Interaction-Induced Adiabatic Cooling and Antiferromagnetism of Cold Fermions in Optical Lattices

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We propose an interaction-induced cooling mechanism for two-component cold fermions in an optical lattice. It is based on an increase of the spin entropy upon localization, an analogue of the Pomeranchuk effect in liquid helium 3. We discuss its application to the experimental realization of the antiferromagnetic phase. We illustrate our arguments with dynamical mean-field theory calculations.

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Cold atoms in optical lattices [1] offer a promising laboratory for the study of strongly correlated systems, bringing quantum optics to have bearing on key issues in condensed matter physics. Pioneering experiments on the Mott insulator to superfluid transition [2] have demonstrated the possibility [3] of probing quantum phase transitions between different ground states of these systems. Recently, great progress has been achieved on cold Fermi gases as well, resulting in the production of molecular condensates in trapped gases [4–7] and the first imaging of Fermi surfaces in a three-dimensional optical lattice [8]. Controllability is one of the most remarkable aspects of these systems, with the possibility of tuning both the tunneling amplitude between lattice sites (t) and the on-site interaction strength (U), by varying the depth of the optical lattice and by varying the interatomic scattering length thanks to Feshbach resonances.

In this Letter, we consider fermionic atoms with two hyperfine (''spin'') states in an optical lattice. When the lattice is deep and the scattering length is small (see below for a precise condition), a one-band Hubbard model is realized. The main physical effect studied in this Letter is the possibility of cooling down the system by increasing the interaction strength adiabatically. As described below, this is due to a higher degree of localization—and hence an increase in spin entropy—as U/t or the temperature is increased. This is a direct analogue of the Pomeranchuk effect in liquid helium 3. This mechanism relies on interactions and should be distinguished from the adiabatic cooling for noninteracting atoms in the lattice discussed in [9,10]. The second main goal of the present Letter is to study how this effect can be used in order to reach the phase with antiferromagnetic (AF) long-range order. For deep lattices (large U/t), the Néel temperature is expected to become very low, of the order of the magnetic superexchange $J_{\mathrm{AF}} = 4t^2/U$. Naively, it would seem that this requires extreme cooling of the gas. Here, we point out that the appropriate concept is actually the entropy along the antiferromagnetic critical line, and that at large U/t this quantity tends to *a finite constant* which depends only on the specific lattice. Hence, cooling the gas down to a temperature corresponding to this finite entropy per atom, and then following equal-entropy trajectories, should be enough to reach the magnetic phase. These physical observations are substantiated by theoretical calculations using, in particular, dynamical mean-field theory (DMFT) [11,12], an approach that has led to important progress on strongly correlated fermion systems in recent years.

We consider the one-band repulsive Hubbard model:

$$H = -\sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where i and j are site indices on the lattice, and $\sigma = \uparrow, \downarrow$ is a spin index associated with the two hyperfine states. The conditions under which two-component fermionic atoms in an optical lattice actually realize such a single-band lattice model will be discussed later. On an unfrustrated bipartite three-dimensional lattice (e.g., the cubic lattice), with hopping between nearest-neighbor sites $t_{ij} = t$, and for one particle per site on average (half filling), the physics of this model is rather well understood (see, e.g., [13]). For temperatures above the Néel critical temperature T_N, the system is a paramagnet with an increasing tendency to Mott localization as U/t is increased (the Mott gap becomes of order U at large U/t). For $T < T_N$, the antiferromagnetic phase (Fig. 1) displays a two-sublattice spin ordering and a doubling of the unit cell. At weak coupling (small U/t), this is a spin-density wave instability with a weak modulation of the sublattice magnetization. In this regime, T_N is exponentially small in t/U, as a simple Hartree mean-field theory suggests. At strong coupling (large U/t), the low-energy sector of the model is described by a Heisenberg exchange Hamiltonian $J_{\mathrm{AF}} \Sigma_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$, with $J_{\mathrm{AF}} = 4t^2/U$. In this Heisenberg limit, $T_N = \theta J_{\mathrm{AF}}$, with θ a numerical constant depending on the lattice ($\theta = 0.957$ for the cubic lattice [13]). These two regimes are connected by a smooth crossover (which is equivalent to the Bose-Einstein-condensation–BCS cross-

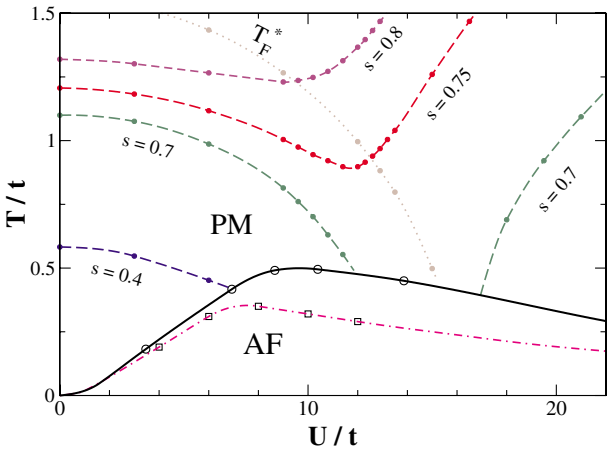

FIG. 1 (color online). Phase diagram of the half-filled Hubbard model on the cubic lattice: antiferromagnetic (AF) and paramagnetic (PM) phases. Transition temperature within DMFT approximation (solid curve, open circles) and QMC calculation of Ref. [13] (dot-dashed curve, squares). Dashed lines: isentropic curves ($s = 0.4, 0.7, 0.75, 0.8$), computed within DMFT. Dotted line: quasiparticle coherence scale $T_F^*(U)$. The DMFT results were obtained with QMC calculations (for T_N) and the IPT approximation [11] (for the isentropics). The transition curves are interpolations, continued at high U/t using the analytical expressions for the Heisenberg regime.

over at half filling). The Néel temperature displays a maximum at intermediate coupling, as a function of U/t. This is illustrated by Fig. 1, in which we display our calculation of T_N vs U/t, using the DMFT approximation on the cubic lattice and the quantum Monte Carlo (QMC) Hirsch-Fye algorithm. DMFT overestimates T_N by about 50% in the intermediate coupling regime, in comparison to the direct QMC calculations of Ref. [13] on the cubic lattice (also displayed in Fig. 1).

We now discuss how the entropy varies as the effective strength of the on-site interaction U/t is changed in the paramagnetic phase. Since all properties depend on the ratios T/t and U/t, we can consider that the hopping is fixed and that T and U are varied, or alternatively that both the temperature and coupling are measured in units of t, the natural unit of kinetic energy. Denoting by f and s the free energy and entropy per lattice site, respectively, one has $s = -\partial f/\partial T$ and $\partial f/\partial U = d$, with d the probability that a given site is doubly occupied: $d \equiv \langle n_{i\uparrow} n_{i\downarrow} \rangle$. We thus obtain

$$\frac{\partial s}{\partial U} = -\frac{\partial d}{\partial T}. \tag{2}$$

This equation can be used to discuss qualitatively the shape of the isentropic curves $T_i = T_i(U)$ in the (U, T) phase diagram, along which $s(T_i(U), U) = \text{const}$. Taking a derivative of this equation yields

$$c(T_i)\frac{\partial T_i}{\partial U} = T_i \frac{\partial d}{\partial T}\bigg|_{T=T_i}, \tag{3}$$

in which $c = T\partial s/\partial T$ is the specific heat per lattice site. Fortunately, the temperature dependence of the probability of double occupancy $d(T)$ has been studied in previous work by one of the authors [14,15] and others [16]. It was observed that, when U/t is not too large, the double occupancy first *decreases* as temperature is increased from $T = 0$ (indicating a higher degree of localization), and then turns around and grows again. This is shown in Fig. 2 using DMFT calculations. This apparently counterintuitive behavior is a direct analogue of the Pomeranchuk effect in liquid helium 3: Since the (spin) entropy is larger in a localized state than when the fermions form a Fermi liquid (in which $s \propto T$), it is favorable to increase the degree of localization upon heating. The minimum of $d(T)$ essentially coincides with the quasiparticle coherence scale $T_F^*(U)$, which is a rapidly decreasing function of U (Fig. 1). This phenomenon therefore applies only as long as $T_F^* > T_N$, and hence when U/t is not too large. For large U/t, Mott localization dominates for all temperatures $T < U$ and suppresses this effect. Since $\partial d/\partial T < 0$ for $T < T_F^*(U)$ while $\partial d/\partial T > 0$ for $T > T_F^*(U)$, Eq. (3) implies that the isentropic curves of the half-filled Hubbard model (for not too high values of the entropy) must have a negative slope at weak to intermediate coupling, before turning around at stronger coupling. In order to substantiate this behavior, inferred on rather general grounds, we have performed DMFT calculations of the isentropic curves, with results displayed in Fig. 1. The entropy $s(T)$ was calculated by integrating the internal energy per site $e(T)$ according to $s(T) = \ln 4 + e(T)/T - \int_T^\infty dT' e(T')/T'^2$, which follows from the thermodynamic relation $\partial_T e = T\partial_T s$. The DMFT equations were solved using the "iterated perturbation theory" (IPT) approximation [11] (using, for simplicity, a semicircular density of

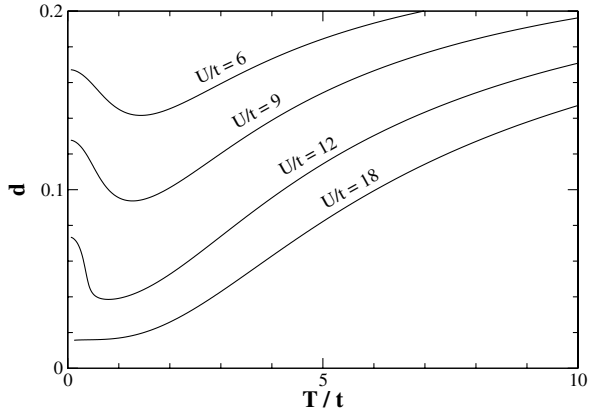

FIG. 2. Double occupancy $d = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ as a function of temperature, for several values of U/t, calculated within DMFT (IPT). The initial decrease is the Pomeranchuk effect responsible for adiabatic cooling.

states), and the internal energy was calculated from the one-particle Green's function.

It is clear from the results of Fig. 1 that, starting from a low enough initial value of the entropy per site, adiabatic cooling can be achieved by either increasing U/t starting from a small value or decreasing U/t starting from a large value (the latter, however, requires one to cool down the gas while the lattice is already present). We emphasize that this cooling mechanism is an interaction-driven phenomenon: indeed, as U/t is increased, it allows one to lower the *reduced temperature* T/t, normalized to the natural scale for the Fermi energy in the presence of the lattice. Hence, cooling is not simply due to the tunneling amplitude t becoming smaller as the lattice is turned on. At weak coupling and low temperature, the cooling mechanism can be related to the effective mass of quasiparticles ($\propto 1/T_F^*$) becoming heavier as U/t is increased, due to Mott localization. Indeed, in this regime, the entropy is proportional to $T/T_F^*(U)$. Hence, conserving the entropy while increasing U/t adiabatically from $(U/t)_i$ to $(U/t)_f$ will reduce the final temperature in comparison to the initial one T_i according to $T_f/T_i = T_F^*(U_f)/T_F^*(U_i)$.

At this stage, let us briefly discuss the validity of the DMFT approach, extensively used in the present work. In this approach, the lattice model is mapped onto a single-site quantum problem coupled to a self-consistent effective medium. This is an approximation, which becomes exact only in the limit of infinite lattice coordination [11]. As a local approach, it underestimates the precursor antiferromagnetic correlations above T_N, which will in turn quench the entropy and ultimately play against the cooling mechanism very close to T_N. However, as long as the correlation length is not too large, a local approximation should be accurate. Indeed, the existence of a minimum in $d(T)$ has been confirmed by the calculations of Ref. [17] using a different method, for a three-dimensional lattice, suggesting that the cooling mechanism discussed here is a robust effect.

The isentropic curves in Fig. 1 suggest that interaction-induced adiabatic cooling could be used in order to reach the magnetically ordered phase. To explore this idea in more details, we focus on the entropy along the Néel critical boundary $s_N(U) \equiv s(T_N(U), U)$. At weak coupling (the spin-density wave regime), $s_N(U)$ is expected to be exponentially small. In contrast, in the opposite Heisenberg regime of large U/t, s_N will reach a finite value s_H, which is the entropy of the quantum Heisenberg model at its critical point. s_H is a pure number which depends only on the specific lattice of interest. Mean-field theory of the Heisenberg model yields $s_H = \ln 2$, but quantum fluctuations will reduce this number. We have performed a Schwinger boson calculation of this quantity, along the lines of [18,19], and found that this reduction is of the order of 50% on the cubic lattice. How does s_N evolve from weak to strong coupling? A rather general argument suggests that it should go through a maximum $s_{\max} > s_H$. In order to see this, we use again (2) and take a derivative of $s_N = s(T_N(U), U)$, which yields

$$\frac{ds_N}{dU} = \frac{c(T_N)}{T_N}\frac{dT_N}{dU} - \left.\frac{\partial d}{\partial T}\right|_{T=T_N}. \tag{4}$$

If only the first term was present on the right-hand side of this equation, it would imply that s_N is maximum exactly at the value of the coupling where T_N is maximum [note that $c(T_N)$ is finite ($\alpha < 0$) for the 3D Heisenberg model [20]]. However, in view of the above properties of the double occupancy, the second term on the right-hand side has a similar variation than the first one: it starts positive, and then changes sign at an intermediate coupling when $T_F^*(U) = T_N(U)$. These considerations suggest that $s_N(U)$ does reach a maximum value at intermediate coupling, in the same regime where T_N reaches a maximum. Hence, $s_N(U)$ has the general form sketched in Fig. 3. This figure can be viewed as a phase diagram of the half-filled Hubbard model, in which *entropy itself is used as a thermometer*, a very natural representation when addressing adiabatic cooling. Experimentally, one may first cool down the gas (in the absence of the optical lattice) to a temperature where the entropy per particle is lower than s_H (this corresponds to $T/T_F < s_H/\pi^2$ for a trapped ideal gas). Then, by branching on the optical lattice adiabatically, one could increase U/t until one particle per site is reached over most of the trap: this should allow one to reach the antiferromagnetic phase. Assuming that the time scale for adiabaticity is simply set by the hopping, we observe that typically $\hbar/t \sim 1$ ms.

Let us now discuss the conditions under which two-component fermions in an optical lattice are accurately described by the Hubbard Hamiltonian (1) (see also [1,3]). The many-body Hamiltonian is written in second-

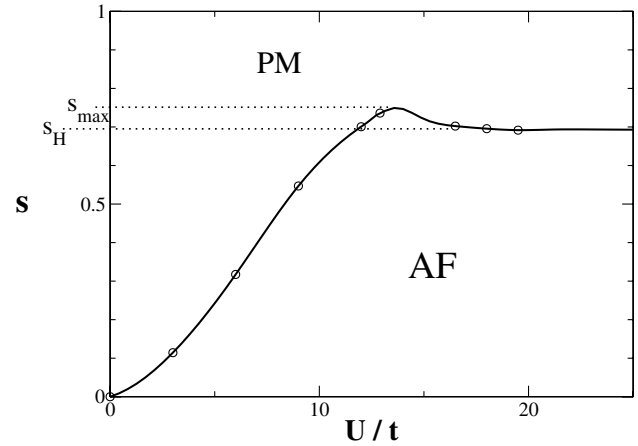

FIG. 3. Phase diagram as a function of entropy. The displayed curve results from a DMFT-IPT calculation (in which case $s_H = \ln 2$), but its shape is expected to be general (with s_H reduced by quantum fluctuations).

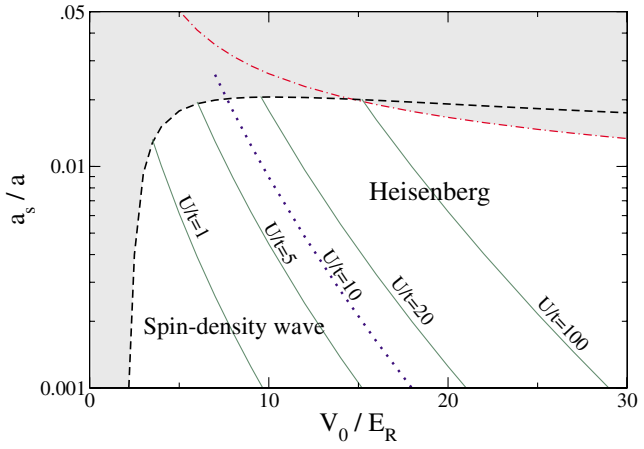

FIG. 4 (color online). Spin-density wave and Heisenberg regimes as a function of the depth of the periodic potential V_0 and the scattering length a_s. The crossover between these regimes is indicated by the dotted line ($U/t = 10$), where T_N/t is maximum (other contour lines are also indicated). In the shaded region, the one-band Hubbard description is no longer valid. Above the dashed line ($U/\Delta > 0.1$), other bands must be taken into account and the pseudopotential approximation fails. Above the dashed-dotted line, non-Hubbard interaction terms become sizeable ($t_d/t > 0.1$, see text).

quantized form using as single-particle basis functions the Wannier functions associated with the periodic potential $V_{\rm opt}(\vec{r}) = V_0 \Sigma_{i=1}^{3} \sin^2(\pi x_i/a)$ (the lattice spacing is $a = \lambda/2$, with λ the wavelength of the laser). The interaction terms are obtained as matrix elements of the low-energy effective potential $V_{\rm int}(\vec{r}_1 - \vec{r}_2) = \frac{4\pi\hbar^2 a_s}{m} \delta^3(\vec{r}_1 - \vec{r}_2)$, where a_s is the scattering length. In general, this results in a multiband model which, besides the on-site Hubbard interaction, involves also more complicated interaction terms such as nearest-neighbor interactions or density-assisted hopping terms of the form $t_d c_i^\dagger c_j n_i$, with i and j neighboring sites. By explicitly computing these terms, as well as the one-body part of the Hamiltonian, we examined under which conditions (i) the reduction to a one-band model is valid and (ii) these non-Hubbard interactions are negligible. This determines a domain in the $(V_0/E_R, a_s/a)$ plane (with $E_R = \hbar^2\pi^2/2ma^2$ the recoil energy), which is depicted in Fig. 4. Condition (i) requires, in particular, that the on-site Hubbard repulsion is smaller than the gap Δ between the first and the second band: $U \ll \Delta$. At large values of V_0/E_R, it can be shown that this is also the condition for our use of the pseudopotential approximation to be valid: $a_s \ll l_0$, with l_0 the spatial extension of the Wannier function of the first band. We found that the stricter condition of type (ii) originates from density-assisted hopping terms which should obey $t_d \ll t$. We also displayed in Fig. 4 some contour lines associated with a given value of U/t. The one associated with $U/t \approx 10$ can be taken as the approximate separatrix between the spin-density wave and Heisenberg antiferromagnetic regions. T_N/t is maximal along this line, and $T_N < 0.015 E_R$ in the allowed region. Thus adiabatic cooling is important to reach the AF phase. Since V_0 and a_s are the two experimentally tunable parameters, Fig. 4 aims at summarizing useful information for such experimental investigations. The detection of the antiferromagnetic long-range order might be achieved by spin-selective Bragg spectroscopy in order to reveal the doubling of the unit cell. The two hyperfine states could be distinguished by their Zeeman splitting or by using polarized light. A different method, which has been recently proposed [21] and investigated experimentally [22], is to use quantum noise interferometry.

To summarize, in this Letter we propose an interaction-induced cooling mechanism for two-component cold fermions in an optical lattice. One possible application of this mechanism is in reaching the phase with antiferromagnetic long-range order.

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