at sufficiently low temperatures first enter the Mott phase with one particle per site, and the subsequent evolution of the gas is then described by the Heisenberg model for the spins alone. The result from the usual mean-field theory is shown for a lattice depth of $6.5E_R$ (where E_R is the recoil energy) by the black curve, and is equal to $k_B \ln(2)$ everywhere above the critical temperature T_c. Since entropy is conserved in adiabatic processes, the final temperature is simply the temperature at which the final entropy in the lattice equals the initial entropy in the trap. Two such processes are shown by the dotted lines for different initial temperatures demonstrating that the gas is sometimes heated and not cooled by the lattice. Nevertheless, mean-field theory leads to the intuitive result that as long as the entropy per particle in the initial state is less than $k_B \ln(2)$, which is the maximum entropy of the Heisenberg model, the Néel state is always reached by adiabatically turning on the optical lattice.

The inclusion of fluctuations leads, however, to a more restrictive condition. To probe the effect of fluctuations, we present an improved mean-field theory which produces a temperature-dependent entropy above T_c, as seen from the inset of Fig. 2. Although this approach is exact at high temperatures, it fails to account for spin waves present at low temperatures and for critical phenomena near T_c. By further extending the improved mean-field theory to reproduce the correct critical and low temperature behavior due to fluctuations, we are able to determine the entropy in the lattice for all temperatures (red curve in Fig. 1). In particular, we find that fluctuations lower the entropy of the atoms in the square lattice at T_c as

$$S(T = T_c) \simeq Nk_B \ln(2) - \frac{3NJ^2}{32k_B T_c^2 (3\nu - 1)}, \quad (1)$$

where ν is the critical exponent of the correlation length ξ. For the case of three dimensions, $\nu = 0.63$ [17]. As a result, the initial temperature required to reach the Néel state is more than 20% lower than that found from the usual mean-field theory, but fortunately remains experimentally acces-

sible. For example, with ^{40}K atoms and a final lattice depth of $8E_R$ the Néel state is achieved when the final temperature in the lattice is $0.012T_F$, which can be obtained with an initial temperature of $0.059T_F$.

II. SINGLE-SITE MEAN-FIELD THEORY

The Hamiltonian for the Hubbard model is given by

$$H = -t \sum_\sigma \sum_{\langle jj' \rangle} c_{j,\sigma}^\dagger c_{j',\sigma} + U \sum_j c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger c_{j,\downarrow} c_{j,\uparrow}, \quad (2)$$

in terms of fermionic creation and annihilation operators, denoted by $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$, respectively, where σ labels the two hyperfine spin states $|\uparrow\rangle$ or $|\downarrow\rangle$ of the atoms. In the first term of this expression, the sum over lattice sites labeled by indices j and j' is over nearest neighbors only and proportional to the hopping amplitude given by

$$t = \frac{4E^R}{\sqrt{\pi}} \left(\frac{V_0}{E^R} \right)^{3/4} e^{-2\sqrt{V_0/E^R}}. \quad (3)$$

Here, $V_0 > 0$ is the depth of the optical lattice potential defined by

$$V(\mathbf{x}) = V_0 [\cos^2(2\pi x/\lambda) + \cos^2(2\pi y/\lambda) + \cos^2(2\pi z/\lambda)], \quad (4)$$

where λ is the wavelength of the lattice lasers. The second term in the Hamiltonian corresponds to an on-site interaction of the strength given in the harmonic approximation by

$$U = 4\pi a \sqrt{\frac{\hbar}{\lambda^3}} \left(\frac{8V_0^3}{m} \right)^{1/4}, \quad (5)$$

where a is the s-wave scattering length which is equal to $174a_0$ for ^{40}K. It is well-known [15] that at half filling and in the limit that $U \gg t$ the ground state of the Hubbard model is antiferromagnetic and that, for $k_B T \ll U$, its low-lying excitations are described by the effective Heisenberg Hamiltonian

$$H = \frac{J}{2} \sum_{\langle jk \rangle} \mathbf{S}_j \cdot \mathbf{S}_k, \quad (6)$$

with $\mathbf{S}$ being one-half times the vector of Pauli matrices. The exchange constant $J = 4t^2/U$ arises from the superexchange mechanism. That is, the system can lower its energy by virtual nearest-neighbor hops only when there is antiferromagnetic ordering.

Within the usual mean-field analysis of the effective Hamiltonian in Eq. (6), the total entropy for N atoms in the optical lattice is given by

$$S = -\frac{\partial F_L(\langle \mathbf{n} \rangle)}{\partial T}, \quad (7)$$

where F_L is the Landau free energy,

$$F_L(\mathbf{n}) = N \left\{ \frac{zJ|\mathbf{n}|^2}{2} - k_B T \ln \left[2 \cosh \left(\frac{zJ|\mathbf{n}|}{k_B T} \right) \right] \right\}, \quad (8)$$

in terms of the staggered, or Néel, order parameter $\mathbf{n} = (-)^j \langle \mathbf{S}_j \rangle$ for the phase transition to the antiferromagnetic

state. In the expression for the free energy, $z = 6$ is the number of nearest neighbors for a three-dimensional simple square lattice on which we focus here, $k_B T$ is the thermal energy, and $\langle \mathbf{n} \rangle$ is the equilibrium value of the order parameter determined from

$$\left. \frac{\partial F_L(\mathbf{n})}{\partial \mathbf{n}} \right|_{\mathbf{n} = \langle \mathbf{n} \rangle} = 0. \tag{9}$$

It is nonzero below a critical temperature $k_B T_c = Jz/4 = (3/2)J$. After solving Eq. (9) the entropy is determined using Eq. (7). The results for S and $\langle \mathbf{n} \rangle$ obtained in this way are plotted as solid black curves in Figs. 1 and 2.

The entropy S_{FG} of the initial normal state before ramping up the optical lattice is the entropy of a trapped ideal Fermi gas. It is most conveniently determined from the grand potential

$$\Omega(\mu, T) = -k_B T \int_0^\infty d\epsilon \, \rho(\epsilon) \ln[1 + e^{-(\epsilon - \mu)/k_B T}], \tag{10}$$

where μ is the chemical potential, and the effect of the harmonic trapping potential with the effectively isotropic frequency $\omega = (\omega_x \omega_y \omega_z)^{1/3}$ is incorporated via the density of states $\rho(\epsilon) = \epsilon^2/(\hbar \omega)^3$ of the atoms. The entropy at fixed total particle number $N(\mu) = -\partial \Omega / \partial \mu$ is then given by $S_{FG} = -\partial \Omega / \partial T|_{\mu(N)}$. At temperatures much lower than the Fermi temperature in the trap, given by $T_F = (3N)^{1/3} \hbar \omega / k_B$, we find in this manner that [16] $S_{FG} = N k_B \pi^2 T / T_F$. Now, by equating the final and initial entropies we calculate the temperature of the Heisenberg spin system that results after adiabatically turning on the optical lattice, in terms of the initial temperature of the trapped Fermi gas.

From the expression for the free energy, Eq. (8), we immediately see that $S = N k_B \ln(2)$ for all temperatures $T > T_c$, as was shown in Fig. 1. Although this is the correct high-temperature limit of the entropy, temperature dependence will lower the entropy at T_c and therefore lower the initial temperature required to achieve the Néel state. To obtain the temperature dependence above T_c, we must thus go beyond single-site mean-field theory to include fluctuations. The simplest such model described below incorporates the interaction of a given site with one of its neighbors exactly and treats interactions with the rest of the neighbors within mean-field theory.

III. TWO-SITE MEAN-FIELD THEORY

The two-site Hamiltonian for neighboring sites labeled "1" and "2" is given by

$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2 + J(z-1)|\mathbf{n}|(\mathbf{S}_1^z - \mathbf{S}_2^z) + J(z-1)|\mathbf{n}|^2, \tag{11}$$

where the last term is a correction to avoid double counting of mean-field effects. Diagonalizing this Hamiltonian we obtain the free energy

$$F_L(\mathbf{n}) = N \left\{ \frac{1}{2}(z-1)J|\mathbf{n}|^2 - \frac{1}{2\beta} \ln \left[2e^{-\beta J/4} \right. \right.$$
$$\left. \left. + 2e^{\beta J/4} \cosh\left(\frac{\beta J}{2} \sqrt{1 + 4(z-1)^2 |\mathbf{n}|^2} \right) \right] \right\}, \tag{12}$$

and find the entropy from Eq. (7) with the condition Eq. (9) as in the single-site model. The results are plotted in Fig. 2, where we see that fluctuations lower the critical temperature and also bring about a 2% depletion of the order parameter which is now less than 0.5 near $T = 0$.

The two-site result carries the exact $1/T^2$ dependence of the entropy of the Heisenberg model at high temperatures. Near $T = 0$, however, the entropy is still exponentially suppressed reflecting the energy cost of flipping a spin. This exponential suppression is an artifact of the mean-field approximation that ignores the Goldstone modes which are present in the symmetry-broken phase. Furthermore, critical behavior cannot be properly accounted for by a one-, two- or higher-site model since, near the onset of Néel order, critical fluctuations extend throughout the entire lattice so one would, in principle, need to include all sites exactly. To overcome these shortcomings, we extend our two-site model below to all temperatures.

IV. FLUCTUATIONS

The two-site mean-field theory produces the correct normal-state entropy behavior in the high-temperature limit,

$$S(T \gg T_c) = N k_B \left[\ln(2) - \frac{3J^2}{64 k_B^2 T^2} \right]. \tag{13}$$

In the low-temperature regime, the entropy is determined from spin-wave fluctuations prevalent near $T = 0$ which give a black-body-like entropy,

$$S(T \ll T_c) = N k_B \frac{4\pi^2}{45} \left(\frac{k_B T}{2\sqrt{3} J \langle \mathbf{n} \rangle} \right)^3. \tag{14}$$

The continuous interpolation between these two regimes has the additional constraint that, near T_c, we should obtain the correct critical behavior of the antiferromagnet, namely, the correct universal ratio of the amplitudes above and below the phase transition A^+/A^- and correct critical exponent $d\nu - 1$ where

$$S(T \simeq T_c) = S(T_c) \pm A^{\pm} |t|^{d\nu-1}, \quad t = (T - T_c)/T_c \to 0^{\pm}. \tag{15}$$

This follows from the fact that the singular part of the free energy density behaves as $F^{\pm}/\xi^d$, where the correlation length diverges like $\xi \sim |t|^{-\nu}$ as $t \to 0$. Explicit expressions for the entropy embodying the correct behavior in the low-, high-, and critical-temperature regimes are presented in the Appendix and plotted as the red curve in Fig. 1 for $d = 3$ using $A^+/A^- \simeq 0.54$ and $\nu = 0.63$ [17] and the Néel temperature of $T_c = 0.957 k_B/J$ [18]. Their value at T_c leads to the

central result of this paper, namely, Eq. (1) which specifies the initial entropy required to reach the Néel state.

V. DISCUSSION AND CONCLUSIONS

As briefly mentioned earlier, there is a limit on the total number of atoms in the trap, beyond which at low temperatures it is energetically more favorable to doubly occupy sites in the center of the trap, thereby destroying the antiferromagnetic state, rather than singly occupying outlying sites where the trap potential is larger than U. Thus, insisting that the system end up in the Mott-insulator state with one particle per site entails the upper bound, $N \leq N_{max} = (4\pi/3)(8U/m\omega^2\lambda^2)^{3/2}$, where m is the mass of the atoms and λ is the wavelength of the lattice lasers. For ^{40}K atoms in a lattice with a wavelength $\lambda = 755$ nm and depth $8E_R$, and with a harmonic trap frequency $\omega/2\pi = 50$ Hz, $N_{max} \simeq 2 \times 10^6$ which is well above the typical number of atoms in experiments.

We have also attempted to determine the effect that fluctuations have on the entropy in a more microscopic manner by studying Gaussian fluctuations about the mean-field $\langle \mathbf{n} \rangle$ for the single-site mean-field theory in the low-temperature regime; but such a random-phase approximation has severe complications related to the fact that $\langle \mathbf{n} \rangle$ enters in the magnon dispersion as $\omega_{\mathbf{k}}^M \propto \langle |\mathbf{n}| \rangle |\mathbf{k}|$. Hence, as can be already seen from Eq. (14), the contribution of the magnons to the entropy diverges when $\langle \mathbf{n} \rangle \to 0$ near T_c. One way to potentially resolve this issue is to start from the Hubbard Hamiltonian Eq. (2) directly but such an analysis is involved [19] and has yet to be carried out.

In the above, we have focused on the $d=3$ case. While our results can easily be extended to the $d=2$ case, a more pertinent way to reach the two-dimensional antiferromagnet most relevant to high-temperature superconductors would be to adiabatically prepare a three-dimensional Néel state, as explained in this paper, and then decrease the tunneling in one direction by changing the intensity of one of the lattice lasers. In this way, the three-dimensional system is changed into a stack of pancakes of atoms in the two-dimensional Néel state. Furthermore, studying doped optical lattices made by introducing a small imbalance in the initial state may shed some light on the physics of high-temperature superconductors and would be an exciting direction for future research.

APPENDIX: ENTROPY FORMULAS

For temperatures above T_c we use

$$\frac{S(T \geq T_c)}{N k_B} \simeq \alpha_1 \left[\left(\frac{T - T_c}{T} \right)^\kappa - 1 + \frac{\kappa T_c}{T} \right] + \ln(2),$$

with $\alpha_1 = 3J^2/32\kappa(\kappa-1)k_B^2 T_c^2$ and $\kappa = 3\nu - 1 \simeq 0.89$ [17]. The first term embodies the correct critical behavior whereas the remaining terms are present to recover the correct high-temperature limit. Below T_c, however, we have

$$\frac{S(T \leq T_c)}{N k_B} = -\alpha_2 \left[\left(\frac{T_c - T}{T_c} \right)^\kappa - 1 + \kappa \frac{T}{T_c} - \frac{\kappa(\kappa-1)}{2} \frac{T^2}{T_c^2} \right]$$
$$+ \beta_0 \frac{T^3}{T_c^3} + \beta_1 \frac{T^4}{T_c^4},$$

where

$$\alpha_2 = \frac{6}{(\kappa-1)(\kappa-2)(\kappa-3)}$$
$$\times \left(\frac{4\pi^2 k_B^3 T_c^3}{135\sqrt{3} J^3} - \alpha_1(\kappa-1) + \beta_1 - \ln(2) \right);$$

$$\beta_0 = \frac{\kappa}{(\kappa-3)} \left(\frac{4\pi^2 k_B^3 T_c^3}{45\sqrt{3}\kappa J^3} + \alpha_1(\kappa-1) - \beta_1 + \ln(2) \right),$$

$$\beta_1 = \ln 2 - J^2 \frac{6(A^+/A^- + 1) + \kappa(\kappa-5)}{64\kappa k_B^2 T_c^2 A^+/A^-} - \frac{4\pi^2 k_B^3 T_c^3}{135\sqrt{3} J^3}.$$

The first and last terms in $S(T \leq T_c)$ embody the critical phenomena and allow for the continuous interpolation with $S(T \geq T_c)$, respectively, whereas the remaining terms are included to retrieve the correct low-temperature behavior.

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