Pseudogap above $T_c$ in a model with $d_{x^2-y^2}$ pairing

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We study the anomalous normal state properties of a simple two-dimensional model whose ground state is a $d$-wave superconductor. Using a self-consistent, conserving formulation, we show that pairing correlations above $T_c$ lead to the appearance of a highly anisotropic pseudogap in the electronic spectral function and the destruction of the Fermi surface. We discuss the similarities and differences between our results and ARPES experiments on underdoped cuprates.

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The deviations from Fermi liquid theory (FLT) in the normal state of high $T_c$ superconductors are now well established. It has recently become clear that the underdoped cuprates exhibit even more remarkable deviations from FLT than the optimally doped materials: not only are the quasiparticles not defined, but the Fermi surface also becomes ill-defined due to the opening of a pseudogap. Early evidence for the suppression of low frequency spectral weight above $T_c$ came from a variety of probes, including NMR, specific heat, and optics. Recent angle-resolved photoemission (ARPES) studies on Bi-2212 compounds have considerably clarified the situation by providing direct evidence for a highly anisotropic pseudogap, for $T_c < T < T^*$, which is similar in its magnitude and in its angular dependence to the $d$-wave superconducting gap below $T_c$.

These observations of a normal state pseudogap find a simple explanation in a theory in which the pairing amplitude develops at a crossover scale $T^*$ higher than the $T_c \sim n_s/m^*$, at which phase coherence sets in. The separation between $T_c$ and $T^*$ naturally occurs in low density, short coherence length superconductors, and leads to striking deviations from FLT in degenerate Fermi systems in 2D. However, rather little is known theoretically about the pseudogap state above $T_c$ in $d$-wave superconductors (since, for technical reasons, the quantum Monte Carlo results are restricted to s-wave pairing). Such a study is clearly important, not only because the experiments show $d$-wave pairing, but also to compare the predictions of these theories with those of RVB-based theories in which spinons pair at $T^*$ and holons condense at $T_c$. An improved understanding of the origin of this pseudogap effect may also be an important clue towards a theory of high temperature superconductivity.

As a first step in this direction, we study a phenomenological model of a 2D $d$-wave superconductor, in a parameter range where the normal state is dominated by $d$-wave pairing correlations. Using a self-consistent, conserving approximation, we show that there is a crossover temperature scale $T^*$ below which normal state spectral functions exhibit anomalous dispersion with a highly anisotropic suppression of spectral weight – pseudogap – near the chemical potential. This also leads to the partial destruction of the Fermi surface along certain directions in the Brillouin zone. Both these effects are very similar to the ARPES experiments. We also find that the normal state spin susceptibility acquires a spin-gap like $T$-dependence.

Let us consider a simple two-dimensional model which has a superconducting ground state with $d_{x^2-y^2}$ symmetry, defined by

$$
H = \sum_{k,\sigma} (\epsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{N} \sum_{k,k',q} V_{k,k'} c_{k\uparrow}^\dagger c_{q-k\downarrow}^\dagger c_{q-k'\downarrow} c_{k'\uparrow}
$$

(1)

where the $d$-wave separable potential is $V_{k,k'} = U_d f(k) f(k')$ with $U_d < 0$ and $f(k) = (\cos k_x - \cos k_y)$. This potential is a piece of the nearest-neighbour interaction used in Ref. to model superconductivity in the cuprates. For simplicity, we study the nearest-neighbor dispersion $\epsilon_k = -2t(\cos k_x + \cos k_y)$, with $t = 1$, on a square lattice with periodic boundary conditions. The chemical potential $\mu$ is adjusted to obtain the required density $n$.

To investigate the finite temperature properties of this model in the intermediate coupling regime ($|U_d|$ of order bandwidth), we use the “fluctuation exchange” (FLEX) approximation. Since the important correlations in this problem are in the particle-particle (p-p) channel, we dress the propagator with these and solve the problem self-consistently. Specifically, the vertex (with two incoming and two outgoing legs) is defined by the standard integral equation written symbolically as:

$$
\Gamma_{k,k'}^q = I_{k,k'}^q - \tilde{I}_{k,k'}^q - \sum_{p} I_{k,p}^q G(p) G(q-p) \Gamma_{p,k'}^q,
$$

(2)

where $I_{k,k'}^q$ is the p-p irreducible vertex and $\tilde{I}$ is the same quantity with twisted outgoing legs. Here and below all the quantities are matrices in spin space, the
four-momentum \( k = (k_i, ik_n) \) with \( ik_n \) a fermion Matsubara frequency \((p \text{ and } k' \text{ have the same nature})\) and the four-momentum \( q = (q_i, iq_m) \) with \( iq_m \) a boson Matsubara frequency, and the symbolic summation means integrating out (with proper factors) intermediate momenta and frequencies and matrix multiplication with respect to spin indices. The Green’s function \( G(k) = [i k_n - \epsilon_k - \mu - \Sigma(k)]^{-1} \) is defined in terms of the self-energy, which satisfies the relation (3)

\[
\Sigma(k) = \sum V_{k,p} G(q-k)G(p)G(q-p)\Gamma^q_{p,k}
\]

where \( V_{k,p} \) is the bare two-body potential.

We now approximate the p-p irreducible vertex by the bare potential from (1), in which case the contribution from \( \tilde{I} \) to \( \Sigma \) vanishes. For the self-energy, this is completely equivalent to the well-known self-consistent T-matrix approximation (14). The advantage of the present approach is that in addition to the one-particle Green’s function \( \Gamma \) also defines the two-particle Green’s functions, and diagrams with “twisted” legs are important for evaluating response functions such as the spin susceptibility (as we will discuss in detail elsewhere (15)).

The coupled integral equations for the self-energy and the vertex part are numerically solved using fast Fourier transforms (16) and the analytic continuation from Matsubara to real frequencies is performed using Padé approximants (17). Technical details, as well as checks on the method and the numerics for the case of the attractive Hubbard model, where we could compare our results against quantum Monte Carlo (18), will be described elsewhere (15).

In this paper we focus primarily on the spectral function \( A(k, \omega) = -(1/\pi)\text{Im}G(k, \omega + i0^+) \), which is closely related to the ARPES intensity (13). We show representative results for \( U_d = -8 \) and \( n = 0.5 \) (quarter-filling, \( n_s = 0.25 \)); qualitatively similar results were found for several other parameter values. All the results are in the non-superconducting state above \( T_c \) (see below). In Fig. 1 we plot the spectral functions at a high temperature \( T = 2.0 \) for \( k \) varying from \((0, 0)\) to \((\pi, 0)\), and see the peaks of \( A(k, \omega) \) disperse through the chemical potential \( \omega = 0 \). We may identify points \( k^* \) in the Brillouin zone such that \( A(k^*, \omega) \) has a dominant peak at \( \omega = 0 \). The “locus of gapless excitations” \( \{k^*\} \) then generalizes (13) the notion of a “Fermi surface” (FS) to finite temperatures without any assumptions about well-defined quasiparticles, and, quite generally, it is a closed contour in the repeated-zone scheme.

It is worth commenting on the lineshapes in Fig. 1 at \((0, 0)\) the peak is actually infinitely sharp for our model, and the small width is put in by hand. Our choice of \( V_{k,k'} \) implies that states along the diagonal \((0, 0)\) to \((\pi, \pi)\) are totally unaffected by interactions. On the other hand, this potential gives rise to very strong effects near \((\pi, 0)\) where the spectral functions acquire very large widths as seen from Fig. 1, so that the quasi-particle nature is completely destroyed. Note that a log scale is used so that this spreading of spectral weight over an enormous frequency range can be easily seen. The sum rule \( \int d\omega A(k, \omega) = 1 \) is satisfied (to very high precision) for each \( k \).
imaginary parts of the (retarded) self-energy as functions of ω. We find that the dominant peak of A(k, ω), which is at ω ≤ 0 for each k in Fig. 2, is associated with a solution of ω − θk − μ − ReΣ(k, ω) = 0 for which dReΣ/dω < 0 and ImΣ is small. The very broad features at ω > 0 come from solutions for which ReΣ has a positive slope and ImΣ is large. It is tempting to describe the “bounce” and multiple-peak structure as a precursor of the Bogoliubov-like dispersion of excitations in the SC state. In the presence of strong self-energy effects, such a simple picture may need to be generalized significantly.

Let us now ask how the pseudogap affects the “Fermi surface” (FS) by studying the “locus of gapless excitations” {k∗} (defined, as before, by the condition that the spectral function at that k has a dominant peak centered at ω = 0). Along (or near) the zone diagonal, (0, 0) to (π, π), interaction effects are absent (or weak) and there is a conventional FS crossing with a well defined k∗. However, along the (0, 0) to (π, 0) there is no FS crossing. By studying the spectral function in the entire zone we find that the anomalous dispersion and large line-widths destroy the notion of a FS as a closed contour of gapless excitations (even in the repeated-zone scheme). The resulting picture emerging from our calculations, and consistent with ARPES experiments, is that the Fermi Surface is destroyed in patches in the Brillouin zone, as schematically depicted in Fig. 3.

A more quantitative understanding of the destruction of the FS can be obtained by studying the angular dependence of the pseudogap and its variation with temperature. In the spirit of the ARPES experiments we estimate the pseudogap by making scans through k-space and noting the position of the spectral function peak which is farthest to the right, i.e. at the largest frequency below zero. We then plot the spectral function pseudogap ∆ps, as a function of θ = arctan(ky/kx). In Fig. 4 we plot the angle-dependence of ∆ps(θ) at two temperatures T = 0.2t and T = 0.75t. The first point to notice is the strong anisotropy of the gap, which is always suppressed to zero in an arc about the diagonal. The extent of the zero gap (nodal) region, and the magnitude of the maximum gap at low T are both sensitive functions of the choice of parameters (see below); we find that the larger the maximum gap, the smaller the nodal region. The second important point to note is the T-dependence of the pseudogap, which suggests a gap collapse due to quasiparticles excited around the nodal regions in a d-wave SC gap, similar to a recent suggestion of Lee and Wen [21]. At high temperatures, the pseudogap gets suppressed and eventually disappears upon further heating; above a crossover scale T* ≃ 1 (for the parameters discussed here) the spectral function peaks disperse through ω = 0 for all fixed-kx scans. Thus we find that we recover a closed contour of gapless excitations above T*.

However, in our model we find that this “Fermi surface” has T-dependence [19]. It is quite remarkable that in the ARPES experiments, there are indications [2] of an underlying Luttinger FS which is T-independent within error bars.

![FIG. 3. Fermi Surface destroyed in patches; solid lines represent gapless excitations and the shaded patches indicate momenta where there is strong scattering and the FS is washed out.](image)

![FIG. 4. The angle dependence of the ∆ps(θ) for temperatures T = 0.2 and T = 0.75 and U_d = −8, n = 0.5.](image)

It is instructive to consider the doping dependence of the effect. In Fig. 5 we show ∆ps(θ) at the same temperature and coupling, for three values of the density. The pseudogap clearly increases rapidly with increasing density.

![FIG. 5. The angle dependence of ∆ps(θ) for densities n = 0.5, n = 0.55 and n = 0.60 and U_d = −8, T = 0.2.](image)

Up to now, we have discussed the pseudogap behaviour in our model in the single-particle spectral weight. In Fig. 6 we show that the temperature dependence of the static, uniform, spin susceptibility also has a spin gap,
similar to what is observed in NMR [1] and has been calculated [7] for the case of the attractive Hubbard model which has s-wave pairing. More details of this calculation will be presented elsewhere [15].

To ensure that we are above the superconducting $T_c$ we calculate the parameter $\lambda = \text{Im} \chi_{pp}(q=0)$ where $\chi_{pp}^0(q) = (T/N) \sum_k f^2(k) G(k) G(q-k)$. The gap equation at $T = T_c$ reduces to the condition $\lambda = 1$, which in our approximation coincides with the appearance of a pole in the full vertex. Thus, one should keep $\lambda < 1$ to be in the normal state. In 2D, there is of course no LRO at non-zero temperatures and one expects $\lambda < 1$ for all $T > 0$. Even though our formalism does not include topological excitations, it is reasonable to expect $\lambda \approx 1$ near the onset of algebraic order. In practice we consider only temperatures for which $\lambda < 0.8$.

We conclude this paper by showing that the pseudogap behavior described above is occuring in a degenerate Fermi system above $T_c$. This is important to establish since gap-like features can be trivially obtained either in a system below $T_c$, or in a strongly coupled regime where all the electrons are tightly bound up into bosonic pairs. The specific heat [8] and the ARPES [9] experiments clearly indicate that in the underdoped systems one is still dealing with a degenerate Fermi system and not bosons. By looking at the momentum distribution $\alpha(k)$ [13], and by ascertaining that the chemical potential $\mu \gg T$, we know that we are in a degenerate Fermi regime.

In this paper we have studied the normal state of a simple model in which d-wave pairing correlations above $T_c$ lead to the appearance of a highly anisotropic pseudogap and the destruction of the Fermi surface, which are remarkably similar to the results of ARPES experiments. Quantitative comparison with the experiments must, however, await a controlled calculation based on a microscopic model which describes how a Mott insulator upon doping goes into a short coherence d-wave superconductor whose normal state is dominated by pairing correlations.

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