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Fermions in 3D Optical Lattices: Cooling Protocol to Obtain Antiferromagnetism

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A major challenge in realizing antiferromagnetic (AF) and superfluid phases in optical lattices is the ability to cool fermions. We determine the equation of state for the 3D repulsive Fermi-Hubbard model as a function of the chemical potential, temperature and repulsion using unbiased determinantal quantum Monte Carlo methods, and we then use the local density approximation to model a harmonic trap. We show that increasing repulsion leads to cooling, but *only in a trap*, due to the redistribution of entropy from the center to the metallic wings. Thus, even when the average entropy per particle is *larger* than that required for antiferromagnetism in the homogeneous system, the trap enables the formation of an AF Mott phase.

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Introduction: One of the most exciting themes in condensed matter physics is how complex states of matter emerge from simple Hamiltonians. In particular, the repulsive Fermi-Hubbard model gives rise to a rich variety of behavior, including a Mott insulating regime, an antiferromagnetically ordered Néel state, and possibly a "high-temperature" d-wave superfluid.

Cold atomic gases are unique in being clean and tunable systems that offer tremendous promise for exploring such Hamiltonians. The Fermi-Hubbard model can be emulated using an optical lattice with two hyperfine species of fermions [1]. Several experimental feats have already been accomplished: the observation of sharp Fermi surfaces for free fermions in an optical lattice [2], and of the Mott insulating regime for repulsively interacting fermions [3, 4]. The next step in this quest is to go to even lower temperatures, where the local moments order to form a Néel antiferromagnet.

In this Letter we present an adiabatic cooling protocol for trapped systems, which we expect to play an important role in the race for finding antiferromagnetism in the repulsive Hubbard model and for opening the door toward the search for the d-wave superfluid state. We first calculate the thermodynamics of a homogeneous system using unbiased determinantal quantum Monte Carlo (DQMC) as a function of filling and temperature, accessing both paramagnetic and AF phases. At half-filling, this allows us to obtain the entropy down to $T = 0.1t$ (see Fig. 1(b)), well below the maximum Néel temperature $T_N \approx 0.36t$ [6], and also well below the temperatures accessed by recent cluster studies [5].

We next use the local density approximation to treat the effect of a harmonic trap. We demonstrate that increasing the repulsion U adiabatically leads to substantial cooling, *but only in the presence of the trap* (see Fig. 2). During this process, the cloud expands and entropy gets redistributed from the center to the metallic wings. Even though the average entropy per particle $S/N \approx 0.65k_B$ is higher than the critical entropy of the homogeneous system ($0.4k_B$ at $U/t = 8$), we see from Fig. 3 that it is possible to generate an AF state at the center; see also Ref. 5.

Model and methods: We consider the Fermi-Hubbard Hamiltonian,

$$\mathcal{H} = - t \sum_{\langle \mathbf{r}\mathbf{r}'\rangle\sigma} (c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma}) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} + \sum_{\mathbf{r}} (V_t\, \mathbf{r}^2 - \mu)(n_{\mathbf{r}} - 1), \quad (1)$$

in which $\mathbf{r}$ labels a site (or well) of a 3D cubic optical lattice, $\sigma = \uparrow$ or $\downarrow$ corresponds to two hyperfine states, t is the nearest-neighbor hopping amplitude, U is the on-site interaction energy, $c_{\mathbf{r}\sigma}$ is the fermion destruction operator at site $\mathbf{r}$ with spin σ, and $n_{\mathbf{r}\sigma} = c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}\sigma}$ with $n_{\mathbf{r}} = \sum_\sigma n_{\mathbf{r}\sigma}$. The curvature $V_t = \frac{1}{2} m\omega_0^2 d^2$ describes harmonic confinement with trap frequency $\omega_0/2\pi$, fermion mass m, and lattice spacing d. The chemical potential μ controls the average density. The parameters t and U can be directly related [8] to the lattice depth, set by the laser intensity, and to the interatomic interaction tuned by a Feshbach resonance. This Hamiltonian is valid in the regime where only a single band is populated in the optical lattice. Following Ref. 4 we define the characteristic trap energy $E_t = V_t(3N/8\pi)^{2/3}$. This is equivalent to using the characteristic density [9] $\tilde{\rho} = N(4V_t/t)^{3/2}$ obtained by normalizing N with the length scale $\xi = (4V_t/t)^{-1/2}$, with $E_t \propto \tilde{\rho}^{2/3}$.

We calculate the density ρ, energy density E, double occupancy $D = \langle n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}\rangle$, and spin correlations for a homogeneous system ($V_t = 0$) as a function of μ, T, and U/t using DQMC simulations [10, 11].

Half-filling: We first focus on the homogeneous case at half-filling ($\mu = 0$) and $U/t = 8$, where the Néel temperature $T_N/t = 0.36$ is highest [6]. At $\mu = 0$ DQMC is free of the fermion sign problem and we can access low temperatures down to $T = 0.1t$, well into the AF phase. We perform extrapolation on $E(T)$ to the limit

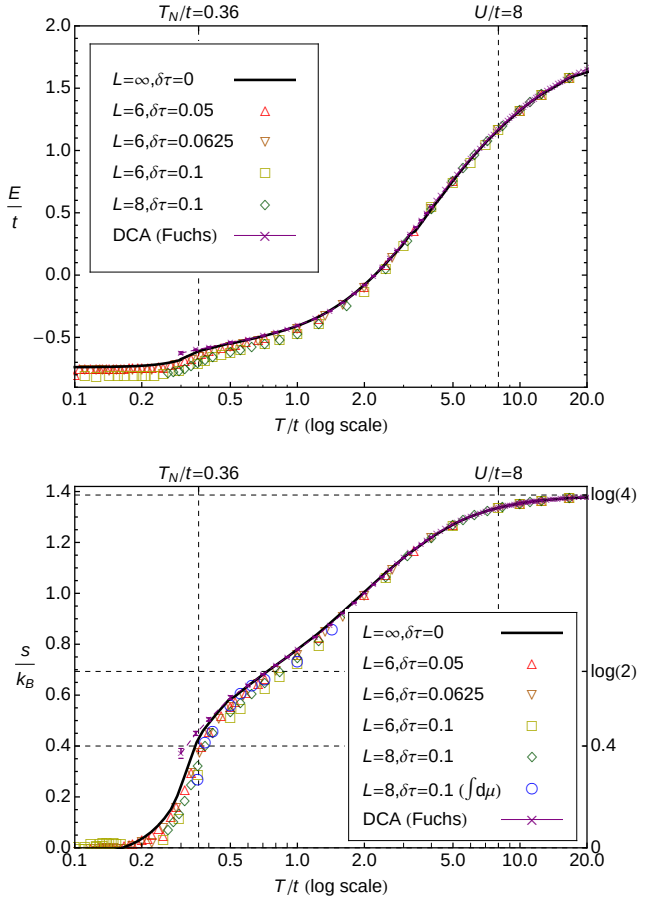

FIG. 1: **(a) Energy per site of homogeneous system** at half-filling and $U/t = 8$, calculated using DQMC down to $T/t = 0.1$. Statistical error bars are smaller than symbols. The solid curve is the entropy extrapolated to $L = \infty$ and $d\tau = 0$ (details in supplement). **(b) Entropy per site** obtained by integrating down from $T = \infty$, showing a shoulder at the Mott scale $T_{\rm Mott} \simeq U$ and a distinct feature at the Néel temperature $T_N \approx 0.36t$ due to critical fluctuations. Errors in E/t and s/k_B are both about 0.02. Our extrapolated results are fully consistent, within error bars, with the DCA results from Fuchs *et al.* [5].

of zero imaginary-time discretization ($\delta\tau = 0$) and infinite system size ($L^3 = \infty$), as described in detail in the supplement. The high statistical accuracy of the DQMC data even reveals critical fluctuations near T_N.

We obtain the ground state energy $E_0/t = -0.74(2)$ and the correct low-temperature behavior ($E \sim T^4$) expected for an antiferromagnet with linearly dispersing spin waves. The results are shown in Fig. 1(a). Integrating $E(T)$ down from infinite temperature, we determine the entropy per site using $s(T) = \ln 4 + E/T - \int_T^\infty dT\, E/T^2$. Our results agree with extrapolated results from the dynamical cluster approximation (DCA) [5], available only in the paramagnetic phase.

We see from Fig. 1(b) that as the temperature is reduced below $U = 8t$, the entropy per site s/k_B decreases from ln(4) to ln(2), due to suppression of double occupancy below the Mott scale for charge fluctuations. At T_N the critical entropy is $s_N/k_B \approx 0.4k_B$, consistent with Ref. 5. Our DQMC results show a steep drop in entropy below T_N resulting from spin ordering.

In Fig. 2(a), we show constant-entropy curves in the (T, U) plane at half-filling. We also plot the Néel temperature as a function of U obtained from previous QMC simulations [6] together with its asymptotic forms at weak and strong coupling. The dashed curve is $0.282T_{\rm MF}(U/t)$ where the mean-field result is given by $2/U = \sum_k \tanh(2\epsilon_k/T_{\rm MF})/\epsilon_k$ and the suppression factor 0.282 arises from $O((U/t)^2)$ vertex corrections [12, 13]. The dotted curve shows the strong-coupling Heisenberg limit result $3.78t^2/U$ [14].

Away from half-filling: We next compute the equation of state $\rho(\mu)$ of the homogeneous system away from half-filling, as this will be needed to study the effect of a trap. We now obtain the entropy by integrating along an isotherm from the empty lattice, $s(\mu) = \int_{-\infty}^{\mu} d\mu\ (\partial s/\partial\mu)_T$, making use of the Maxwell relation $(\partial s/\partial\mu)_T = (\partial\rho/\partial T)_\mu$, where $(\partial\rho/\partial T)_\mu$ is evaluated using a finite difference scheme. This gives results (indicated by symbols labelled "$\int d\mu$" in Fig. 1(b)) consistent with integration of $E(T)$ as described above.

We model the trap using the local density approximation (LDA), in which local observables are given by their homogeneous values evaluated at a chemical potential $\mu(r) = \mu_0 - V_t\mathbf{r}^2$. The LDA is very accurate for *local* quantities such as entropy or number density, as has been established by QMC calculations in the presence of a trap [15, 16]. The chemical potential at the trap center μ_0 is determined from the total fermion number $N = \int_0^\infty dr\ 4\pi r^2\rho(\mu(r))$. We obtain density, entropy, and local spin correlation profiles such as those in Figs. 3 and 4, from which we can deduce a route to achieving cooling in optical lattices.

Cooling: Note the contrast between the constant-entropy curves in the homogeneous system at half-filling (Fig. 2(a)) and in a harmonic trap with $E_t = 3.28t$ (Fig. 2(b)). For a given entropy per particle S/N the temperature of the trapped system is already lower than that of the homogeneous system at $U = 0$. Furthermore, as U is ramped up, the trapped system exhibits significant cooling compared to the homogeneous system. Thus we see that for $E_t = 3.28t$ and any starting entropy less than $0.65k_B$, one can obtain an AF core by adiabatic cooling (see Fig. 2(c)).

We gain further insight from the profiles shown in Fig. 3(a,b,c). As the interaction is ramped up from $U/t = 0$ to 8, the cloud expands and the density at the center decreases towards 1, characteristic of a Mott insulator (MI). This MI has a gap to charge excitations and thus a low entropy. On the other hand, the metallic state in the wings, with its low-energy spin and charge excitations, can act as an entropy sink. Although the central entropy density changes non-monotonically with

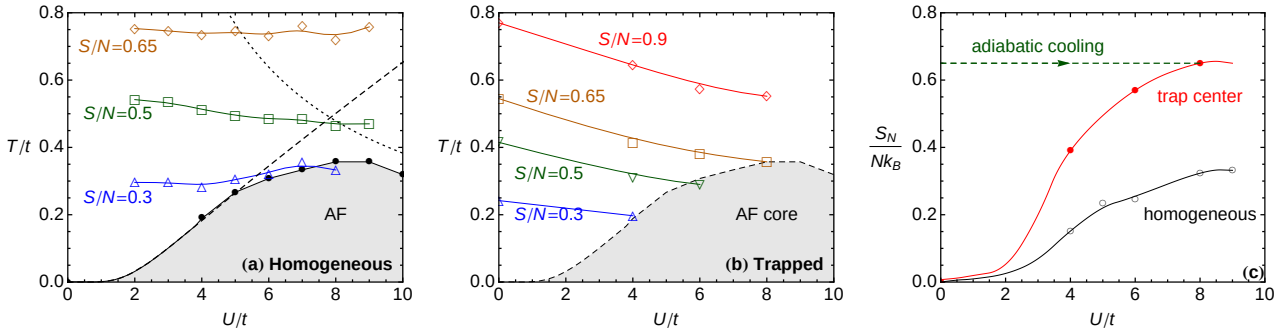

FIG. 2: (a) Constant-entropy curves of a homogeneous system at half-filling [7]. There is no clear evidence for "Pomeranchuk" cooling as U is increased adiabatically, in marked contrast to (b). The filled symbols are QMC values for T_N from Ref. 6, and the dashed and dotted curves are weak- and strong-coupling asymptotic forms (see text). (b) In a harmonic trap with $E_t = 3.28t$, ramping up U adiabatically produces significant cooling due to entropy redistribution. An AF state can be produced in the trap center even for an overall entropy per particle $S/N \approx 0.65k_B$. (c) Average entropy per particle in a harmonic trap below which AF order exists at the center. This is significantly higher than the critical entropy of a homogeneous system.

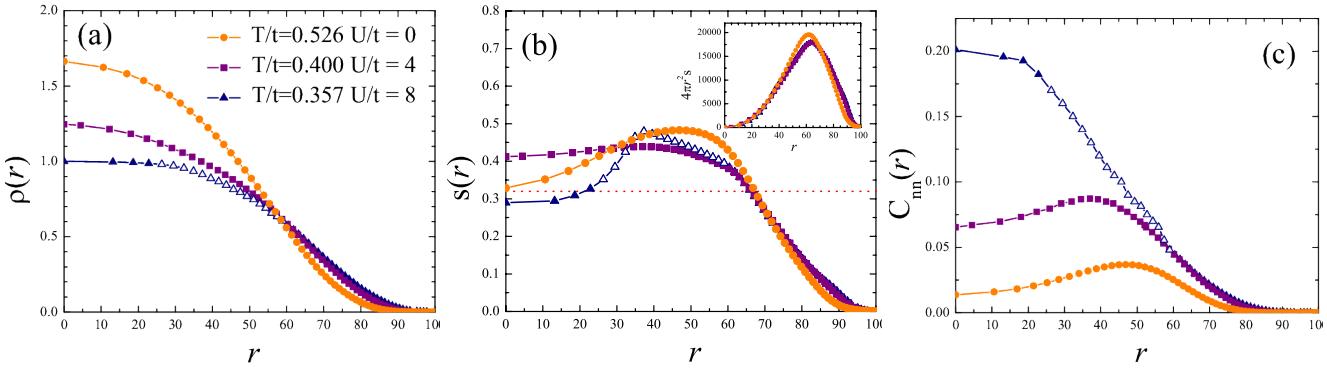

FIG. 3: **Cooling by increasing interaction:** Adiabatic evolution of a cloud of $N = 1.3 \times 10^6$ particles with increasing interaction U for a fixed total entropy per particle $S/N = 0.65k_B$ and trap compression $E_t/t = 3.28$. In going from $U/t = 0$ to 8, entropy is ultimately transferred from the core to the wings (or outer shell) at $r > 70$, with $S = \int_0^\infty dr\ 4\pi r^2 s(r)$ remaining constant. The integrand $4\pi r^2 s(r)$ is shown in the inset.

U, eventually there is a transfer of entropy from the center to the wings leading to a Mott core.

During this process the temperature falls from $T/t = 0.53$ to $0.36 \approx T_N$. In the final state, the entropy density $s(r)$ at the center is near the critical value for AF ordering indicated by the dashed line [7]. We see the growth of local antiferromagnetic correlations from the nearest-neighbor spin-spin correlation $C_{nn}(r) = -\langle \mathbf{S_r} \cdot \mathbf{S_{r+\hat{x}}} \rangle$, where $\mathbf{S_r} = \frac{1}{2} \sum_{\alpha\beta} \boldsymbol{\sigma}_{\alpha\beta} c^\dagger_{\mathbf{r}\alpha} c_{\mathbf{r}\beta}$ is the spin at site $\mathbf{r}$.

Our analysis shows that the adiabatic cooling in a trap results from entropy redistribution, and not from a Pomeranchuk effect in the homogeneous equation of state [17, 18] as discussed below. In any case, we do not find a significant Pomeranchuk effect $(\partial T/\partial U)_S < 0$ in DQMC, either in 3D (see Fig. 2(a)) or in 2D [19, 20].

Another way to cool in a trap is to use adiabatic expansion, a standard cryogenic technique, the results for which are shown in Fig. 4. We see that as E_t/t decreases from 21.93 to 3.28, the core goes from a band insulator to an antiferromagnetic MI.

In Figs. 3 and 4 the open symbols used only at the lowest temperature ($T/t = 0.36t$) denote regions of the trap away from half-filling where the DQMC sign problem is significant. In this range we have used a combination of interpolation and results from smaller systems (for which the sign problem is less severe).

We now remark on the temperature dependence of the double occupancy D of the homogeneous system at half-filling, shown in Fig. 5. As T decreases below the U, D is generally suppressed due to Mott physics, so that $(\partial D/\partial T)_U > 0$. At low temperature for intermediate $U/t = 4$ to 6, D shows anomalous behavior in that $(\partial D/\partial T)_U < 0$ over a range of T close to T_N. Using a Maxwell relation, $(\partial D/\partial T)_U = (\partial D/\partial S)_U (\partial S/\partial T)_U = (\partial T/\partial U)_S \times C/T$, so that $(\partial T/\partial U)_S < 0$, suggesting the possibility of "Pomeranchuk cooling" [17] by adiabatically increasing the interaction. This effect is smaller in DQMC than predicted by DMFT. When corrections for finite $\delta\tau$ are made, the DQMC and DCA [5] data are in fact in very good agreement [21]. Thus the "Pomer-

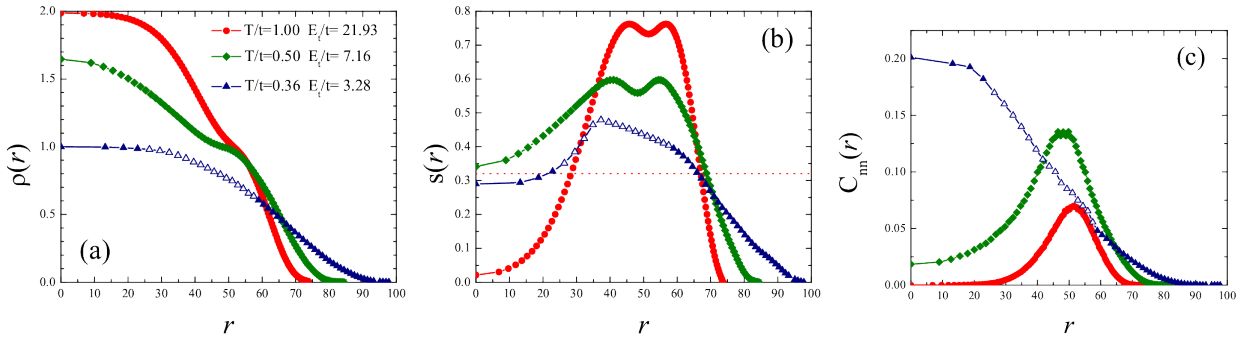

FIG. 4: **Cooling by expansion:** Adiabatic evolution of a cloud of $N = 1.3 \times 10^6$ particles with decreasing trap energy E_t for a fixed total entropy per particle $S/N = 0.65k_B$ at interaction $U/t = 8$.

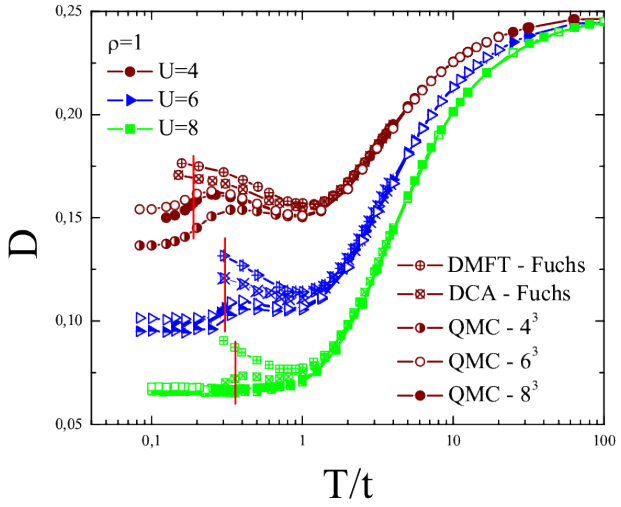

FIG. 5: **Double occupancy** $D(T)$ for the homogeneous system at half-filling for $U/t = 4, \delta\tau = 0.125$; $U/t = 6, \delta\tau = 0.125$; and $U/t = 8, \delta\tau = 0.1$. The vertical red lines correspond to $T_N(U)$.

anchuk effect" in a homogeneous system is insignificant, as already shown in Fig. 2(a).

Discussion and conclusion: To conclude, our most significant observation is that it is possible to lower the temperature of the *trapped* system by suitable adiabatic processes. Cooling results from entropy redistribution in a trap with the metallic wings acting as entropy sinks. We find that an average entropy per particle in the trap $S/N = 0.65k_B$ is sufficiently low to produce an AF state at the center using our adiabatic cooling protocol [5]. In order to go well below T_N a correspondingly lower entropy is required.

The results for the trapped system are markedly different from those for the homogeneous system. First, the maximum critical entropy of a homogeneous AF state occurring at $U = 8t$ is $0.4k_B$, considerably lower than the average value required in a trap. Second, adiabatically increasing U in the homogeneous case does not lead to significant cooling.

We finally discuss the implications for optical lattice experiments [3, 4]. Before the lattice is turned on, the initial temperature of a trapped gas is typically $T_i \sim 0.1T_F$ where the Fermi temperature $k_B T_F = \hbar\omega_0(3N)^{1/3}$. For non-interacting fermions, an initial temperature $T_i/T_F \approx 0.06$, within the reach of current experiments, corresponds to an average entropy per particle $S/N = 0.65k_B$ in the trap. As noted above, this leads to an AF state at the center, which can be probed by the growth of nearest-neighbor spin-spin correlations. Thus, the results presented here imply that antiferromagnetism is achievable in optical lattices, provided that adiabaticity can be maintained during our cooling protocol.

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