Role of Symmetry and Dimension in Pseudogap Phenomena

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The attractive Hubbard model in $d = 2$ is studied through Monte Carlo simulations at intermediate coupling. There is a crossover temperature T_X where a pseudogap appears with concomitant precursors of Bogoliubov quasiparticles that are *not* local pairs. The pseudogap in $A(\mathbf{k}_F, \omega)$ occurs in the renormalized classical regime when the correlation length is larger than the direction-dependent thermal de Broglie wavelength, $\xi_{\text{th}} = \hbar v_F(\mathbf{k})/k_B T$. The ratio T_X/T_c for the pseudogap may be made arbitrarily large when the system is close to a point where the order parameter has SO(n) symmetry with $n > 2$. This is relevant in the context of SO(5) theories of high T_c but has more general applicability.

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Normal state pseudogaps observed in angle-resolved photoemission experiments [1] and tunneling [2] have become the focus of much of the research on high temperature superconductors. Theoretically, strong-coupling models of this phenomenon include repulsive doped insulator models [3] and attractive models with preformed local pairs [4–6]. At intermediate coupling, resonant pair scattering has been invoked [7]. In weak coupling, antiferromagnetic or superconducting fluctuations also lead to pseudogap formation before long range order is established [8–11]. Finally, arguments about the relevance of phase fluctuations [12] do not specify whether the small superfluid density comes from strong coupling or from thermal fluctuation effects.

Although the effect of superconducting fluctuations on the density of states was studied long ago [13], the relevance of these critical fluctuations on pseudogap phenomena in high temperature superconductors has been questioned mainly because, even in low dimension, the critical region should be quite small compared with the size of the pseudogap region observed in high temperature superconductors. Indeed, even for the Kosterlitz-Thouless (KT) transition in two dimensions, the range of temperatures where superconducting phase fluctuations occur is of order $k_B T_c^2/E_F$ unless disorder depresses T_c [14]. Another question for the original critical-fluctuation calculations is that, contrary to density of states pseudogaps, a pseudogap can appear in the single-particle spectral weight $A(\mathbf{k}_F,\omega)$ only when the fluctuation-induced scattering rate at the Fermi surface $\mathrm{Im}\Sigma(\mathbf{k}_F, \omega = 0)$ increases with decreasing temperature, a behavior that is opposite to that predicted by the traditional phase-space arguments of Fermi liquid theory.

The last objection has already been answered [8] by showing that in $d = 2$ the Fermi liquid arguments fail when one enters the so-called renormalized classical (RC) regime of fluctuations ($d = 3$ is the upper critical dimension [8]). This RC regime is the one where critical slowing down leads to increasing dominance of classical fluctuations ($\hbar\omega_c < k_B T$) as temperature is lowered. However, the question of the large temperature range where pseudogaps appear has to be addressed theoretically both at the qualitative and at the quantitative levels. On the quantitative side, the dependence of the critical region on interaction strength and quasi two dimensionality is not obvious, but it has been argued [15] that specific models can give large critical regions even at intermediate coupling. On the qualitative side, a factor that may considerably enlarge the size of the pseudogap regime is the proximity to a point where the order-parameter symmetry is SO(n) with $n > 2$. Indeed, in $d = 2$ the critical region can become much larger when $n > 2$ since then the Mermin-Wagner theorem implies that the transition temperature is pushed down to $T = 0$. We argue that both conditions, namely, $d = 2$ and higher symmetry, are generic for high temperature superconducting materials. Indeed, in the underdoped region, where the pseudogap is largest, these materials are highly anisotropic (quasi two dimensional) and it has been proposed that the order parameter may have both antiferromagnetic and superconducting characters corresponding to approximate SO(5) symmetry [16].

The attractive Hubbard model may be used to illustrate the properties of pseudogaps that appear in such situations of approximate high symmetry in $d = 2$. For our purposes, the important characteristic of this model is that the long-wavelength critical behavior is as follows for all values of interaction U. At half filling, there is a zero-temperature phase transition that breaks the finite-temperature SO(3) symmetry [17] while away from half-filling, there is a KT transition at finite temperature. The corresponding ground state breaks SO(2) symmetry. While the details of this model are clearly inappropriate for high temperature superconductors, it is useful to illustrate a number of general points that should be applicable to models with transition temperatures that are pushed down from

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their mean-field value by a combination of low dimension and high order-parameter symmetry SO($n > 2$) [16].

In this paper, we present Monte Carlo simulations for the $d = 2$ Hubbard model at $U = -4t$, a value that is slightly on the BCS side of the BCS to Bose-Einstein crossover curve $[U < U(T_c^{\max})]$ [18]. We use units where nearest-neighbor hopping is $t = 1$, lattice spacing is unity, $\hbar = 1$, and $k_B = 1$. Previous numerical work charted the phase diagram [19]. They have also investigated the pseudogap phenomenon mostly in strong coupling where, we stress, the physics is different from the case discussed here [18,20,21]. On the weak-coupling side of the BCS to Bose-Einstein crossover, there have been numerical studies of KT superconductivity [22] as well as several discussions of pseudogap phenomena in the spin properties and in the total density of states at the Fermi level [5,20,23]. The only study of $A(\mathbf{k}, \omega)$ was restricted to regions far from the SO(3) symmetric point [21].

Here we establish a dynamical connection between the appearance of the RC regime in the pairing collective modes and pseudogap formation in single-particle quantities. In particular, we show the following: (a) Close to a high symmetry point, pseudogaps can appear at a crossover temperature T_X that scales with the mean-field transition temperature while the real transition may occur at much lower temperature, T_c, leading to a wide temperature range for the pseudogap. (b) At the crossover temperature, one enters the RC regime where the characteristic frequency for fluctuations becomes smaller than the temperature. (c) Pseudogaps in weak-to-intermediate coupling do not require resonance in the two-particle correlations [24]. (d) To have a pseudogap in $A(\mathbf{k}_F,\omega)$ for a given wave vector, it is not enough to have the collective mode (two-particle) correlation length satisfy $\xi > 1$. It is necessary that ξ becomes larger than the single-particle thermal de Broglie wavelength $\xi_{\mathrm{th}} = v_F(\mathbf{k})/T$. This implies, in particular, that even for an isotropic interaction, as temperature decreases a pseudogap opens first near the zone edge, where v_F is small, and it opens last along the zone diagonal where v_F is largest. This anisotropy would be amplified for an anisotropic interaction of d-wave type [15]. For $U = -4$, the condition $\xi > \xi_{\mathrm{th}}$ is realized near the zone edge for ξ not so large. Analytical arguments for the above results have appeared elsewhere [9,10,25].

Let us first recall a few results at half filling, $\langle n \rangle = 1$, where the chemical potential μ vanishes. There the canonical transformation $c_{i\downarrow} \to (-1)^{i_x + i_y} c_{i\downarrow}^{\dagger}$ maps the attractive model onto the repulsive one at the same filling. The $\mathbf{q} = 0$, s-wave superconducting fluctuations and the $\mathbf{Q} = (\pi, \pi)$ charge fluctuations are mapped onto the three components of antiferromagnetic spin fluctuations of the repulsive model and hence they are degenerate. Because of this degeneracy, the order parameter at half filling has SO(3) symmetry [17], hence, by the Mermin-Wagner theorem, in two dimensions the phase transition is at $T_c = 0$. Results for the attractive model are easily extracted from simulations of the canonically equivalent repulsive model. The pair structure factor $S_\Delta = \langle \Delta^\dagger \Delta + \Delta \Delta^\dagger \rangle$ with $\Delta = (1/\sqrt{N}) \sum_{i=1}^{N} c_{i\uparrow} c_{i\downarrow}$ and the $\mathbf{Q} = (\pi, \pi)$ charge structure factor $S_c = \langle \rho_{\mathbf{Q}} \rho_{-\mathbf{Q}} \rangle$ are identical, showing an increase as temperature decreases and then size-dependent saturation. The sudden rise of S_Δ as temperature decreases indicates a crossover to a RC regime with a concomitant opening of the pseudogap [8,9,26] in $A(\mathbf{k}_F, \omega)$. The crossover temperature is a sizable fraction of the mean-field transition temperature.

Slightly away from half filling, the SO(3) symmetry is formally broken by the chemical potential [17] since it couples only to the charge part of the triplet. However, in the regime where the temperature is larger than the symmetry breaking field, the symmetry is approximately satisfied. [10] For filling $\langle n \rangle = 0.95$, we have $T > |\mu|$ for the whole range of temperature shown in Fig. 1(a) ($\mu \sim -0.07$ at $T = 0.125$). In this figure, superconducting (S_Δ, filled symbols) and charge (S_c, open symbols) structure factors are of comparable size when one enters the RC regime, showing that we have approximate SO(3) symmetry for various sizes $L \times L$. The beginning of the RC regime, that occurs at a temperature nearly identical to the crossover temperature [8] T_X identified at half filling, is signaled by the increase in the magnitude of correlations. Eventually, the concomitant increase of ξ leads to the size dependence apparent at lower temperature in Fig. 1(a). The plot in Fig. 1(a) resembles the result at half filling. [9,27]. The near equality of superconducting and charge fluctuations at the crossover to the RC regime should be contrasted with the case $\langle n \rangle = 0.8$ in Fig. 1(b) where the charge fluctuations show basically no critical behavior when the superconducting correlations begin to do so. Hence, at this filling, there is little SO(3) symmetry left at T_X. This is expected since the symmetry breaking field $|\mu(T_X)| = |\mu(0.25)| = 0.26$ is comparable to T_X. One basically enters directly into the RC regime of a SO(2) KT transition [19]. In this regime $dT_c(n)/dn > 0$.

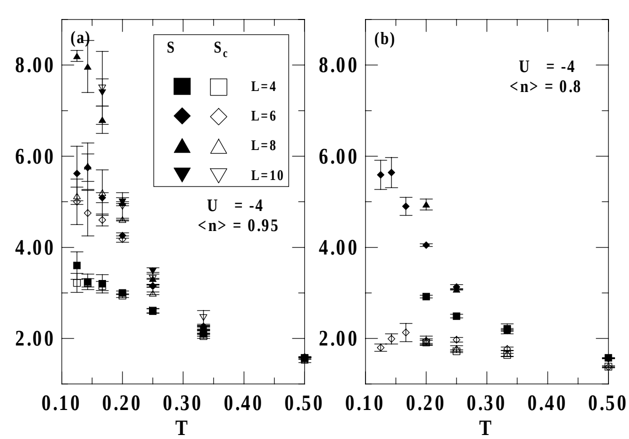

FIG. 1. Pair (filled symbols) and charge (open symbols) structure factors for $U = -4$ and various system sizes. (a) Filling $\langle n \rangle = 0.95$. (b) Filling $\langle n \rangle = 0.8$.

Let us go back to the filling $\langle n \rangle = 0.95$. At this filling, it has been estimated [19] that $T_c < 0.1$ and $dT_c(n)/dn < 0$. We already showed that at this filling one has approximate SO(3) symmetry. One can confirm that the increase of S_Δ and S_c at T_X comes from RC fluctuations by calculating the spectral weight for superconducting fluctuations χ''_Δ (imaginary part of the T *matrix*), $\chi''_\Delta(\omega) = \int dt \, \frac{1}{2}\langle[\Delta(t), \Delta^\dagger]\rangle e^{i\omega t}$. The even part [28] of $\chi''_\Delta(\omega)/\omega$ was obtained from a Monte Carlo calculation of the imaginary-time quantity $\langle \Delta(\tau)\Delta^\dagger + \Delta^\dagger(\tau)\Delta \rangle$ followed by maximum entropy inversion [29]. The even part of $\chi''_\Delta(\omega)/\omega$ is plotted in Fig. 2 for an 8×8 system and various temperatures. The symbols are for a 6×6 system at $T = 1/5$. The maximum is at zero frequency, as for an overdamped mode $\chi_\Delta^{-1}(\mathbf{q}, \omega) \propto \xi^{-2} + q^2 - i\omega/\omega_0$. The characteristic frequency, given by the half width at half maximum, is $\omega_c = \omega_0/\xi^2$ with ω_0 a microscopic relaxation rate. There is a marked narrowing of the width in frequency as temperature decreases. One enters the RC regime when $\omega_c \simeq 1/4 \simeq T_X$, a temperature larger than $T_c(<0.1)$. At $T = 1/5$, the correlation length is becoming comparable with the system size since the 6×6 system gives a result that differs from 8×8.

The effect of RC collective fluctuations on single-particle quantities is illustrated in Figs. 3(a) to 3(c) that show density plots of the single-particle spectral weight $A(\mathbf{k},\omega)$ for an 8×8 system at, respectively, $T = 1/3, 1/4$, and $1/5$. When temperature reaches $T = 1/4$ one notices that a minimum (*pseudogap*) around $\mathbf{k} = (0, \pi)$, $\omega = 0$ develops along with two maxima away from $\omega = 0$. The latter maxima are *precursors* of the Bogoliubov quasiparticles of the ordered state [9,30]. The pseudogap becomes deeper and deeper as temperature decreases, the distance between maxima remaining about constant, as observed in high temperature superconductors [2]. The condition for the appearance of a pseudogap in $A(\mathbf{k},\omega)$ is not only that we should be in the RC regime and in low dimension but also that ξ/ξ_{th} should be large [8,9]. This illustrated by the fact that the pseudogap at $\mathbf{k} = (\pi/2, \pi/2)$, where the Fermi velocity is larger, is not opened yet at $T = 1/4$ despite the fact that at $T = 1/5$ the pseudogap is of comparable size both around $\mathbf{k} = (0, \pi)$ and at $\mathbf{k} = (\pi/2, \pi/2)$, in concordance with the equality of the gaps at these two points in the zero-temperature spin-density wave state. From the slopes in Figs. 3(a) to 3(c), v_F is clearly larger at $(\pi/2, \pi/2)$ meaning that the condition $\xi > \xi_{\text{th}} = v_F/T$ is harder to satisfy at this wave vector. Numerical estimates show that ξ is nearly isotropic, by contrast with v_F. These estimates are consistent with the appearance of the pseudogap in $A(\mathbf{k},\omega)$ when $\xi \sim \xi_{\text{th}}$.

As in any numerical simulation, finite-size effects should be considered carefully. There are two important intrinsic lengths in this problem, namely, ξ_{th} and ξ. When $L \ll \xi_{\text{th}}$, the system acts as if it was basically in the quantum zero-temperature limit of a finite system. We have checked that, at $T = 1/8$, $A(\mathbf{k}, \omega)$ shows real gaps, instead of pseudogaps, that appear at progressively higher temperature in systems of smaller size. For $T = 1/3, 1/4$, on the other hand, estimates of ξ_{th} and of ξ as well as calculations for 6×6 systems and a few 10×10 systems suggest that our numerical results for $A(\mathbf{k},\omega)$ on 8×8 systems are free of appreciable size effects, i.e., $L > \xi, \xi_{\text{th}}$. This can also be checked by the size dependence of the results in Figs. 1(a) and 2. While size effects become important in $\chi''_\Delta(\omega)/\omega$ when ξ exceeds L, as long as $\xi_{\text{th}} < L$ it is possible to see thermally induced pseudogap effects in $A(\mathbf{k}, \omega)$ even if $\xi > L$ [8].

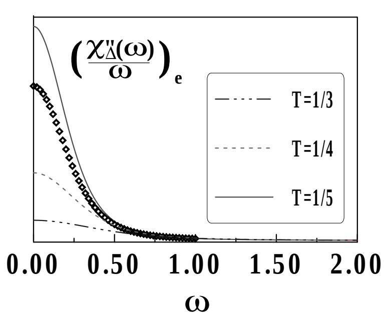

FIG. 2. Even part of the pair spectral weight $\chi''_\Delta(\omega)/\omega$ obtained from analytic continuation of imaginary time Monte Carlo data for $U = -4$, $\Delta\tau = 1/10$, $\langle n \rangle = 0.95$, and size 8×8, except for symbols that are for 6×6 at $T = 1/5$. About 10^5 sweeps were done in each case.

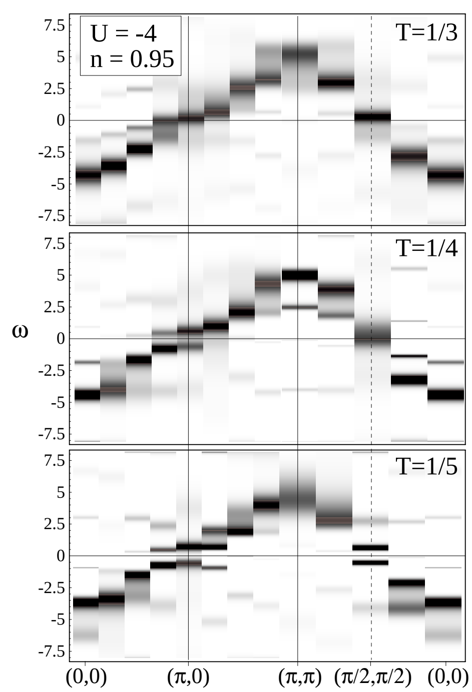

FIG. 3. Density plot of the single-particle spectral weight $A(\mathbf{k}, \omega)$ from about 10^5 Monte Carlo sweeps for $U = -4$, $\Delta\tau = 1/10$, $\langle n \rangle = 0.95$, and size 8×8. Top to bottom, $T = 1/3, 1/4, 1/5$. The dilation by $\sqrt{(2)}$ of the axis from (π, π) to $(0, 0)$ allows a comparison of Fermi velocities.

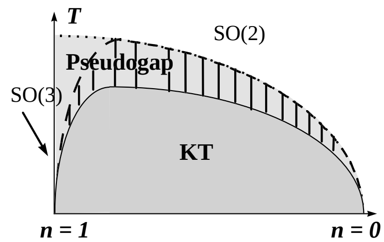

FIG. 4. Schematic crossover diagram for the $d = 2$ attractive Hubbard model in the weak-coupling regime. The shaded area above the KT phase, up to the dotted line, is the RC pseudogap regime. The KT critical regime is hatched.

In summary, the qualitative phase diagram for the attractive Hubbard model in $d = 2$ sketched in Fig. 4 shows that near a point with high order parameter symmetry the transition temperature decreases, while the pseudogap temperature increases along with the mean-field transition temperature and the zero-temperature gap. In the region where $dT_c/dn < 0$, the crossover to KT critical behavior occurs in the RC pseudogap regime when T is less than the symmetry breaking field. In our simulations we would need a larger system size to reach the KT critical regime. Contrary to the scenario of Ref. [7], in our case, dimension and symmetry contribute to create a wide pseudogap region, there is no critical coupling strength, and furthermore one enters the RC regime without sharp resonance in $\chi''_\Delta(\omega)/\omega$. Also, the precursors of Bogoliubov quasiparticles in $A(\mathbf{k}, \omega)$ occur under conditions very different from those for strong-coupling Cooper pairs that are local and do not need low dimension or large ξ/ξ_{th}. Comparisons with nonperturbative many-body calculations should appear elsewhere [30].

In high T_c superconductors the competition is between antiferromagnetism and superconductivity. Recent time-domain transmission spectroscopy experiments [31] suggest that the RC regime for the KT transition (hatched region in Fig. 4) has been observed. Close enough to the transition there is dimensional crossover to $d = 3$. For antiferromagnetic fluctuations, there are suggestions from NMR of a RC regime [32], but there is no definite proof.

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