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ATTRACTIVE HUBBARD MODEL AND SINGLE-PARTICLE PSEUDOGAP CAUSED BY CLASSICAL PAIRING FLUCTUATIONS IN TWO-DIMENSIONS

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Abstract—It is shown that in the two-dimensional attractive Hubbard model, the mean-field phase transition is replaced by a renormalized classical regime of fluctuations where a pseudogap opens up in the single-particle spectral weight. It is argued that this pseudogap and precursors of the ordered state quasiparticles can occur only in strongly anisotropic quasi two-dimensional materials. This precursor phenomenon differs from preformed local pairs. Further, while critical antiferromagnetic fluctuations would also lead to a pseudogap in the repulsive model, there are some important differences with the superconducting case. © 1998 Elsevier Science Ltd. All rights reserved

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For several years, experimental evidence about the existence of gap-like features in the normal phase of underdoped high-temperature superconductors was accumulating. In the last year or so, photoemission experiments have convincingly shown that fermionic excitations do develop a pseudogap on the Fermi surface [1, 2]. This pseudogap, that forms well above the superconducting transition temperature, suggests a normal-state precursor of the superconducting gap. It has a similar angular dependence and basically the same magnitude. Several explanations of this gap were put forward. They range from strong coupling effects, to magnetic effects, to preformed local pair effects [3, 4] (for a review see Ref. [5]). In this paper, we present a Quantum Monte Carlo study of the attractive Hubbard model to show how precursors of the superconducting quasiparticles may occur in the normal state, creating pseudogap features in the single-particle weight $f(\omega)A(\mathbf{k},\omega)$ measured in angular resolved photoemission experiments (ARPES). Pseudogap features caused by superconducting fluctuations have a very long history, dating back to film studies in the 1970s [6, 7] (for a review see Ref. [8]). Such fluctuations were proposed again more recently under the name of phase fluctuations [9] as a cause of the pseudogap. The pseudogap features discussed before were in the total density of states. Conditions for a pseudogap in the momentum-dependent $f(\omega)A(\mathbf{k},\omega)$ are more stringent. These conditions were studied in the magnetic context [10] and analogies with the superconducting case have also been pointed out [11].

In this paper, we show that classical thermal fluctuations are sufficient to obtain precursors of superconducting quasiparticles at arbitrarily small coupling as long as: (a) the system is quasi two-dimensional; (b) the superconducting correlation length ξ grows faster with decreasing temperature than the single-particle thermal de Broglie wavelength $\xi_{\rm th} = v_{\rm F}/T$. This last condition is always satisfied in the vicinity of Kosterlitz-Thouless or meanfield transitions, although it is more stringent than the condition $\xi > a$ (a is the lattice constant) assumed by several authors. The physics of this effect is very different from that of the so-called preformed local pairs that destroy the Fermi surface in any dimension but only for sufficiently strong coupling.

The attractive Hubbard model, that leads to an s-wave state, is used here because it is easier to simulate, allowing us to check the sufficient conditions obtained analytically for the appearance of precursors of the superconducting quasiparticles in the normal state. All simulations are done for $U = -4t$ and units are chosen such that $t = 1$, $a = 1$, $\mathbf{k}_{\rm B} = 1$, $\hbar = 1$.

At half-filling, where the chemical potential μ vanishes, the canonical transformation $c_{i\downarrow} \rightarrow (-1)^{i_x + i_y} c^{\dagger}_{i\downarrow}$ maps the attractive model onto the repulsive one. The $\mathbf{q} = 0$ s-wave superconducting fluctuations and the $\mathbf{q} = (\pi,\pi)$ charge fluctuations are mapped onto the three antiferromagnetic spin components of the repulsive model and, hence, they are degenerate. Because of this degeneracy, the order parameter at half-filling has $O(3)$ symmetry and therefore by the Mermin-Wagner theorem, in two-dimensions the phase transition cannot be at finite temperature. At half-filling the transposition of the results for the repulsive case shows that the pair

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structure factor $S_\Delta = (<\Delta^\dagger\Delta> + <\Delta\Delta^\dagger>)$ with $\Delta = 1/(\sqrt{N})\sum_i c_{i\uparrow}c_{i\downarrow}$ becomes size-dependent and saturates at low temperature. This saturation signals a superconducting ground state. Instead of a finite temperature phase transition, the sudden rise of S_Δ as temperature decreases indicates a crossover to a renormalized classical regime where the correlation length ξ increases exponentially. In an infinite system, a pseudogap opens up all the way from the crossover temperature T_X to zero temperature. The opening of this pseudogap is signaled by a sharp decrease with temperature of the following measure of the single-particle spectral weight near the Fermi energy:

$$\tilde{z}(T) = -2G(\mathbf{k}_F, \beta/2) = \int \frac{d\omega}{2\pi} \frac{A(\mathbf{k}_F, \omega)}{\cosh(\beta\omega/2)}$$

[12].

Away from half-filling, the $O(3)$ symmetry is broken down to $O(2)$ by the finite chemical potential. The charge fluctuations are suppressed compared with the superconducting ones. The size-dependent data can be scaled like at half-filling with an exponentially growing correlation length, showing that, for the accessible temperature range, this is still an appropriate scaling. It is noteworthy that at the crossover temperature T_X the charge fluctuations are still comparable to the superconducting ones. Despite the fact that a finite-temperature Berezinski-Kosterlitz-Thouless (KT) transition is possible with an $O(2)$ symmetry, the rapid rise of superconducting correlations apparent from Fig. 1(a) is a crossover to a renormalized classical regime, not a finite-temperature KT transition. [13] The fact that this is a crossover is demonstrated by Fig. 1(b) which shows the ratio of the classical (zero Matsubara frequency) to quantum contribution to the pair structure factor. We see that the classical contribution

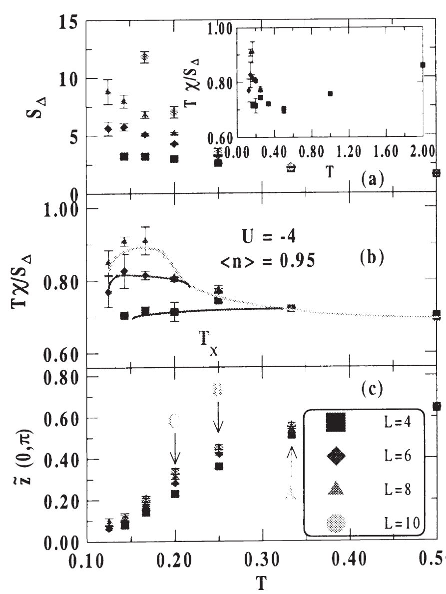

Fig. 1. (a) Pair structure factor; (b) Classical contribution. Lines are guides to the eye; (c) Weight at Fermi surface.

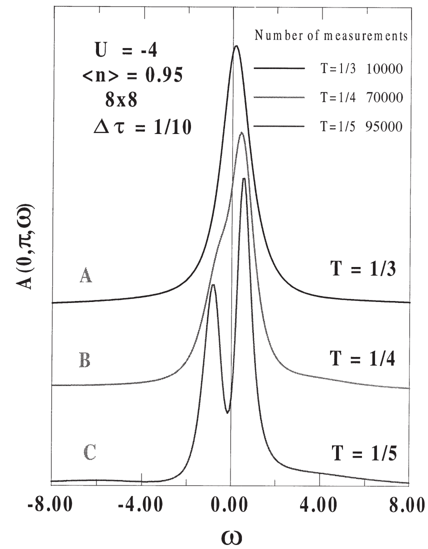

Fig. 2. Precursors near the zone edge.

decreases as temperature decreases (from $T = 2$ to $T = 1/2$ in the inset of Fig. 1(a) and then it starts to rise again at a lower temperature signaling the onset of the renormalized classical regime at $T_x(n)$. The downturn at a lower temperature indicates that as temperature becomes smaller than the minimal energy of the pairing fluctuations in the given finite system, the finite system returns back to a quantum regime and eventually $S_\Delta(L, \mathbf{q} = 0)$ saturates to its zero-temperature value in the superconducting ground state. It is known from classical-spin simulations that the KT transition is seen in finite-size systems only for much larger lattice sizes than those accessible here, namely when at least several vortices can fit inside.

In the renormalized-classical regime that exists between T_X and T_{KT} one should observe features in the single-particle spectral weight that are precursors of the superconducting ground state quasiparticles. This is suggested by the drop in $\tilde{z}(T)$ in Fig. 1(c) that coincides with T_X. To show the precursors more explicitly, consider in Fig. 2 the Fermi surface single-particle spectral weight $A(\mathbf{k}_F,\omega)$ obtained from analytical continuation of Monte Carlo data using maximum-entropy techniques. Temperature decreases from $T = 1/3$ to $1/5$ from the top to the bottom curve. These temperatures correspond respectively to the points marked *A*, *B*, *C*, in Fig. 1(c). Clearly, the Fermi liquid quasiparticle that exists at high temperature, $T = 1/3$, starts to split into two superconducting-like quasiparticles around $T = 1/4$, opening a pseudogap at the Fermi level. The splitting at $T = 1/4$ occurs in a size-independent regime (6×6 near 8×8) while at $T = 1/5$ we start to be in the size-dependent regime of Fig. 1(a).

The above results may be understood by analytical methods that were validated in detail in the half-filled case [11] [12]. Assuming some effective coupling constant g between quasiparticles and pairing fluctuations, one can obtain for the classical contribution to the spectral weight

$$A(\mathbf{k},\omega) \cong \frac{-2\sum_{cl}''(\mathbf{k},\omega)}{\left(\omega-\tilde{\epsilon}_k-\frac{g}{2\pi}\frac{T\ln\xi}{\omega+\tilde{\epsilon}_{-k}}\right)^2+\sum_{cl}''(\mathbf{k},\omega)^2} \quad (1)$$

As long as ξ increases exponentially, it is clear that $\Delta^2 \propto gT\ln\xi$ will be finite so that the spectral weight will have a maximum at a frequency given by a BCS-like dispersion $\omega^2=\tilde{\epsilon}_{\mathbf{k}}^2+\Delta^2$. Clearly the above effects can exist even in the weak coupling limit. This has to be contrasted with the case of preformed local pairs that appear when the coupling strength becomes of the order of the bandwidth. The latter is certainly not the case in High-T_c materials where the gap is about 30 meV while the bandwidth is, of the order W $\approx$ 2 eV. Also, preformed local pairs can occur for $U > W$ in arbitrary dimensions. Here however, phase space considerations for the integral defining the renormalized classical contribution show that in three dimensions one does not obtain the singular form $T\ln\xi/(\omega+\tilde{\epsilon}_{-\mathbf{k}})$ for Σ' that is necessary to obtain finite-frequency precursor quasiparticles. Nevertheless the imaginary part of Σ in three dimensions is weakly (logarithmically) divergent close to T_c which leads to a pseudogap in the total density of states $N(\omega)=\Sigma_k A(\mathbf{k},\omega)$. Note that approximations that include self-consistency in the Green's functions without the corresponding vertex corrections (FLEX like approximations) fail to reproduce the precursor of superconducting bands in the $\mathbf{k}-$ resolved spectral function $A(\mathbf{k},\omega)$[11].

Physically, precursor effects exist because in the Kosterlitz-Thouless picture the magnitude of the order parameter is locally non-zero starting below a crossover temperature T_X that is larger than the transition temperature T_{KT}. It is only the phase that is globally decorrelated above T_{KT}. Another way to understand the precursor effects is that the superfluid density and the gap are finite as $T \to T_{K.T.}^-$ and, hence, a two peak structure in $A(\mathbf{k}_F,\omega)$ exists even as the phase transition point is approached from the low-temperature side. This two peak structure should not immediately disappear when one increases the temperature slightly above T_{KT}. In quasi two-dimensional systems these high energy precursors should persist. By contrast, in an isotropic three-dimensional system, the gap vanishes at the transition point and there is no finite frequency precursors even though there may be a low-frequency depletion of the total density of states [11].

It is tempting to speculate that the physical origin of the decrease of T_c in the underdoped materials is similar to what happens in the attractive Hubbard model due to the fact that T_{KT} must go to zero when the number of components of the order parameter is larger than $N > 2$ ($O(3)$ in the attractive model). However, at present the size of the fluctuating regime of the phase transition in high-T_c materials is controversial. Recent infrared experiments [14] suggesting a pseudogap even in the overdoped regime are consistent with the mechanism discussed here. Clearly however, present ARPES experiments [1], show large backgrounds that are unexplained by the above approach. Finally, let us contrast precursor effects due to magnetic and superconducting fluctuations. Our criterion for the appearance of a pseudogap shows that even for the s-wave interaction the superconducting pseudogap should open up from the zone edge (smaller v_F) as temperature decreases until the whole Fermi surface is gapped. This is, obviously, even more so for the d-wave like interaction, when one has nodes along the diagonal direction. In the case of an antiferromagnetic pseudogap, the region near the hot spots is gapped, but a whole segment of the Fermi surface near the diagonal direction remains gapless even when one approaches a phase transition.

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