Magnetism and Pairing of Two-Dimensional Trapped Fermions

Simone Chiesa,[1,2] Christopher N. Varney,[3,4] Marcos Rigol,[3] and Richard T. Scalettar[2]

[1]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA
[2]Department of Physics, University of California, Davis, California 95616, USA
[3]Department of Physics, Georgetown University, Washington, D.C. 20057, USA
[4]Joint Quantum Institute, University of Maryland, College Park, Maryland 20742, USA

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The emergence of local phases in a trapped two-component Fermi gas in an optical lattice is studied using quantum Monte Carlo simulations. We treat temperatures that are comparable to or lower than those presently achievable in experiments and large enough systems that both magnetic and paired phases can be detected by inspection of the behavior of suitable short-range correlations. We use the latter to suggest the interaction strength and temperature range at which experimental observation of incipient magnetism and d-wave pairing are more likely and evaluate the relation between entropy and temperature in two-dimensional confined fermionic systems.

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Strong electron correlations in solids are believed to be at the origin of a remarkable host of phenomena that range from anomalous insulating states and magnetism to high temperature superconductivity [1]. The Hubbard Hamiltonian [2], a model which provides a simplified picture of the band structure and electron interactions, is thought to contain the necessary ingredients to describe such spectacular diversity. In the strongly interacting limit the half filled model describes a Mott insulator, and, on a two-dimensional (2D) square lattice, quantum Monte Carlo simulations [3,4] have convincingly established the existence of antiferromagnetism at $T = 0$. This conjunction of insulating behavior and long-range antiferromagnetic order accurately describes the low-temperature physics of the undoped parent compounds of the cuprate superconductors.

Despite intensive analytical and computational work, what happens as one dopes the antiferromagnet has remained controversial and many important questions remain unanswered [5–7]. A promising new route to study the model has recently emerged in the form of experiments with fermionic gases in optical lattices. The appeal of these experiments lies in the high degree of control over the different parameters of the system and the ensuing possibility of a close realization of a ‘‘pure’’ Hubbard Hamiltonian [8], free of the complexity characterizing solid state systems. Groundbreaking achievements include loading an ideal quantum degenerate Fermi gas in a three-dimensional (3D) lattice [9] and the realization of the Mott metal-insulator transition in 3D [10,11].

Optical lattice experiments require the presence of a confining potential, usually harmonic, and are accordingly modeled by the Hamiltonian

$$H = -t \sum_{\langle ij\rangle,\sigma} (c^{\dagger}_{j\sigma} c_{i\sigma} + \text{H.c.}) + \sum_i (V_i n_i + U n_{i\uparrow} n_{i\downarrow}), \quad (1)$$

with $V_i \equiv V r_i^2$. The curvature V causes the density to vary across the lattice, resulting in a situation at odds with the homogeneous system that one would like to emulate. This is a potential problem because numerical studies on related models [12] have indicated the existence of many competing phases with vastly different physical properties. Understanding the extent to which the delicate balance between these phases is affected by the presence of the trap is, therefore, of importance for assessing whether fermionic gases can be taken as accurate simulators of homogeneous models. Thanks to improvements in quantum Monte Carlo (QMC) codes [4,13–16], this and other issues can now be quantitatively investigated at temperatures that are comparable to or below those of the latest optical lattice experiments [10,11].

Here we report results from state-of-the-art determinant QMC (DQMC) simulations [17] of the trapped 2D Fermi-Hubbard Hamiltonian. We found clear signatures of magnetic and pairing correlations at temperatures of the order of the magnetic scale $J = 4t^2/U$, a perhaps surprising observation considering that the corresponding temperature range in strongly correlated solid state systems is well above T_c. We note, however, that the properties that we compute are local in character, and that recent advances in optical lattice experiments [18–20] have made possible the imaging of individual sites and short-range correlations around them. Hence, our results suggest that the purity of optical lattices and the novel probes used in these experiments could allow the observation of local pairing signatures at higher temperatures than possible in a condensed matter environment.

We analyze the properties of the trapped system in terms of the spatial dependence of the local density $n(i) = \langle n_i \rangle$, the density fluctuations $\delta(i) = \langle n_i^2 \rangle - \langle n_i \rangle^2$, and the spin correlations $C_{xy}(i) = 4\langle S^z_{i+(x,y)} S^z_i \rangle$. Pairing is analogously discussed by defining a local d-wave pair creation operator,

$$\Delta_i^{d\dagger} = \frac{1}{2}(\Delta^\dagger_{i,i+\hat{x}} + \Delta^\dagger_{i,i-\hat{x}} - \Delta^\dagger_{i,i+\hat{y}} - \Delta^\dagger_{i,i-\hat{y}}),$$

$$\text{with } \Delta^\dagger_{ij} = \frac{1}{\sqrt{2}}(c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} + c^\dagger_{j\uparrow}c^\dagger_{i\downarrow}), \tag{2}$$

and a corresponding correlation function $P_{xy}(i) = \langle \Delta^d_{i+(x,y)}\Delta_i^{d\dagger}\rangle$. To isolate the effect of the pairing vertex [21], we focus on the connected correlation function in which suitable products of single particle propagators are subtracted from P_{xy}.

In Fig. 1, we examine the spatial dependence of different properties at $U = 6t$, $V = 0.04t$, and $T = 0.31t$ for a system of 560 fermions. In this parameter regime, the average sign in DQMC simulations is 0.3 and decreases exponentially as T is lowered. $T = 0.31t$ is therefore very close to the bound that the sign problem [22,23] imposes on the lowest achievable temperature. Despite this restriction, the emergence of a Mott insulator is clearly visible and depicted in Fig. 1(a), which shows a density plateau region of commensurate filling, $n(i) \simeq 1$, and in Fig. 1(b) through the formation of a pronounced minimum in the density fluctuations. This domain is also distinguished by enhanced antiferromagnetism [Fig. 1(c)] and d-wave pairing [Fig. 1(d)]. These last two properties are represented by the local order parameters

$$M(i) = \sum_{x,y}(-1)^{x_i+y_i+x+y}C_{xy}(i), \qquad \chi(i) = \sum_{x,y}P_{xy}(i),$$

which are expected to diverge if long-range order develops around site i.

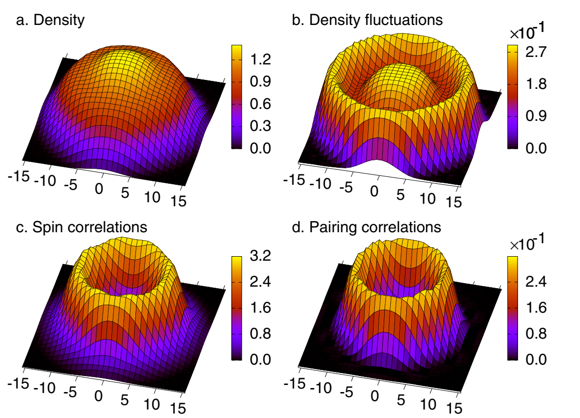

FIG. 1 (color online). (a) Local density $n(i)$, (b) density fluctuations $\delta(i)$, (c) local staggered magnetization $M(i)$, and (d) d-wave pairing $\chi(i)$ are shown for $U = 6t$, $T = 0.31t$, $\mu_0 = 3.0t$, and $V = 0.04t$. A Mott insulating domain is emerging in the density profile of (a), in the form of a half filled ring 6–10 lattice spacings from the trap center. The density fluctuations are minimized in this region. The staggered magnetization and the d-wave pairing, however, show a pronounced maximum in the Mott domain.

Given that the temperature $T = 0.31t$ is of the order of the antiferromagnetic exchange J, the sharp signal in $M(i)$ is clearly due to the formation (and partial ordering) of local moments in the Mott domain. The appearance of the peak in $\chi(i)$ in the same region is, however, surprising—one would expect the peak to occur away from the insulating phase. This shows that $M(i)$ or $\chi(i)$ can be accurate indicators of the appearance of local phases only at temperatures sufficiently low that the order parameter is dominated by long-range contributions. As Fig. 1(d) demonstrates, this is not the case in our simulations nor in current experiments. However, we shall argue that the temperature and interaction dependence of spin and pairing correlations, when examined at distances which are sensitive to the appropriate energy scales, can provide compelling evidence of incipient order [24].

Using this argument, we proceed to determine the temperature and entropy scale that experimentalists need to achieve in trapped 2D lattices in order to observe the onset of antiferromagnetic and pairing correlations. Note that a related analysis has been recently carried out for the entropy scale of the half filled homogeneous model [25].

As the temperature is lowered from $T = 1.14t$ to $T = 0.31t$ ($U = 6t$), the density distribution [Fig. 2(a)] is slightly compressed, the entropy per particle S [shown in Fig. 2(a) inset] decreases monotonically, and there is a marked increase in the total double occupancy in the system D [see inset in Fig. 2(b)], which is generated by the increase of the double occupancy at the trap center. We determine the entropy, $S = \beta(\langle E\rangle - F)$, by first computing the Helmholtz free energy using constant-temperature coupling-constant integration over an identical set of traps containing approximately 560 fermions and increasing U [24]. The Mott insulating region $n(i) \simeq 1$ is characterized

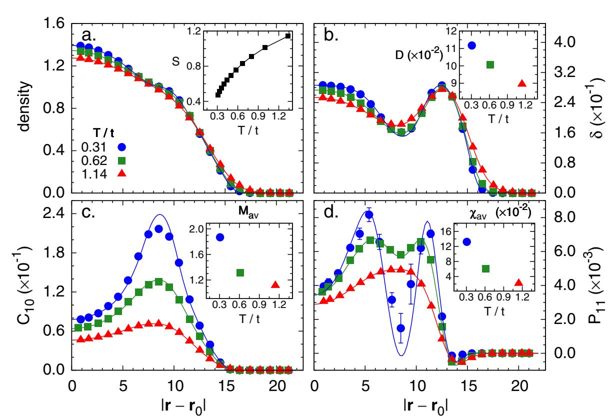

FIG. 2 (color online). Temperature dependence of the (a) density, (b) density fluctuations, (c) nearest-neighbor spin correlations $C_{10}(i)$, and (d) next-nearest-neighbor d-wave pairing $P_{11}(i)$ for $U = 6t$. Lines are results within the local density approximation. The insets of (a) and (b) show the temperature dependence of the entropy and the double occupancy normalized to the number of particles, respectively, while the insets of (c) and (d) are the averages over the lattice of the local staggered magnetization and d-wave pairing.

by a deepening of the minimum in the density fluctuations $\delta(i)$ [Fig. 2(b)] and by a threefold increase in the nearest-neighbor spin-spin correlation $C_{10}(i)$ [Fig. 2(c)]. As the latter may be the easiest way to observe the onset of antiferromagnetic correlations in experiments, Fig. 2(c) makes clear that, although a weak signal may be visible at the highest T, a clear maximum in the Mott domain will only be apparent when $T < t$.

When analyzing pairing correlations it is important to realize that $P_{00}(i)$ and $P_{10}(i)$ contain large contributions from $C_{10}(i)$ and, consequently, carry little information on the actual pairing amplitude in the vicinity of a given site. This is analogous to the more familiar statement that local moment formation cannot be taken as indication of short-range magnetic order. $P_{11}(i)$ [Fig. 2(d)] is therefore the shortest-distance correlation that can be used to gain insights on the development of off-diagonal order; it is characterized by two maxima around the Mott region, sharply peaked at densities ($n = 0.8$ and $n = 1.2$) that lie in the center of the superconducting dome of the cuprate phase diagrams [26]. The analogous correlation for pairs in an extended s-wave state (see [24]) is also significantly enhanced in a broad ring around $n = 0.6$. Although the local character of P_{11} and the high temperature do not allow a characterization of the dominant low-temperature pairing symmetry, our results suggest that d-wave and extended s-wave pairing may be detected as leading pairing symmetries in spatially distinct regions, in agreement with existing ground state calculations on related homogeneous models [27,28].

Another important piece of information that will help experimentalists observe antiferromagnetism and pairing is the optimal value of the ratio U/t at which those correlations are expected to be maximal. In order to address this issue, we first investigate the interaction dependence of the same physical properties represented in Fig. 2 but at constant $T = 0.5t$ (Fig. 3), and then show that our conclusions are unaltered if it is S to be held constant.

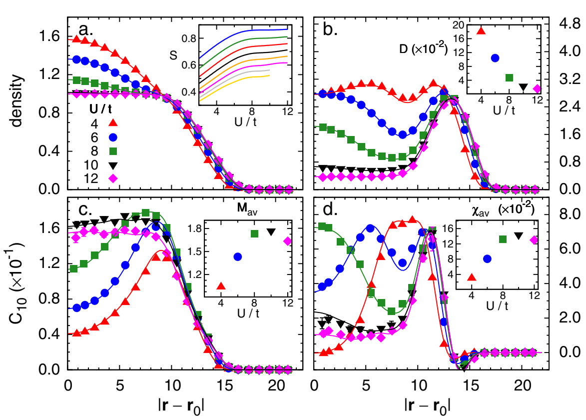

FIG. 3 (color online). Same quantities of Fig. 2 but as a function of interaction strength U/t at constant $T = 0.50t$. The inset of (a) shows the entropy for temperatures $T/t = 0.67$, 0.57, 0.50, 0.44, 0.40, 0.36, 0.33, and 0.31 (top to bottom).

At intermediate coupling ($U = 4t$), the smallness of the gap, the curvature of the trapping potential, and thermal fluctuations make it impossible for a flattening in the density profile to appear. Note, however, that signals of incipient insulating behavior are clear in the structure of density fluctuations [Fig. 3(b)]. At large interaction strength ($U = 10t$, $12t$), the existence of a Mott insulating domain can be directly inferred by inspection of the density profile: the large central plateau comprising about 300 sites is indicative of a phase with vanishing compressibility. Nearest-neighbor spin correlations acquire their largest value at $U = 8t$. While the double occupancy is monotonically suppressed as U increases, the staggered magnetization shows a similar behavior to $C_{10}(i)$, reaching a maximum when U is of the order of the bandwidth. It is therefore -clear that the optimal interaction strength must be near the bandwidth and that future experiments should focus their attention on this regime. Similarly, $P_{11}(i)$ exhibits a sharp maximum at $n(i) = 0.8$ for $U \simeq 8t$, but contrary to what is observed for $C_{10}(i)$, there is no weakening when going from $U = 8t$ to $U = 12t$ and no dependence of the "optimal" density for pairing on U. The latter is reminiscent of the properties of cuprate superconductors where optimal doping is constant across the entire family of these materials.

One might wonder what would happen in the experimentally relevant case of a (quasi)adiabatic evolution, i.e., a system at constant entropy, as a function of U. In the inset of Fig. 3(a), we show the evolution of the entropy per particle as a function of the interaction strength for various fixed temperatures. As U is increased at constant S, we find that the system cools down and goes, for instance, from $T = 0.5t$ at $U = 2t$ to $T = 0.31t$ at $U = 10t$, while S is held fixed at 0.5. Since this cooling is mild beyond $U = 8t$, isothermal and adiabatic evolution in this parameter regime are essentially equivalent. For $U < 8t$, an adiabatic increase of U is accompanied by progressively lower temperatures, and this, in turn, implies that $U = 8t$ remains the optimal interaction strength to observe strong-correlation phenomena.

We finally touch on the extent to which properties in a trap are a faithful representation of those in a homogeneous system. To this aim we use DQMC simulations on homogeneous 8×8 clusters to estimate local properties as a function of chemical potential and plot the corresponding local density approximation (LDA) results in Figs. 2 and 3 as continuous lines. The agreement with the *ab initio* results is excellent with the sole exception of the half filled region at $T = 0.31t$ [Fig. 2(c)]. This discrepancy is a characteristic failure of the LDA when applied to the interface between coexisting phases [29].

A more dramatic failure of the LDA is expected when examining longer-range correlations. Since in the fermionic Hubbard model the development of a certain type of order corresponds with a rather narrow density interval, different phases in a trap appear with a narrow-ring-like topology. If one disregards interfacial effects, these regions can be thought of as one-dimensional homogeneous strips where

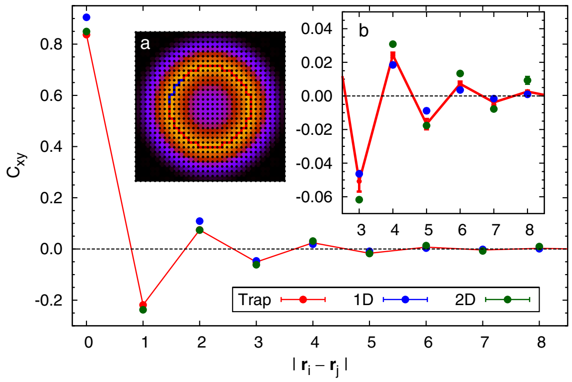

FIG. 4 (color online). Spin correlations $C_{xy}(i)$ [for fixed site i and variable separation (x, y)] along the path illustrated in inset (a) around the trap center. Inset (b) is an enlarged view of the longer correlations. $C_{xy}(i)$ exhibits the alternating sign characteristic of antiferromagnetism. The correlations decrease rapidly, but nevertheless extend out to several lattice spacings. The spin correlations are also shown in the LDA approximation for $d = 1$ and $d = 2$.

the long-range character of correlations is determined by the strip width. An example of such a situation is given by the development of long-range magnetic order in the half filled annulus found in our simulations at $U = 6t$. In particular, Fig. 4 shows that 2D correlations, computed on a half filled homogeneous cluster at the same temperature, represent a good approximation to the correlations in a trap only at short distances, overestimating the correct long-range value. Analogous results for a 1D chain fail at all distances and, in particular, decay too quickly at large separation. This behavior is generic and expected for the superfluid regions as well. When the system size increases, these quasi-1D regions grow both in width and length and their correlations ultimately cross over to a pure 2D character. This dimensionality effect must be taken into account when using finite size systems to infer the critical behavior.

In summary, we have addressed finite temperature properties of inhomogeneous Fermi-Hubbard systems using an *ab initio* approach. Our findings of enhanced antiferromagnetic and pairing correlations just below the temperature scale $T \sim t$ thus open important perspectives for current experiments with ultracold fermions in optical lattices. While the lowest temperatures reported here are well above the d-wave coherence temperature, the enhanced signal in local properties is a promising sign: these results and the purity of the experimental optical lattice suggest that, in contrast to solid state systems, temperatures of the order of the hopping scale may be enough to observe clear local signature of *both* magnetic and pairing correlations. Tuning experiments to be in the regime where the on site interactions are of the order the bandwidth ($U \sim 8t$) provides the sharpest signal of the many-body effects. Our computation of the entropy S indicates that adiabatic cooling occurs in the 2D Hubbard Hamiltonian with a position dependent (confining) potential as the interaction strength U is increased via, e.g., a Feshbach resonance. This allows our conclusions concerning the observability of spin and pairing order to be relevant to experiments at constant entropy.

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