Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity

Thereza Paiva,[1] Richard Scalettar,[2] Mohit Randeria,[3] and Nandini Trivedi[3]

[1]*Instituto de Fisica, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[2]*Department of Physics, University of California, Davis, California 95616, USA*
[3]*Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA*

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One of the major challenges in realizing antiferromagnetic and superfluid phases in optical lattices is the ability to cool fermions. We determine constraints on the entropy for observing these phases in two-dimensional Hubbard models using determinantal quantum Monte Carlo simulations. We find that an entropy per particle $\simeq \ln 2$ is sufficient to observe the insulating gap in the repulsive Hubbard model at half-filling, or the pairing pseudogap in the attractive case. Observing antiferromagnetic correlations or superfluidity in 2D systems requires a further reduction in entropy by a factor of 3 or more. In contrast with higher dimensions, we find that adiabatic cooling is not useful to achieve the required low temperatures. We also show that double-occupancy measurements are useful for thermometry for temperatures greater than the nearest-neighbor hopping energy.

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An exciting new development in cold atoms is the ability to realize in the laboratory simple models of strongly correlated fermions in optical lattices [1–7]. These studies are motivated by their relevance to spectacular phenomena in condensed matter physics, like high T_c superconductivity, that are not fully understood. The best known model is the fermion Hubbard Hamiltonian [8,9] that captures the physics of antiferromagnetism and, at least qualitatively, d-wave superconductivity in two dimensions (2D). The Hubbard model is well understood in one dimension (1D), using exact solutions and bosonization [10], and also in the limit of large dimensions, using dynamical mean field theory (DMFT) [11]. The *two-dimensional* problem, of direct relevance to layered high T_c superconductors, is the least well understood theoretically. New insights into the 2D Fermi Hubbard model can come from cold atom emulators, given their high degree of tunability (interaction, chemical potential) and absence of disorder and material complications.

In cold atom experiments it is the entropy, rather than temperature, that is directly controlled and measured. However, much of our intuition about Hubbard models is as a function of T. Hence it is important to gain insight into various physical phenomena, such as formation of moments or pairs and their ordering, as functions of the *entropy* and interaction parameters. In this Letter we address these questions for 2D Hubbard models using determinantal quantum Monte Carlo (QMC) simulation [8], an unbiased, nonperturbative method which gives exact results (within controlled error bars) on finite lattices.

We investigate two systems, (a) the 2D repulsive ($U > 0$) Hubbard model at half-filling and (b) the 2D attractive ($U < 0$) Hubbard model at any filling, for the following reasons. First, determinantal QMC simulation is free of the fermion ''sign problem'' [12] in both cases. Second, these systems exhibit phenomena of fundamental interest: strong antiferromagnetic correlations and Mott physics for $U > 0$, and a Berezinskii-Kosterlitz-Thouless (BKT) transition to an s-wave superfluid [13] with a pairing pseudogap [14] above T_c for $U < 0$. Finally, both models are realizable in optical lattice experiments, where a Feshbach resonance can be used to change the sign of the interaction.

Our main result is the determination of the characteristic entropy scales as functions of the interaction. These scales correspond to the opening of the insulating gap and to development of significant spin correlations in the $U > 0$ case, and to the pairing pseudogap crossover at T^* and the superfluid phase transition at T_c for $U < 0$. We find that, in the (U/t, s) phase diagram, the characteristic scales saturate to *constant* values of s, the entropy per particle, in the strong coupling $|U|/t \gg 1$ limit, which is qualitatively different from their more familiar behavior in the (U/t, T/t) phase diagram. We present a scaling argument to understand why the ''critical entropy'' at the phase transition saturates, in marked contrast to T_c which decreases in strong coupling. This implies that once the entropy per particle is lowered to a certain value, $s = S/Nk_B \simeq 0.1$, then one can access the broken symmetry phase for arbitrarily large interaction strengths.

In addition, our results on the T dependence of the double occupancy shed light on two distinct questions. We point out the difficulty of using adiabatic cooling in 2D, and determine the regime in which double occupancy can be used for thermometry.

The Hubbard Hamiltonian is $\mathcal{H} = -t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_i(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu\sum_i n_i$. Here i labels a site, or well, of a 2D square optical lattice, with unit lattice spacing $a = 1$, and $\sigma = \uparrow, \downarrow$ corresponds to two hyperfine states of the atom. The hopping t sets the scale for the kinetic energy and U is the on site interaction energy. $c_{i\sigma}$ is

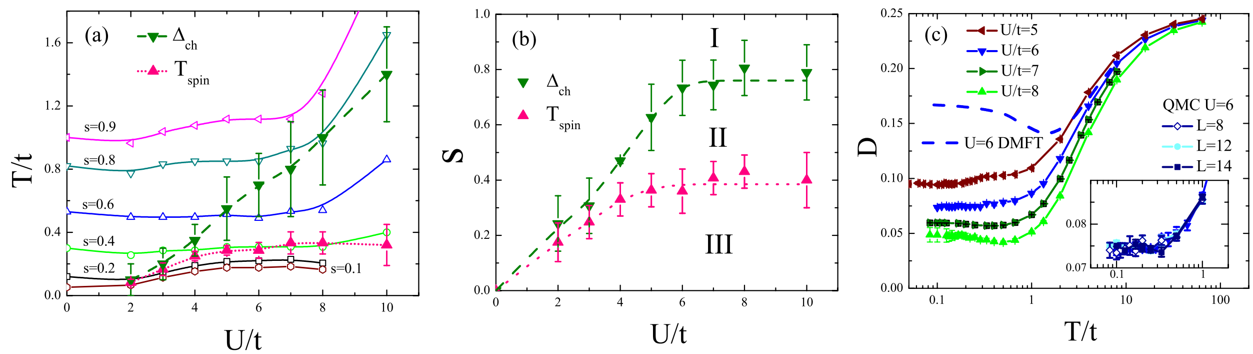

FIG. 1 (color online). (a) Phase diagram of the repulsive ($U > 0$) 2D Hubbard Model at half-filling in the $(U/t, T/t)$ plane obtained from QMC simulations on $N = 10^2$ lattices. Two important crossover scales are denoted by filled symbols: the insulating gap $\Delta_{\rm ch}$ (obtained from the compressibility) and $T_{\rm spin}$ (obtained from the peak in the uniform magnetic susceptibility). We also show curves of constant entropy per particle $s = S/Nk_B$. (b) Phase diagram in the $(s, U/t)$ plane showing the two crossover scales. In the regime I, the system is effectively gapless; in regime II, the insulating gap develops and local moments form; and in regime III, the spins get correlated over ever increasing distances. (c) Temperature dependence of the double-occupancy $D(T)$ for various U/t. Dynamical mean field theory (DMFT) [20] shows a much more pronounced anomalous region with $dD/dT < 0$ compared to our QMC results. The inset shows that D is insensitive to linear system size L.

the fermion destruction operator at site i with spin σ, and densities $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and $n_i = \sum_\sigma n_{i\sigma}$. We need to tune the chemical potential μ to obtain the desired density $\rho = \sum_i \langle n_i \rangle / N$ on an N-site lattice. The hopping t, determined by the overlap of single-particle wave functions localized on near-neighbor sites, leads to the kinetic energy $\epsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a)$. The parameters t and U can be directly related [6,15] to the lattice depth V_0, tuned by the laser intensity, and to the interatomic interaction tuned by a Feshbach resonance. The Hubbard model is valid in the regime where only a single band is populated in the optical lattice.

We first describe the results for the repulsive ($U > 0$) model at half-filling $\rho = 1$. We then turn to the attractive ($U < 0$) case at arbitrary filling $\rho \neq 1$. Taken together, this permits us to discuss the parallels between these two systems and extract some general lessons about 2D lattice fermions.

Repulsive Hubbard model at half-filling.—Our calculations are done at fixed T; thus we begin with the phase diagram in the $(U/t, T/t)$ plane shown in Fig. 1(a). From this we determine the $(U/t, s)$ phase diagram in Fig. 1(b) as explained below. Note that, for the $U > 0$ model at $\rho = 1$, there are no finite temperature phase transitions in 2D. The ground state has long range antiferromagnetic (AFM) order, but, in the thermodynamic limit, this order is destroyed by thermal fluctuations [16] at all $T > 0$ (in contrast to the 3D case). We, nevertheless, see two important *crossover* scales, denoted by filled symbols in Fig. 1(a). The high T crossover corresponds to the opening of the insulating gap, and the low T crossover is due to the growth of AFM order, so that the system appears ordered on *finite* lattices. As described next, both these crossovers have characteristic signatures in physical observables.

(i) Insulating gap: At sufficiently high temperatures, the effect of interactions can be ignored. As we lower the temperature, interactions lead to the opening of an insulating gap in the spectrum of fermionic excitations at half-filling. This results in a characteristic feature in the compressibility: $d\rho/d\mu$ is very small (vanishing at $T = 0$) for $|\mu| < \Delta_{\rm ch}$, which is called the "charge gap". The U/t dependence of the gap $\Delta_{\rm ch}$, obtained from QMC data on the compressibility [15], is shown in Fig. 1(a).

The crossover at $T \approx \Delta_{\rm ch}$ separates the regime of effectively gapless behavior for $T \gg \Delta_{\rm ch}$, from the presence of an insulating gap for $T \ll \Delta_{\rm ch}$. For large U, $\Delta_{\rm ch}$ scales linearly with U and is called the Mott gap, but it becomes (exponentially) small for low U. The qualitative behavior of $\Delta_{\rm ch}$ as a function of U/t is correctly described by a simple mean field theory (MFT), but surprisingly the QMC value of $\Delta_{\rm ch}$ is much smaller [15] than MFT (by as much as a factor of 4 at $U/t = 8$).

We note that the evolution [17] from a weak coupling spin-density wave insulator to a strong coupling Heisenberg-Mott insulator in the $U > 0$ Hubbard model at $\rho = 1$ is the analog of the BCS to Bose-Einstein condensation (BEC) crossover in attractive Fermi systems.

(ii) Spin correlations: For moderate to large U, once the insulating gap is well developed, the double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ is strongly suppressed, as shown in Fig. 1(c), and there are well-defined "spins" or "local moments" formed on each of the lattice sites. At even lower temperatures the moments begin to order, with a correlation length that grows rapidly with decreasing T. We have examined the growth of spin correlations using a variety of observables as functions of T and U/t. These include [15] the magnetic susceptibility $\chi(T)$, spin-spin correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle$, and its Fourier transform, the structure factor $S(\mathbf{q})$.

We plot in Fig. 1(a) the U/t dependence of the characteristic scale $T_{\rm spin}$ for spin correlations. We determine [15] $T_{\rm spin}$ by looking at the maximum in the magnetic suscep-

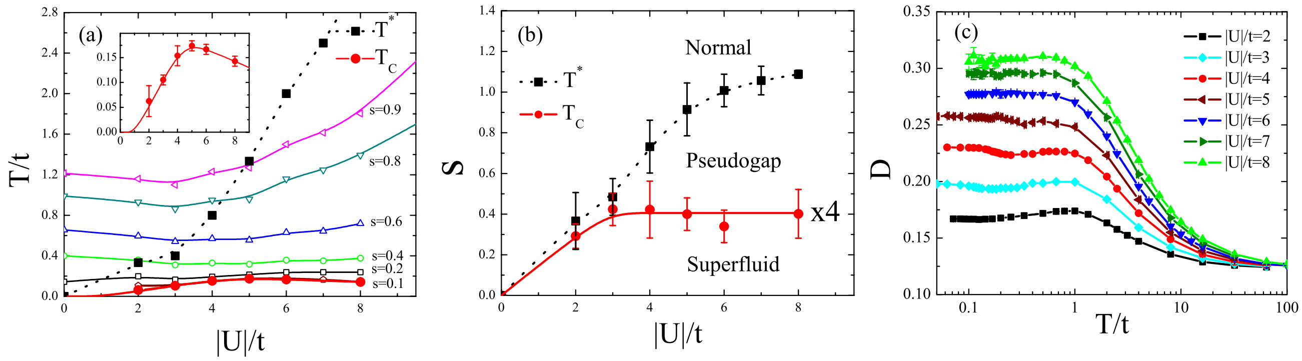

FIG. 2 (color online). (a) Phase diagram of the attractive ($U < 0$) 2D Hubbard Model at $\rho = 0.7$ (away from half-filling) obtained on $N \geq 10^2$ lattices. We show the crossover scale T^* corresponding to the pairing pseudogap (obtained from the susceptibility) and the critical temperature T_c [estimated from the superfluid density $\rho_s(T)$]. We also show curves of constant entropy *per site* $s = S/Nk_B$, Inset: $|U|$-dependence of the superfluid T_c. (b) Phase diagram in the ($|U|/t$, s) plane showing the three regions: normal, pseudogap, and superfluid. (c) Temperature dependence of the double-occupancy $D(T)$ for various $|U|/t$.

tibility $\chi(T)$. Except in weak coupling $U/t \ll 1$, where the charge and spin scales are essentially identical, we find in Fig. 1(a) that the two scales are quite different for $U/t > 1$. In the large U (Mott) limit we expect $\Delta_{\mathrm{ch}} \sim U \gg T_{\mathrm{spin}} \simeq J_{\mathrm{AF}} = 4t^2/U$, although the $1/U$ dependence is not yet observed at $U/t = 8$ in the QMC data of Fig. 1(a). We note that T_{spin} would set the maximum scale for $T_{\mathrm{N\acute{e}el}}$ if we were to couple 2D layers to stabilize AFM order in a layered system like the parent insulators of the high T_c superconductors.

(iii) Entropy: We now wish to represent all of the insights gained above in the (U/t, s) plane, since the entropy density s can be monitored more easily than the temperature in cold atom experiments. We calculate $S(T)$ from QMC calculations in two different ways [18,19] which agree to within a few percent [15], and plot curves of constant entropy density $s = S/Nk_B$ in the (U/t, T/t) phase diagram of Fig. 1(a). We can thus obtain the (U/t, s) phase diagram of Fig. 1(b), where the characteristic crossovers are represented as the entropy as a function of U/t at the insulating gap scale Δ_{ch} and the spin scale T_{spin}.

At weak coupling, both scales are exponentially small and the system looks like a highly degenerate normal Fermi gas with a low entropy. It is only for very low $s \ll \ln 4 \simeq 1.386$ that one observes either the insulating gap or buildup of spin correlations for $U/t \leq 1$. For larger coupling $U/t \geq 5$ we see that the entropy at the gap scale is approximately $s = \ln 2 \simeq 0.693$. By lowering the entropy to $s \sim 0.4$ it is already possible to cross T_{spin}.

We also note that both the characteristic curves in the (U/t, s) plane saturate to *constant* values of s in the $U/t \gg 1$ limit. This is in marked contrast to the more familiar (U/t, T/t) phase diagram, where Δ_{ch} grows linearly in U and T_{spin} is expected to decrease with $J = 4t^2/U$ in strong coupling. We can understand this from a scaling argument for s, analogous to the one we present in detail below for the attractive Hubbard model.

(iv) Cooling and thermometry: We next turn to a beautiful suggestion [20] for adiabatic cooling, that exploits the anomalous T dependence of the double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ observed in dynamical mean field theory. The idea is as follows. The entropy and D are related to the free energy F via $S = -\partial F/\partial T$ and $D = \partial F/\partial U$, so that $\partial S/\partial U = -\partial D/\partial T$. For $U > 0$, the "natural" expectation is $dD/dT > 0$ since raising T gives more thermal energy to overcome the on site repulsion U. Thus T increases along a constant S curve upon increasing U/t. The DMFT observation of an anomalous region with $dD/dT < 0$, beginning at very weak coupling and extending up to $U/t = 12$, implies that we can follow a curve of constant S and cool the system as the lattice is turned on, i.e., as U/t is increased.

We show in Fig. 1(c) the DMFT curve [20] for $D(T)$ at $U = 6t$ contrasted with 2D QMC results. The absence of an anomalous regime with $dD/dT < 0$ in 2D is likely a result of short range spin correlations that are important in low dimensional systems but neglected in DMFT. We see that the constant-s curves in Fig. 1(a) do not show a significant negative slope and thus one cannot obtain adiabatic cooling in 2D.

From Fig. 1(c) we see that the double-occupancy $D(T)$ is quite weakly T dependent for $T < t$, but its monotonic T dependence at higher temperature suggests that $D(T)$, which can be measured in cold atom experiments [3], can be used for thermometry in the range $1 < T/t < 10$. Such a thermometer would need QMC results for $D(T)$ calibration. We show in the insert to Fig. 1(c) that the double occupancy, that is a local observable, has no significant system size dependence and can indeed be very accurately determined by QMC simulations.

Attractive Hubbard model at arbitrary filling.—QMC simulations of the *attractive* Hubbard model are free of the fermion sign problem [12] for arbitrary values of the filling ρ. Moreover, this model shows superfluidity of s-wave pairs [13] and a BCS to BEC crossover [14] as a function of $|U|/t$. We will work away from half-filling where the ground state is a superfluid of s-wave pairs; for concreteness we present results at $\rho = 0.7$.

(i) Pairing pseudogap: The "pseudogap" or pairing scale T^* below which pairs form [14] in the attractive Hubbard model, is the analog of the gap scale below which moments form in the repulsive model. Since pairing represents the onset of singlet correlations, we can easily determine [15] T^* from the susceptibility $\chi(T)$, which is strongly suppressed for $T \le T^*$. The pairing T^* is plotted as a function of $|U|/t$ in Fig. 2(a). T^* has essentially the same $|U|$ dependence as the $T = 0$ pairing gap: exponentially small in $|U|/t$ for the weak coupling BCS limit and proportional to U in the strong coupling Bose limit. For $T < T^*$ there is a pseudogap [14] due to pairing correlations above T_c, that leads to the suppression of low-energy spectral weight in the density of states.

(ii) Berezinskii-Kosterlitz-Thouless (BKT) transition: At lower temperature there is a transition to a superfluid phase in the attractive Hubbard model (for $\rho \neq 1$). In 2D this is a BKT transition, with algebraic order in the pair-pair correlation function [13] below T_c and a nonzero superfluid density ρ_s.

We determine [15] the BKT T_c from the jump in the superfluid density ρ_s. While T_c is exponentially small in the weak coupling BCS limit, it goes as $T_c \sim t^2/|U|$ at strong coupling, for a BEC of hard-core bosons with hopping energy $t^2/|U|$. The nonmonotonic $|U|/t$ dependence of T_c shown in the inset to Fig. 2(a), though expected on general grounds, has never been computed before.

(iii) Entropy: We calculate the entropy [15] and plot curves of constant s in the $(|U|/t,\ T/t)$ plane in Fig. 2(a). From this, we obtain the $(|U|/t,\ s)$-phase diagram of Fig. 2(b). We see that for $|U|/t \ge 5$ one needs to lower the entropy $s \lesssim 0.8$ to enter the pseudogap regime below T^*. To observe superfluidity below the BKT transition requires $s \lesssim 0.1$.

We note that, while $T^* \sim |U| \to \infty$ and $T_c \sim t^2/|U| \to 0$ for $|U|/t \gg 1$, the corresponding s values in Fig. 2(b) saturate at large $|U|$. This striking difference between the strong coupling behavior of the characteristic crossovers and phase transitions in $(U/t,\ T/t)$ and $(U/t,\ s)$ phase diagrams is common to both the attractive and repulsive Hubbard models.

We now give a scaling argument to understand this qualitative difference. We exploit the fact that the entropy density $s = S/Nk_B$ is a dimensionless, intensive, bounded function of $|U|$, t, T, for a given ρ. To understand the pairing crossover in the $(|U|/t,\ s)$ plane, we note that in the $|U|/t \gg 1$ limit, $s(T^*) = \mathcal{F}(T^*/|U|, t/|U|) \to \mathcal{F}(\text{const}, 0)$, which depends only on ρ and is bounded above by ln 4. To estimate s at the phase transition we must use the degeneracy scale, which goes like $t^2/|U|$ in the $|U|/t \gg 1$ limit. Then $s(T_c)$ must be of the form $s(T_c) = \mathcal{G}(T_c/(t^2/|U|))$, which goes to a constant for $|U|/t \gg 1$. Why does the same reasoning *not* lead to the patently false answer that the characteristic scale goes to a constant in the opposite $|U|/t \ll 1$ limit? The reason is that, in the limit of small $|U|$, the degeneracy scale is t and we thus find $s(T_c) \sim T_c/t \to 0$, consistent with Fig. 2(b).

(iv) Cooling and thermometry: The double-occupancy $D(T)$ for $U < 0$ in Fig. 2(c) shows a rather small regime of anomalous behavior, which now corresponds to $dD/dT > 0$. Thus the prospects of using adiabatic cooling [20] in 2D do not look promising for the attractive case either. However, Fig. 2(c) does suggest that $D(T)$ can be used as an effective thermometer for the range $t < T < 10t$.

Conclusions.—Current fermion optical lattice experiments [4] have achieved an entropy per particle $\simeq$ ln2, sufficient to observe the insulating gap in the repulsive Hubbard model or the pairing pseudogap in the attractive case. Observing antiferromagnetic correlations or superfluidity in 2D systems will require a further reduction in the entropy by a factor of 3 or more. It is possible that the inhomogeneous density in a trap can lead to a redistribution of entropy with some regions having a much lower entropy than others.

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