Systematic Study of *d*-Wave Superconductivity in the 2D Repulsive Hubbard Model

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The cluster size dependence of superconductivity in the conventional two-dimensional Hubbard model, commonly believed to describe high-temperature superconductors, is systematically studied using the dynamical cluster approximation and quantum Monte Carlo simulations as a cluster solver. Because of the nonlocality of the *d*-wave superconducting order parameter, the results on small clusters show large size and geometry effects. In large enough clusters, the results are independent of the cluster size and display a finite temperature instability to *d*-wave superconductivity.

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Despite years of active research, the understanding of pairing in the high-temperature "cuprate" superconductors (HTSC) remains one of the most important outstanding problems in condensed matter physics. While conventional superconductors are well described by the BCS theory, the pairing mechanism in HTSC is believed to be of entirely different nature. Strong electronic correlations play a crucial role in HTSC, not only for superconductivity but also for their unusual normal state behavior. Hence, models describing itinerant correlated electrons, in particular, the two-dimensional (2D) Hubbard model and its strong-coupling limit, the 2D *t*-*J* model, were proposed to capture the essential physics of the CuO planes in HTSC [1,2]. Despite the fact that these models are among the mostly studied models in condensed matter physics, the question of whether they contain enough ingredients to describe HTSC remains an unsolved problem.

Many different techniques, from analytic to numerical, have been applied to study superconductivity in these models. The Mermin-Wagner theorem [3] and the rigorous results in Ref. [4] preclude $d_{x^2-y^2}$ superconducting long-range order at finite temperatures in the 2D models. Superconductivity may, however, exist—as in the attractive Hubbard model—as topological order at finite temperatures below the Kosterlitz-Thouless (KT) transition temperature [5]. Recent renormalization group studies indicate that the ground state of the doped weak-coupling 2D Hubbard model is superconducting with a $d_{x^2-y^2}$-wave order parameter [6]. The possibility of $d_{x^2-y^2}$-wave pairing in the 2D Hubbard and *t*-*J* models was also indicated in a number of numerical studies of finite system size [for a review, see [7]]. Only recent numerical calculations for the *t*-*J* model provided evidence for pairing at $T = 0$ in relatively large systems for physically relevant values of J/t [8]. Quantum Monte Carlo (QMC) simulations are also employed to search for such a transition [9]. These studies indicate an enhancement of the pairing correlations in the $d_{x^2-y^2}$ channel with decreasing temperature. Unfortunately the Fermion sign problem limits these studies to temperatures too high to study a possible KT transition. Another difficulty of these methods arises from their strong finite-size effects, often ruling out the reliable extraction of low-energy scales. In fact, a reliable finite-size scaling has only recently been achieved in the negative-U model [10], where the relevant temperature scales are much higher. The available results for the positive-U model so far have thus been inconclusive, and a treatment within a nonperturbative scheme that goes beyond the conventional finite-size techniques is clearly necessary to resolve the controversy as to whether there exists finite temperature superconductivity in these models.

In this Letter we use the dynamical cluster approximation (DCA) [11] [for a review, see [12]] to explore the superconducting instability in the 2D Hubbard model

$$H = -t \sum_{\langle ij\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c_{i\sigma}^{(\dagger)}$ (creates) destroys an electron with spin σ on site i, $n_{i\sigma}$ is the corresponding number operator, t the hopping amplitude between nearest neighbors $\langle \ldots \rangle$, and U the on-site Coulomb repulsion. In the DCA we take advantage of the short length scale of spin correlations in optimally doped HTSC [13] to map the original lattice model onto a periodic cluster of size $N_c = L_c \times L_c$ embedded in a self-consistent host. Thus, correlations up to a range $\xi \lesssim L_c$ are treated accurately, while the physics on longer length scales is described at the mean-field level. By increasing the cluster size, it thus allows us to systematically interpolate between the single-site dynamical mean-field result and the exact result while remaining in the thermodynamic limit. We solve the cluster problem using QMC simulations [14].

We present results of large cluster calculations—up to 26 sites—that indicate that the 2D Hubbard model has a superconducting instability at a finite temperature. This conclusion is reached due to several factors: simulations on small clusters, where *d*-wave order is topologically allowed, show large finite-size and geometry effects leading to inconclusive results. However, since the average sign in DCA-QMC simulations is significantly larger than in finite-size QMC counterparts, exploring lower temperatures and larger clusters becomes possible. In addition, the advent of new parallel vector machines, such as the Cray X1 at ORNL, improves the speed of these calculations by more than 1 order of magnitude compared to conventional architectures, making simulations on large clusters with a small average sign feasible. Within the limits of current computational capability, we observe finite transition temperatures in the largest affordable clusters. There the results are independent of cluster size within the error bars, although we cannot preclude a further small reduction in transition temperatures in yet larger clusters.

Previous DCA simulations with a cluster of four sites, the smallest cluster that can capture $d_{x^2-y^2}$-wave pairing, with U equal to the bandwidth $W = 8t$, show good general agreement with HTSC [15]. In the paramagnetic state, the low-energy spin excitations become suppressed below the crossover temperature T^*, and a pseudogap opens in the density of states at the chemical potential. At lower temperatures, we find a finite temperature transition to antiferromagnetic long-range order at low doping, while at larger doping, the system displays an instability to $d_{x^2-y^2}$-wave superconducting long-range order. This apparent violation of the Mermin-Wagner theorem is a consequence of the small cluster size studied [see also [16]]. More recent results obtained with a similar quantum cluster algorithm confirm the presence of antiferromagnetism and superconductivity in the ground state of the 2D Hubbard model [17].

With increasing cluster size, however, the DCA progressively includes longer-ranged fluctuations while retaining some mean-field character. Larger clusters are thus expected to systematically drive the Néel temperature to zero and hence recover the Mermin-Wagner theorem in the infinite cluster size limit. In contrast, superconductivity may persist as KT order even for large cluster sizes.

Since the large cluster simulations presented here are at the limit of current computational capabilities, we are restricted in our ability to explore both the parameter space and different cluster sizes. We choose the parameters to favor superconducting and antiferromagnetic order. In our study of superconductivity, we choose $U = 4t = W/2$ (we take t as our unit of energy). While we observe that larger values of U yield higher transition temperatures in the 4-site cluster, the smaller value of U greatly reduces the sign problem and thus allows us to simulate larger cluster sizes. We focus on a doping of 10%, where the pairing correlations are maximal for $U = W/2$. To study antiferromagnetism, we focus on the undoped model and set $U = 8t$, where the Néel temperature is highest.

Furthermore, we have to be careful in selecting different cluster sizes and geometries. Much can be learned from simulations of finite-size systems, where periodic boundary conditions are typically used. Betts and Flynn [18] systematically studied the 2D Heisenberg model on finite-size clusters and developed a grading scheme to determine which clusters should be used. The main qualification is the "imperfection" of the near-neighbor shells: a measure of the (in)completeness of each neighbor shell compared to the infinite lattice. In finite-size scaling calculations they found that the results for the most perfect clusters fall on a scaling curve, while the imperfect clusters generally produce results off the curve. Here, we employ some of the cluster geometries proposed by Betts (see Fig. 1) to study the antiferromagnetic transition at half filling and generalize Betts' arguments to generate a set of clusters appropriate to study d-wave superconductivity.

To illustrate that the DCA recovers the correct result as the cluster size increases, we plot in Fig. 2 the DCA results for the Néel temperature T_N at half filling as a function of the cluster size N_c. T_N decreases slowly with increasing cluster size N_c. As spin correlations develop exponentially with decreasing temperature in 2D, the $N_c > 4$ data fall logarithmically with N_c, consistent with $T_N = 0$ in the infinite size cluster limit. Thus, the Mermin-Wagner theorem is recovered for $N_c \to \infty$. The clusters with $N_c = 2$ and $N_c = 4$ are special because their coordination number is reduced from four. For $N_c = 2$ the coordination number is one and hence a local singlet is formed on the cluster for temperatures below $J \sim t^2/U$. In the $N_c = 4$ site cluster,

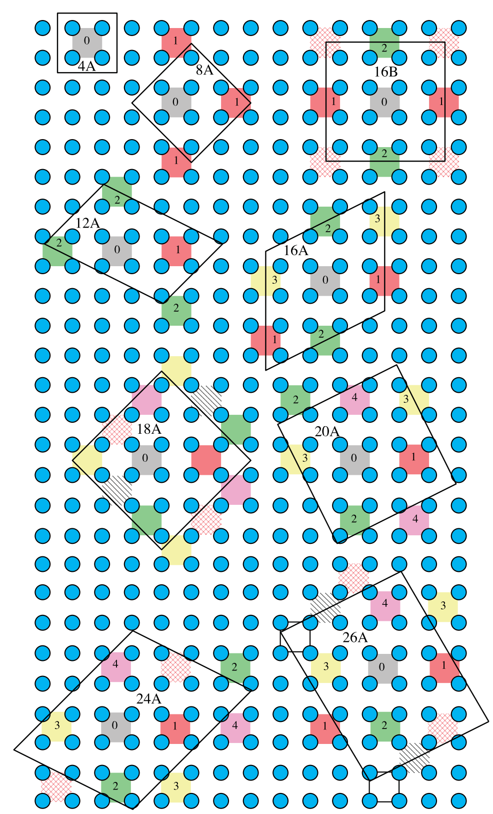

FIG. 1 (color). Cluster sizes and geometries used in our study. The shaded squares represent independent d-wave plaquettes within the clusters. In small clusters, the number of neighboring d-wave plaquettes z_d listed in Table I is smaller than 4, i.e., than that of the infinite lattice.

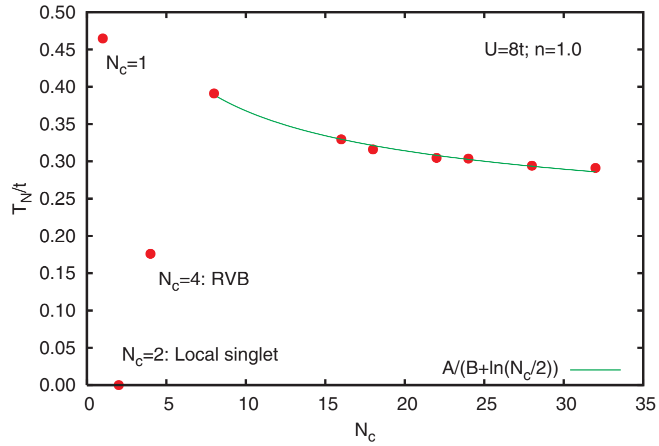

FIG. 2 (color online). Néel temperature at half filling when $U = 8t$ vs the cluster size. T_N scales to zero in the infinite cluster size limit. The solid line represents a fit to the function $A/[B + \ln(N_c/2)]$ obtained from the scaling ansatz $\xi(T_N) = L_c$. For $N_c = 2$ a local singlet and for $N_c = 4$ the RVB state suppresses antiferromagnetism.

the coordination is two, so fluctuations of the order parameter are overestimated and the resonating valence bond (RVB) state [1] is stabilized. Hence, antiferromagnetism is suppressed in these cluster sizes and their corresponding T_N does not fall on the curve.

We now turn to the main focus of this Letter, i.e., the search for a possible KT instability to the superconducting state. To check that the DCA formalism is able to describe such a transition, we first tested the DCA-QMC code on the negative U, i.e., attractive Hubbard model which is known to exhibit a KT instability to an s-wave superconducting state [10]. We find that the DCA indeed produces a finite temperature s-wave instability to the KT superconducting state. Because of the local nature of the s-wave order parameter, the DCA results converge rather quickly with cluster size. The DCA values for T_c agree with those recently obtained in finite-size QMC simulations [10]. In addition, we checked that our DCA-QMC code reproduces the results of other DMFT codes when $N_c = 1$, and those of finite-size QMC codes when the coupling to the self-consistent host is turned off.

To identify a possible KT transition in the positive U Hubbard model we calculate the $d_{x^2-y^2}$-wave pair-field susceptibility P_d for the clusters $N_c = $ 4A, 8A, 16A, 16B, 18A, 20A, 24A, and 26A. In contrast to the s-wave order parameter in the attractive model, the d-wave order parameter is nonlocal and involves four bonds or sites. Thus, large size and geometry effects have to be expected in small clusters. Similar to the cluster grading scheme Betts developed for magnetic order, we can classify the different clusters according to their quality for d-wave order. At low temperatures, local d-wave pairs will form, but phase fluctuations of the pair wave function prevent the system from becoming superconducting. Since the DCA cluster has periodic boundary conditions, each four-site d-wave plaquette has four neighboring d-wave plaquettes. However, as illustrated in Fig. 1, in small clusters, these are not necessarily independent and the effective dimensionality may be reduced.

Figure 1 shows the arrangement of independent d-wave plaquettes in the clusters used in our study and their corresponding number z_d is listed in Table I. In the infinite system, $z_d = 4$. The $N_c = 4$ cluster encloses exactly one d-wave plaquette ($z_d = 0$). When a local d-wave pair forms on the cluster, the system becomes superconducting, since no superconducting phase fluctuations are included. Thus, the $N_c = 4$ result corresponds to the mean-field solution. In the 8A cluster, there is room for one more d-wave pair, thus the number of independent neighboring d-wave plaquettes $z_d = 1$. Since this same neighboring plaquette is adjacent to its partner on four sides, phase fluctuations are replicated and hence overestimated as compared to the infinite system. The situation is similar in the 16B cluster, where only two independent (and one next-nearest neighbor) d-wave plaquettes are found ($z_d = 2$). In contrast, $z_d = 3$ in the oblique 16A cluster. We thus expect d-wave pairing correlations to be suppressed in the 16B cluster as compared to those in the 16A cluster. With the exception of the 18A cluster, where neighboring d-wave plaquettes share one site and thus are not independent, the larger clusters 20A, 24A, and 26A all have $z_d = 4$ and are thus expected to show the most accurate results. Hence, as the number of independent neighboring d-wave plaquettes, z_d, is reduced from four, phase fluctuations are replicated due to periodic boundary conditions and thus overemphasized, suppressing pairing correlations and consequently T_c. Note that the effects of finite-size energy levels on the pairing correlations were pointed out in QMC simulations of Hubbard ladders [19].

Figure 3 shows the temperature dependence of the inverse d-wave pair-field susceptibility, $1/P_d$, in the 10% doped system. Since a proper error propagation is severely hampered by storage requirements, we obtain the error bars shown on the 16A results from a number of independent runs initialized with different random number seeds. Error

TABLE I. Number of independent neighboring d-wave plaquettes z_d and the values of T_c^{KT} and T_c^{lin} obtained from the Kosterlitz-Thouless and linear fits of the pair-field susceptibility in Fig. 3, respectively.

Cluster	z_d	T_c^{KT}/t	T_c^{lin}/t
4	0 (MF)	0.046	0.056
8A	1	−0.014	−0.006
18A	1	−0.043	−0.022
12A	2	0.011	0.016
16B	2	0.010	0.015
16A	3	0.021 ± 0.008	0.025 ± 0.002
20A	4	0.019	0.022
24A	4	0.016	0.020
26A	4	0.020	0.023

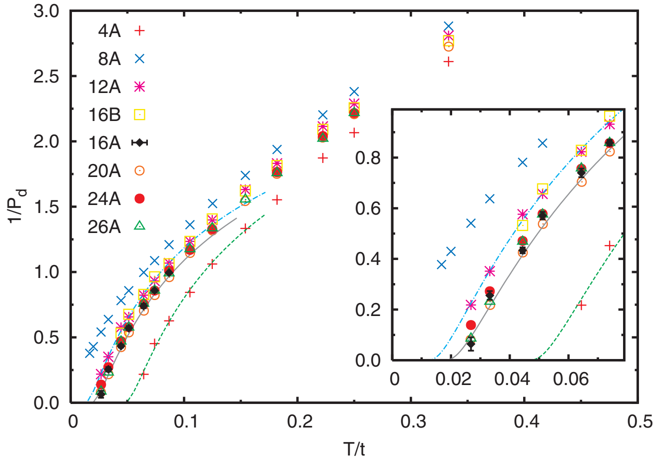

FIG. 3 (color). Inverse d-wave pair-field susceptibility as a function of temperature for different cluster sizes at 10% doping. The continuous lines represent fits to the function $P_d = A\exp[2B/(T - T_c)^{0.5}]$ for data with different values of z_d. Inset: magnified view of the low-temperature region.

bars on larger cluster results are expected to be of the same order or larger. The results clearly substantiate the topological arguments made above.

As noted before, the $N_c = 4$ result is the mean-field result for d-wave order and hence yields the largest pairing correlations and the highest T_c. As expected, we find large finite-size and geometry effects in small clusters. When $z_d < 4$, fluctuations are overestimated and the d-wave pairing correlations are suppressed. In the 8A cluster where $z_d = 1$ we do not find a phase transition at finite temperatures. Both the 12A and 16B cluster, for which $z_d = 2$, yield almost identical results. Pairing correlations are enhanced compared to the 8A cluster and the pair-field susceptibility P_d diverges at a finite temperature. As the cluster size is increased, z_d increases from 3 in the 16A cluster to 4 in the larger clusters, the phase fluctuations become two-dimensional, and as a result, the pairing correlations increase further (with exception of the 18A cluster). Within the error bars (shown for 16A only), the results of these clusters fall on the same curve, a clear indication that the correlations which mediate pairing are short ranged and do not extend beyond the cluster size.

The low-temperature region can be fitted by the KT form $P_d = A\exp[2B/(T - T_c)^{0.5}]$, yielding the KT estimates for the transition temperatures T_c^{KT} given in Table I. We also list the values T_c^{lin} obtained from a linear fit of the low-temperature region, which is expected to yield more accurate results due to the mean-field behavior of the DCA close to T_c [12]. For all clusters with $z_d \geq 3$ we find a transition temperature $T_c \approx 0.023t \pm 0.002t$ from the linear fits. We cannot preclude, however, the possibility of a very slow, logarithmic cluster size dependence of the form $T_c(N_c) = T_c(\infty) + B^2/[C + \ln(N_c)/2]^2$ where $T_c(\infty)$ is the exact transition temperature. In this case it is possible that an additional coupling between Hubbard planes could stabilize the transition at finite temperatures.

In summary, we have presented DCA-QMC simulations of the 2D Hubbard model for clusters up to $N_c = 32$ sites. Consistent with the Mermin-Wagner theorem, the finite temperature antiferromagnetic transition found in the $N_c = 4$ simulation is systematically suppressed with increasing cluster size. In small clusters, the results for the d-wave pairing correlations show a large dependence on the size and geometry of the clusters. For large enough clusters, however, the results are independent of the cluster size and display a finite temperature instability to a d-wave superconducting phase at $T_c \approx 0.023t$ at 10% doping when $U = 4t$.

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