МАТЕРІАЛОЗНАВСТВО ТА МАШИНОБУДУВАННЯ

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ANOMALOUS ONE-PARTICLE PROPERTIES IN THE NORMAL STATE OF A MODEL WITH $d_{x^2-y^2}$ SUPERCONDUCTIVITY

The main purpose of this study is to investigate the influence of the strong superconducting fluctuations in the *d*-wave channel on the normal state properties of a simple two-dimensional strongly correlated Fermi-system. We achieve this goal using a thermodynamically self-consistent Baym–Kadanoff conserving Green's function approximation (formulation is based on a well-defined free energy and conserving particle number, momentum, and energy), which is known to produce reliable results for the *s*-wave superconductors well beyond the weak coupling limit up to the range where the interaction strength is comparable to the bandwidth of the quasiparticle spectrum. The research shows 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 conclude that our results are in remarkable agreement with the available experimental angle-resolved photoemission data on the high temperature superconductors.

Introduction

The deviations from Fermi liquid theory (FLT) in the normal state of high T_c superconductors are now well established [1]. 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 fuzzy 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 [2], specific heat [3] and optics [4]. Recent angle-resolved photoemission (ARPES) studies [5, 6] on various families of the high-T_c 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 [7–9] in which the pairing amplitude develops at a crossover scale T^* higher than the $T_c \sim n_s/m^*T$ [10, 11] 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 [8]. 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 [8] 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 [7, 8, 11] with those of RVB-based theories [12] 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.

Problem setting

We propose a strongly correlated model with the *d*-wave superconductivity in the ground state. This model is used to investigate the anomalies of the normal state properties in the presence of strong superconducting fluctuations. The influence of the fluctuations is related to the anomalous pseudogap behavior experimentally observed on the cuprate superconductors.

Constructing a model with *d*-wave superconductivity in the ground state

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

$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) c^{\dagger}_{k,\sigma} c_{k,\sigma} + \\ + \sum_{k,k',q} V_{k,k'} c^{\dagger}_{k\downarrow} c^{\dagger}_{q-k\downarrow} c_{q-k'\downarrow} c_{k'\uparrow}, \qquad (1)$$

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-neighbor interaction used in Ref. [13] to model superconductivity in the cuprates. For simplicity, we study the nearest-neighbor dispersion $\varepsilon_k = -2t(\cos k_x + \cos k_y)$ on a square lattice with periodic boundary conditions. The chemical potential μ 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 [14]. 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 [15]:

$$\Gamma^q_{k,k'} = I^q_{k,k'} - \tilde{I}^q_{k,k'} + \sum_p I^q_{k,p} G_p G_{q-p} \Gamma^q_{p,k'},$$

where $I^q_{k,k'}$ is the particle-particle (p-p) irreducible vertex and $\tilde{I}^q_{k,k'}$ is the same quantity with twisted outgoing legs. Here and below all the quantities are matrices in spin space, the four-momentum $k = (k, i\omega_n)$ with $i\omega_n$ a fermion Matsubara frequency (p, k and k' have the same nature) and the four-momentum $q = (q, i\nu_n)$ with $i\nu_n$ 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 $G_k = 1/[i\omega_n - (\varepsilon_k - \mu) - \Sigma_k]$ is defined in terms of the self-energy, which satisfies the relation [15]:

$$\Sigma_k = \sum_{p,q} V_{k,p} G_{q-k} G_p G_{q-p} \Gamma^q_{p,k},$$

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 $\tilde{I}^q_{k,k'}$ to Σ vanishes. For the self-energy, this is equivalent to the well-known self-consistent T-matrix approximation [16]. The advantage of the present approach is that in addition to the one-particle Green's function Γ 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 discuss in detail elsewhere [17]).

The coupled integral equations for the self-energy and the vertex part are numerically solved iteratively, using fast Fourier transforms [18] and the analytic continuation from Matsubara to real frequencies is performed using Pade approximants [19]. The FFT works reliably with functions that decay as $1/\omega^2$ (or faster) at large ω because of the necessity of a cutoff. For the present model a cutoff 10 to 20 times the bandwidth was necessary. Our runs were typically for 64×64 lattices with a uniform ω mesh of 512 points. Technical details, as well as checks on the method and the numerics for the case of the attractive Hubbard model, where we could provide extensive comparison of our results to other techniques (see, e.g. [8]), will be described in future publications.

Attractive Hubbard model

For our present purposes, to validate our approach in the chosen parameter range, we applied this approximation to the attractive Hubbard model, for which the Monte-Carlo calculations are available to compare against [20]. The Hamiltonian is given by:

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \\ - \mu \sum_{i,\sigma} n_{i,\sigma} + \frac{U}{N} \sum_{k,k',q} c^{\dagger}_{k\uparrow} c_{k'\uparrow} c^{\dagger}_{q-k\downarrow} c_{q-k'\downarrow},$$

where $c^{\dagger}_{k,\sigma}$ creates an electron in the state k with spin projection σ, $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{j,\sigma}$ is the number operator on site i, the sum $\langle i, j \rangle$ runs over pairs of nearest-neighbor lattice sites, U is the strength of the potential ($U < 0$), t is the nearest-neighbor hopping amplitude, and μ is the chemical potential. The detailed report on the calculations for the attractive Hubbard model will be presented in the

future publications. Here we only show that the density of states, calculated within the framework of the proposed approach is in good agreement with the Monte-Carlo calculation results available in the current literature for the attractive Hubbard. This provides confidence in our results for the model with the *d*-wave superconductivity, for which the Monte-Carlo studies are not readily available yet.

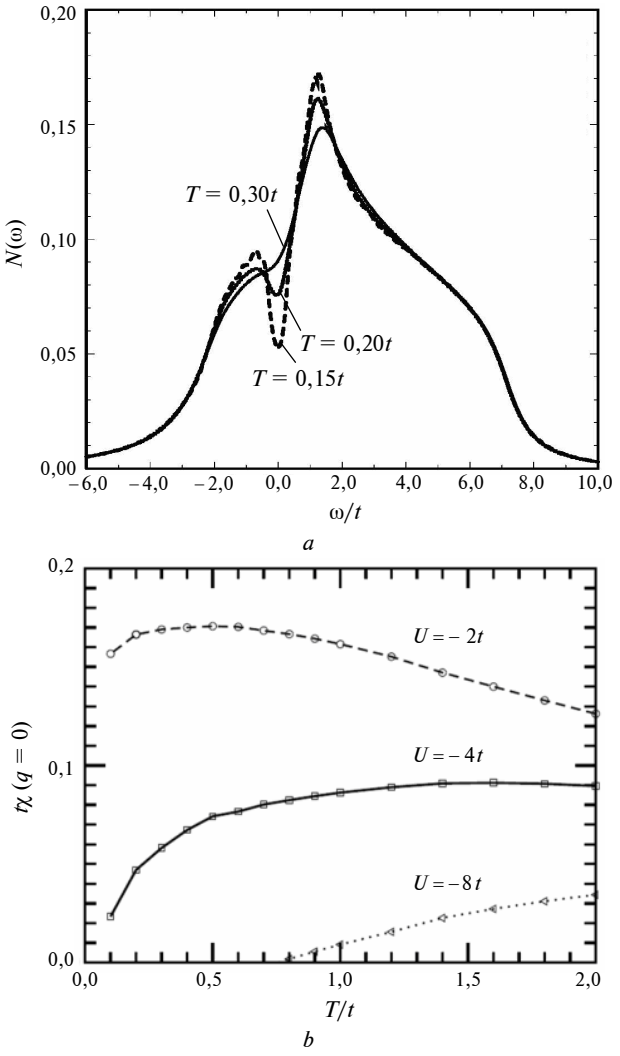


Fig. 1. Density of states (*a*) and the uniform static spin susceptibility (*b*) vs temperature for the attractive Hubbard model. Pseudogap develops near the chemical potential ($\omega = 0$) as the temperature decreases, in agreement with the available Monte-Carlo data (to compare with the Monte-Carlo simulation for the same parameters see [21]). The uniform static spin susceptibility (a two-particle property) also reveals the tendency to the diamagnetism as the temperature drops, in remarkable agreement with [22]

The results were obtained at intermediate coupling $U = -4t$ and moderate density $\langle n \rangle = 0,5$ corresponding to the quarter-filled system. The final temperature Green's function was analytically continued to the complex plane, which allowed to extract the position of leading poles and study their temperature and momentum behavior. The density of states $N(\omega) = (1/N)\Sigma_k A(k,\omega)$ is plotted on Fig. 1, *a* at different temperatures. This picture is in striking agreement with the Monte-Carlo calculations [21] and shows a nontrivial feature of the normal state of the Fermi-system with on-site two-particle attraction: the depletion of the spectral weight at the chemical potential level (on the figure it is at $\omega = 0$). The uniform static spin susceptibility (a two-particle property) also reveals the tendency to the diamagnetism as the temperature drops, in remarkable agreement with [22], as it seen on Fig. 1, *b*. All this suggests that approach is solid for the intermediate coupling strengths, and can be applied to study systems, that are much larger than those accessible by other numerical methods, like quantum Monte-Carlo, or exact diagonalization.

Pseudogap in the model with the *d*-wave pairing

In this paper we focus primarily on one-particle properties of the system, such as the spectral function $A(k,\omega) = -(1/\pi)\mathrm{Im}\,G(k,\omega + i0^+)$, which is closely related to the ARPES intensity [23]. We show representative results for $U_d = -8t$ and $n = 0,5$ (quarter-filling, $n_\sigma = 0,25$); qualitatively similar results were found for several other parameter sets. All the results are in the non-superconducting state above T_c (see below). Note that the strength of the *d*-wave potential $U_d = -8t$ corresponds to the attractive Hubbard potential $U_d = -4t$, as it can be easily seen by averaging $V_{k,k'} = U_d f(k) f(k')$ over the first Brillouin zone. In Fig. 2, *a* we plot the spectral functions at a high temperature $T = 2,0t$ 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 [24] 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. The

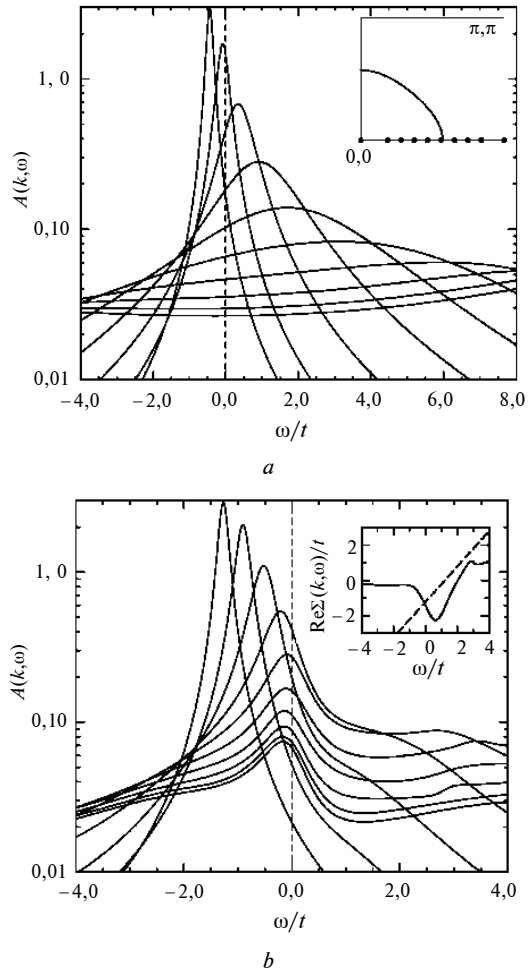


Fig. 2. (*a*) $A(k,\omega)$ for a sequence of momenta $k = (xp/32;0)$; $x = \{0; 6; 9; 12; 15; 18; 21; 24; 27; 32\}$ for $U_d = -8t$ and $n = 0{,}5$ at a high temperature $T = 2{,}0t$. In the inset the points indicate the momenta k and the solid curve shows the $T = 0$, non-interacting FS. The potential gives rise to very strong effects near $(\pi, 0)$ where the spectral functions acquire very large widths, the quasiparticle nature is completely destroyed; (*b*) $A(k,\omega)$ for the same set of parameters as in (*a*) except for much lower temperature $T = 0{,}2t$. The dominant peaks of $A(k,\omega)$ exhibit very anomalous dispersion: as k varies from (0, 0) to $(\pi, 0)$, the peak approaches $\omega = 0$, but never crosses it (in full agreement with the latest ARPES, see text). In addition it acquires a hump-like structure above $\omega = 0$ line, accessible by IPES probes

gapless locus for a strongly correlated system at finite temperatures, need not posses all of the properties that we associate with the usual $T = 0$ definition of a FS in a Fermi liquid. For instance, there is no guarantee that the volume enclosed by this locus is T-independent. Nevertheless, by focusing on gapless excitations, it seems to be a very natural generalization.

It is worth commenting on the line shapes in Fig. 2, *a*: 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 (π, π) 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. 2, *a*, so that the quasiparticle 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 $\int d\omega A(k,\omega)$ is satisfied (to very high precision) for each k.

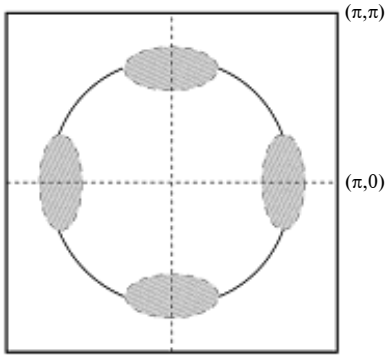
As the temperature is lowered below a scale $T^* \simeq 1{,}0t$ (for the same choice of parameters as in Fig. 2, *a*), remarkable changes takes place in the spectra, as seen from Fig. 2, *b*, which shows results at $T \simeq 0{,}2t$ (but still above T_c). First, we find that spectra which showed one broad feature at high T now show a multiple peak structure (see further below). Second, the dominant peaks of $A(k,\omega)$ exhibit very anomalous dispersion: as k varies from (0, 0) to $(\pi, 0)$, the peak approaches $\omega = 0$ (from below, i.e. from the area accessed by ARPES), but never crosses it, either "bouncing back" towards negative ω or "stalling" (depending on parameter values), in complete contrast to the high T results described above. This is exactly like the pseudogap behavior seen in ARPES experiments [5, 6] on underdoped cuprates in the temperature regime $T_c < T < T^*$, and corresponds to the emergence of the Bogoliubov behavior, albeit above T_c. In addition it acquires a hump-like structure above $\omega = 0$ line, accessible by the inverse photoemission (IPES) probes. Note that modern day IPES experiments have not yet attained the necessary accuracy to provide conclusive comparison, but in general are in agreement with the presented model [5].

To understand the multiple peak structure of the spectral functions it is useful to look at plots of the real and imaginary parts of the (retarded) self energy as functions of ω. We find that the dominant peak of $A(k,\omega)$, which is at $\omega \le 0$ for each k in Fig. 2, *b* is associated with a solution of to the following equation: $\omega - (\varepsilon_k - \mu) - \mathrm{Re}\,\Sigma(k,\omega) = 0$ for which $d\,\mathrm{Re}\,\Sigma / d\omega < 0$ and $\mathrm{Im}\,\Sigma$ is small. The presence of such solution is clearly observed in the

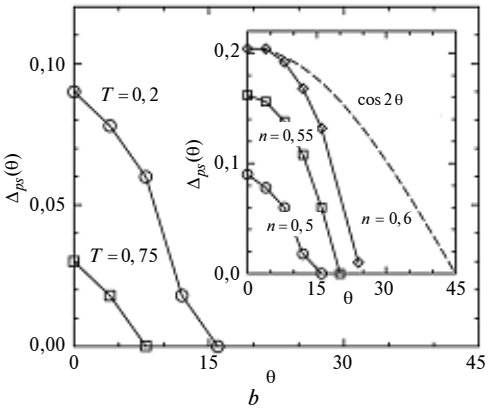
inclusion on Fig. 2, *b*, where the line $\omega - (\varepsilon_k - \mu)$ crosses the curve $\mathrm{Re}\,\Sigma(k,\omega)$. As to the unusual very broad features at $\omega > 0$, they come from those solutions for which $\mathrm{Re}\,\Sigma$ has a positive slope and $\mathrm{Im}\,\Sigma$ is large. Above T_c these solutions strictly speaking do not occur, but $\omega - (\varepsilon_k - \mu)$ approaches $\mathrm{Re}\,\Sigma(k,\omega)$ very closely, as clearly seen on the enclosure in Fig. 2, *b* at $\omega \sim 3,0t$, and corresponds to the position of the emerging hump in the spectral function. It is natural to perceive the "bounce" and multiple-peak normal state structure of the spectral function as a precursor of the Bogoliubov-like dispersion of excitations in the SC state. On the other hand, in the presence of strong self-energy effects, such a simple picture may need to be somewhat generalized.

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 $\omega = 0$). 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 $(\pi,0)$ 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 [5, 6, 25], is that the Fermi Surface is destroyed in patches in the Brillouin zone, as schematically depicted in Fig. 3, *a* (for experiments see, e.g. [26]).

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 Δ_{ps} as a function of $\theta = \arctan(k_y/k_x)$. In Fig. 3, *b* we plot the angle-dependence of $\Delta_{ps}(\theta)$ 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 known suggestion of Lee and Wen [27]. At high temperatures, the pseudogap gets suppressed and eventually disappears upon further heating; above a crossover scale $T^* = 1,0t$ (for the parameters discussed here) the spectral function peaks disperse through $\omega = 0$ for all fixed-k_y scans. Thus we find



a



b

Fig. 3. (*a*) 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 destroyed (see text); (*b*) the angle-dependence of $\Delta_{ps}(\theta)$ (in the units of t, i.e. $t = 1$) at two temperatures $T = 0,2t$ and $T = 0,75t$. In the enclosure we show $\Delta_{ps}(\theta)$ at the same temperature and coupling, for three values of the density. The dependence $\cos(2\theta)$ (the ideal *d*-wave symmetry of the gap) is plotted (dashed line) as the guide to the eyes

that we recover a closed contour of gapless excitations above T^*. However, in our model we find that this "Fermi surface" has T-dependence [24]. It is quite remarkable that in the ARPES experiments, there are indications [6] of an underlying Luttinger FS which is T-independent within error bars.

It is instructive to consider the doping dependence of the effect. In the enclosure to Fig. 3, *b* we show $\Delta_{ps}(\theta)$ at the same temperature and coupling, for three values of the density. The dependence $\cos(2\theta)$ (the ideal *d*-wave symmetry of the gap) is plotted (dashed line) as the guide to the eyes. The value of the pseudogap clearly increases rapidly with increasing density.

To ensure that we are *above* the superconducting T_c we calculate the parameter $\lambda = |U_d|\chi_{pp}(q=0)$, where $\chi_{pp}(q) = (T/N)\sum_k f^2(k) G_k G_{(q-k)}$ is the pair susceptibility. The gap equation at $T = T_c$ reduces to the condition $\lambda = 1$ [17], which in our approximation coincides with the appearance of a pole in the full vertex. In practice we consider only temperatures for which $\lambda < 0,9$.

Conclusions

We conclude this paper by showing that the pseudogap behavior described above is occurring 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 [3] and the ARPES [5, 6] 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 $n(k)$ [17], and by ascertaining that the chemical potential $\mu >> T$, we know that we are in a degenerate Fermi regime.

In conclusion, this paper studies the one-particle properties of 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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