Persistence of pseudogap formation in quasi-2D systems with arbitrary carrier density

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Abstract

The existence of a pseudogap above the critical temperature has been widely used to explain the anomalous behaviour of the normal state of high-temperature superconductors. In two dimensions the existence of a pseudogap phase has already been demonstrated in a simple model. It can now be shown that the pseudogap phase persists even for the more realistic case where coherent interlayer tunneling is taken into account. The effective anisotropy is surprisingly large and even increases with increasing carrier density.

Key words: quasi-2D metal, arbitrary carrier density, normal phase, pseudogap phase, superconducting Berezinskii-Kosterlitz-Thouless phase

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1 Introduction

The anomalous behaviour of the normal state of high-temperature superconductors (HTSC) \cite{1,2} (including the behaviour of the spin susceptibility, resistivity, specific heat and photo-emission spectra) has been recently interpreted in terms of the formation of a pseudogap above the critical temperature, $T_c$ \cite{3,4}.

The formation of a pseudogap phase above $T_c$ has been explicitly demonstrated in a model non-relativistic 2D fermi-system \cite{5,6}. The work is based on the peculiarities of the Berezinskii-Kosterlitz-Thouless (BKT) phase formation (see also \cite{7}), which is a two stage process. For a 2D system one must rewrite the order parameter $\Phi(x)$, where $x = r, \tau$ denotes the position and imaginary time, in terms of its modulus $\rho(x)$ and its phase $\theta(x)$ i.e. $\Phi(x) = \rho(x) \exp[-i\theta(x)]$. This was originally stated by Witten in the context of 2D quantum field theory \cite{8}. It is clearly impossible to obtain $\Phi \equiv \langle \Phi(x) \rangle \neq 0$ at finite $T$ since this corresponds to the formation of homogeneous long-range (superconducting) order which is forbidden by the Coleman-Mermin-Wagner-Hohenberg theorem. However it is possible to obtain $\rho \equiv \langle \rho(x) \rangle \neq 0$ but at the same time $\Phi = \rho \langle \exp[-i\theta(x)] \rangle = 0$ due to random fluctuations in the phase $\theta(x)$. We stress that $\rho \neq 0$ does not imply long-range superconducting order (which is destroyed by the phase fluctuations) and is therefore not in contradiction with the above-mentioned theorem.

Thus one has three regions in the 2D phase diagram \cite{9}. The first is the superconducting (BKT) phase, where $\rho \neq 0$. In this region there is algebraic order and a power law decay of the correlations. The second is the pseudogap phase where $\rho$ is still non-zero but the correlations decay exponentially. The third is the normal (Fermi-liquid) phase where $\rho = 0$. Note that $\Phi = 0$ everywhere. The unusual properties of the second region, which lies between the superconducting and normal phases, have previously been used in \cite{3} to explain the pseudogap behaviour in HTSC. For example in the mean-field calculation of the paramagnetic susceptibility \cite{6} the parameter $\rho$ plays the role of the energy gap $\Delta$ in the theory of ordinary superconductors. Thus in this calculation one has the opening of an energy gap $\rho$ (or equivalently a lowering of the density of states) above the superconducting transition.
The description of the phase fluctuations and the BKT transition closely resembles that
given by Emery and Kivelson [9]. However in their phenomenological approach the field \(\rho(x)\)
does not appear while in the present microscopic approach based on [8] it appears rather
naturally.

Although the description in terms of modulus and phase variables is essential from a
mathematical point of view, the physical implications for the theory of superconductivity
have not been fully understood. Previous work [8] was at zero temperature but the applica-
tion to condensed matter requires the extension to finite temperature where \(\rho\) is a function
of the temperature \(T\). It makes sense therefore to define the temperature \(T_\rho\) at which \(\rho\)
becomes zero. This temperature is then interpreted as the temperature at which the pseudogap
opens. Since in [5, 7] and in the present work \(\rho(x)\) has only been treated in the mean-field
approximation i.e. one has neglected the fluctuations in both \(\rho(x)\) and \(\theta(x)\), a second-order
phase transition was obtained. However it is well known experimentally that the formation
of the pseudogap phase does not display any sharp transition. It can be argued however that
the fluctuations may convert the obtained sharp transition to a crossover [5].

An important question is whether the pseudogap phase (PP) forms in real HTSC, which
are only quasi-2D systems. Another related question is whether the pseudogap phase, if
present, remains large enough to explain the experimentally observed anomalies even when
interlayer tunneling is included.

This paper will study PP formation for a quasi-2D system with arbitrary carrier density.
Note that this problem is further complicated by the formation in quasi-2D systems of the
ordinary bulk superconducting phase with homogeneous long-range order (LRO) at critical
temperature \(T_c\) (see for example [10]). Since the BKT phase formation corresponds to
the formation of two-dimensional order while true LRO is three dimensional one expects
that for weakly coupled layers \(T_c \leq T_{\text{BKT}}^a\), where \(T_{\text{BKT}}^a\) denotes the critical temperature for
the BKT transition in the quasi-2D system. \(T_{\text{BKT}}^a\) represents the temperature at which the
system becomes superconducting in the layers (planes) while \(T_c\) is the critical temperature for
bulk superconductivity. Thus \(T_{\text{BKT}}^a\) is the maximum temperature at which superconducting
behaviour is present. The temperature range $T_c \leq T \leq T_{\text{BKT}}^q$ corresponds to a crossover region where the effect of the interlayer tunneling is insufficient to produce three dimensional behaviour and the behaviour remains BKT-like. There is in fact some experimental evidence for the existence of this crossover region ($\sim 1K$) in optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$ [11].

The size of this region is obviously critically dependent on the anisotropy, the carrier density and the precise form of the interlayer tunneling. At very low densities (i.e. in the Bose limit of isolated pairs) and for physically reasonable values for the parameters, it has been shown for quasi-2D system [3, 12, 13] that long-range order is only established well below $T_{\text{BKT}}$. However these densities are not realised physically. It can also be shown that $T_c$ approaches the BCS critical temperature asymptotically in the high-density limit [14] so that both this region and the pseudogap phase must vanish asymptotically. At the intermediate carrier densities found in HTSC we find that the pseudogap phase remains large enough to explain the observed anomalies. However the experimentally observed superconducting transition is practically three dimensional [11] so that one expects $T_c \lesssim T_{\text{BKT}}^q$ at these densities and this is the subject of current investigations.

For these reasons we only calculate the temperatures $T_{\text{BKT}}^q$ and $T_\rho$ as functions of the carrier density $n_f$ to establish the boundaries of the PP. Here $T_{\text{BKT}}^q$ denotes the critical temperature for the BKT transition in the quasi-2D system.

We show that the value of $T_\rho$ is practically identical in the 2D and the quasi-2D systems, while for realistic model parameters $T_{\text{BKT}}^q > T_{\text{BKT}}$. More importantly, even at relatively low anisotropy (for example that observed in the compound YBa$_2$Cu$_3$O$_{7-\delta}$), the difference between $T_{\text{BKT}}^q$ and $T_{\text{BKT}}$ is too small to destroy the PP at all carrier densities. In addition the difference at high doping levels can be shown to tend to zero logarithmically. This enables one to seriously consider the pseudogap phase explanation claimed in reference 5 even in the quasi-2D case.
2 Model and Formalism

The nature of the interplane tunneling in HTSC is not yet well established [15] and several different models exist. Here we choose the simplest possible Hamiltonian density, often employed for studying HTSC [12, 16],

\[ H = -\psi^\dagger(x) \left[ \frac{\nabla_\perp^2}{2m_\perp} + \frac{1}{m_z d^2} \cos(id\nabla_z) + \mu \right] \psi_\sigma(x) - V\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x), \quad (1) \]

where \( x \equiv \tau, r_\perp, r_z \) (with \( r_\perp \) being a 2D vector); \( \psi_\sigma(x) \) is a fermion field, \( \sigma = \uparrow, \downarrow \) is the spin variable; \( m_\perp \) is the effective carrier mass in the planes (for example CuO\(_2\) planes); \( m_z \) is an effective mass in the \( z \)-direction; \( d \) is the interlayer distance; \( V \) is an effective local attraction constant; \( \mu \) is a chemical potential which fixes the carrier density \( n_f \); and we take \( \hbar = k_B = 1 \).

The Hamiltonian proposed proves to be very convenient for the study of fluctuation stabilization by weak 3D one-particle inter-plane tunneling. We have omitted in (1) the two particle (Josephson) tunneling considering it to be less important than the one-particle coherent tunneling already included. There can be situations where Josephson tunneling is more important. In fact some authors consider the most important mechanism for HTSC to be the incoherent inter-plane hopping (through, for instance, the impurity (localized) states or due to the assistance of phonons). We will not however consider Josephson tunneling here. We do however take into account the layered structure of HTSC which is a vitally important extension to the 2D models usually considered.

It is significant that the large anisotropy in the conductivity cannot be identified with the corresponding anisotropy in the effective masses \( m_z \) and \( m_\perp \). In particular, HTSC with rather large anisotropy in the \( z \)-direction do not display the usual metal behaviour at low temperatures [17]. However this semiconducting behaviour is not directly related to the pseudogap phenomena [17] and the Hamiltonian (1) may be used to study the qualitative features of pseudogap opening.

The Hubbard-Stratonovich method was applied to study the system described by (1). In this method the statistical sum \( Z(\nu, \mu, T) \) is given as a functional integral over the Fermi-fields (Nambu spinors) and the auxiliary field \( \Phi(x) = V\psi^\dagger_\uparrow\psi^\dagger_\downarrow \). In contrast to the usual method
where one calculates $Z$ in terms of the $\Phi(x)$ and $\Phi^*(x)$ variables, the parameterisation $\Phi(x) = \rho(x) \exp [-i\theta(x)]$ should be used [3] (see also [13, 19]). In addition to this reparameterisation one must make the replacement $\psi_\sigma(x) = \chi_\sigma(x) \exp [i\theta(x)/2]$. This representation splits the charged fermion field $\psi_\sigma(x)$ into a neutral fermion field $\chi_\sigma(x)$ and a charged boson field part $\exp [i\theta(x)/2]$. This resembles the spinons and holons in Anderson’s approach.

This particular choice of parameterisation ensures that $\Phi(x)$ is single-valued with period $2\pi$. As a result one obtains

$$Z(v, \mu, T) = \int \rho \mathcal{D}\rho \mathcal{D}\theta \exp [-\beta \Omega(v, \mu, T, \rho(x), \partial\theta(x))],$$

(2)

where

$$\Omega = \frac{T}{V} \int_0^\beta d\tau \int d\rho^2 - T \text{Tr} \ln G^{-1}$$

(3)

is the one-loop effective action which now depends on the modulus-phase variables. The action (3) is expressed in terms of the Green function $G$ of the initial (charged) fermions which now has the following operator form

$$G^{-1}[\rho(x)] = -\hat{I}\partial_\tau + \tau_3 \left[ \frac{\nabla^2}{2m_\perp} + \frac{1}{m_z d^2} \cos(id\nabla_z) + \mu \right] + \tau_1 \rho(x);$$

(4)

$$\Sigma[\partial\theta(x)] = \tau_3 \left[ \frac{i\partial_z\theta}{2} + \frac{(\nabla^2 \theta)^2}{8m_\perp} + \frac{(\nabla_z \theta)^2}{8m_z} \cos(id\nabla_z) \right] -$$

$$\hat{I} \left[ \frac{i\nabla^2 \theta}{4m_\perp} + \frac{i\nabla^2 z \theta \cos(id\nabla_z)}{4m_z} + \frac{i\nabla_\perp \theta \cdot \nabla_z}{2m_\perp} + \frac{i\nabla_z \theta \sin(id\nabla_z)}{2m_z d} \right].$$

(5)

Here $G$ is the Green function for the neutral fermions.

Note that in $\Sigma$ we have omitted higher order terms in $\nabla_z \theta$ but in order to keep all relevant terms in the expansion of $\sin(id\nabla_z)$ the necessary resummation was done. Since the low-energy dynamics in the phases in which $\rho \neq 0$ is determined by the long-wavelength fluctuations of $\theta(x)$, only the lowest order derivatives of the phase need be retained in what follows. This gives the one-loop effective action as

$$\Omega \simeq \Omega_{\text{kin}}(v, \mu, T, \rho, \partial\theta) + \Omega_{\text{pot}}^{\text{MF}}(v, \mu, T, \rho)$$

(6)

where

$$\Omega_{\text{kin}}(v, \mu, T, \rho, \partial\theta) = T \text{Tr} \sum_{n=1}^\infty \frac{1}{n} (G\Sigma)^n \bigg|_{\rho=\text{const}}$$

(7)
and

$$
\Omega_{\text{pot}}^{\text{MF}}(v, \mu, T, \rho) = \left( \frac{1}{V} \int d\mathbf{r} \rho^2 - T \text{Tr} \ln G^{-1} \right) \bigg|_{\rho=\text{const}} .
$$

(8)

Given the representation (8) one can obtain the full set of equations for $T_{\text{BKT}}^3$, $\rho(T_{\text{BKT}}^3)$ and $\mu(T_{\text{BKT}}^3)$ at given $\epsilon_F$. While the equation for $T_{\text{BKT}}^3$ only depends on the kinetic part (7) of the effective action, the equations for $\rho(T_{\text{BKT}}^3)$ and $\mu(T_{\text{BKT}}^3)$ can to a good approximation be obtained using the mean field potential (8). In the phase where $\rho \neq 0$ the mean-field approximation for $\rho$ describes the system well due to the nonperturbative character of the Hubbard-Stratonovich method.

We note that the expression for the potential (8) in terms of $\rho^2$ is identical to the mean-field potential in the BCS approximation but with $|\Phi|^2$ replaced by $\rho^2$ [6]. Thus $T_\rho$, the temperature at which $\rho = 0$, is in this approximation identical to the BCS mean field temperature $T_c^{\text{MF}}$. However, although $T_\rho = T_c^{\text{MF}}$ in the mean-field approximation for $\rho(x)$, the two temperatures have a very different basis, both mathematically and physically. This becomes evident when one includes the fluctuations. Not only does $T_\rho$ remain finite in two dimensions due to the structure of the perturbation theory in the new modulus-phase variables, but it is also bounded below by $T_{\text{BKT}}$. On the other hand $T_c^{\text{MF}}$ approximates the temperature $T_c$ where $\Phi$ becomes non-zero (onset of long-range order) which is zero in two dimensions.

The modulus-phase representation introduced here is a good tool to consider different types of short range order. The success of the BCS approximation is related to the fact that in 3D system with large carrier density short and long range order set in simultaneously because the fluctuations do not change the situation drastically.

3 The Berezinskii-Kosterlitz-Thouless transition in quasi-2D theory

If the model under consideration reduced to some known model describing the BKT phase transition, we could easily write the equation for $T_{\text{BKT}}$. Indeed, in the lowest orders the
kinetic term (7) coincides with classical spin quasi-2D XY-model [21] (see also [10]) which has the following continuum Hamiltonian

\[ H = \frac{1}{2d} \int dr \{ J_\perp [\nabla \perp \theta(r)]^2 + J_z [\nabla_z \theta(r)]^2 \}. \]  

(9)

Here \( J \) and \( J_z \) are constant coefficients (\( J_z \ll J \)). Unfortunately the temperature for the BKT transition in the quasi-2D case is not as well investigated as in the pure 2D case. In fact only in the highly anisotropic case, \( \alpha \equiv J_z/J \ll 1 \), when the vortex ring excitations are irrelevant has the transition temperature been derived [20]. In this limit the temperature \( T_{\text{BKT}}^q \) for the BKT transition in the quasi-2D system is close to that in the pure 2D case and determined by the equation

\[ T_{\text{BKT}}^q = \frac{\pi}{2} J \left[ 1 + \frac{8\pi}{\ln^2 \alpha} \right]. \]  

(10)

This equation was given in [20] and employed to calculate \( T_{\text{BKT}}^q \) for the relativistic quasi-2D four-Fermi theory [10]. The equation was derived using the renormalization group technique, which takes into account the non-single-valuedness of the phase \( \theta \). Thus, the fluctuations of the phase are taken into account at a higher approximation than Gaussian. Below the temperature \( T_{\text{BKT}}^q \) the correlation function

\[ \langle e^{i\theta(r)} e^{-i\theta(0)} \rangle \rightarrow \alpha^{T/4\pi J} \quad r \rightarrow \infty, \]  

(11)

while above \( T_{\text{BKT}}^q \) this correlator decreases exponentially. This is the BKT transition in the classical quasi-2D XY model. The small correction to the unit in the brackets of Eq. (10) corresponds to the influence of the third direction. We note that the equation is only correct in the limit \( \alpha \ll 1 \). From a physical point of view it is evident that the BKT phase cannot form for \( \alpha \sim 1 \), which corresponds to the 3D limit. Moreover, if the temperature \( T_c \) of the LRO formation approaches \( T_{\text{BKT}}^q \) from below, the BKT phase will not form and one will have a superconducting transition directly into a phase with LRO. This may well correspond to the experimental situation and we hope to study this question in detail in our future work.

To expand \( \Omega_{\text{kin}} \) up to \( \sim (\nabla \theta)^2 \), it is sufficient to consider only the terms with \( n = 1, 2 \) in the expansion (10). The method is the same as that in [3, 21], and gives

\[ \Omega_{\text{kin}} = T \int_0^\beta d\tau \int d\mathbf{r} \left[ J(\mu, T, \rho(\mu, T))(\nabla_\perp \theta)^2 + J_z(\mu, T, \rho(\mu, T))(\nabla_z \theta)^2 + \ldots \right]. \]
\[
K(\mu, T, \rho(\mu, T))(\partial_r \theta)^2 + n_F(\mu, T, \rho(\mu, T))i\partial_r \theta, \tag{12}
\]

where

\[
J(\mu, T, \rho) = \frac{d}{4m_\perp} n_F(\mu, T, \rho) - \frac{T}{8\pi^2} \int_0^{2\pi} dt \int_{-\infty}^\infty \frac{w \cos t}{2T} \frac{dx}{\cosh^2 \sqrt{x^2 + \frac{\rho^2}{4T^2}}} \left[ \frac{x + \mu/2T + w \cos t/(2T)}{2T} \right], \tag{13}
\]

\[
J_z(\mu, T, \rho) = \frac{m_\perp}{4m_z (2\pi)^2} \left[ \int_0^{2\pi} dt \cos t \left\{ \frac{w \cos t + \sqrt{(w \cos t + \mu)^2 + \rho^2}}{T} \right\} - 2T \ln \left[ 1 + \exp \left( \frac{\sqrt{(w \cos t + \mu)^2 + \rho^2}}{T} \right) \right] \right] - w \int_0^{2\pi} dt \sin^2 t \int_{-\infty}^\infty \frac{1}{\cosh^2 \sqrt{x^2 + \frac{\rho^2}{4T^2}}} d\theta \tag{14}
\]

\[
K(\mu, T, \rho) = \frac{m_\perp}{(4\pi)^2} \int_0^{2\pi} dt \left( 1 + \frac{w \cos t + \mu}{\sqrt{(w \cos t + \mu)^2 + \rho^2}} \tanh \frac{\sqrt{(w \cos t + \mu)^2 + \rho^2}}{2T} \right), \tag{15}
\]

and where we have introduced the bandwidth in the z-direction \( w = (m_z d^2)^{-1} \). Here

\[
n_F(\mu, T, \rho) = \frac{m_\perp}{(2\pi)^2 d} \int_0^{2\pi} dt \left\{ \mu + \sqrt{(w \cos t + \mu)^2 + \rho^2} \right\} + 2T \ln \left[ 1 + \exp \left( \frac{\sqrt{(w \cos t + \mu)^2 + \rho^2}}{T} \right) \right] \tag{16}
\]

takes the form of a fermi-quasiparticle density. Note that \( J(\mu, T, \rho = 0) = J_z(\mu, T, \rho = 0) = 0 \). This property of the phase stiffness is present in the 2D model where it implies that \( \rho \neq 0 \) at \( T_{BKT} \) and thus \( T_\rho \geq T_{BKT} \). The continued presence of this property in the quasi-2D case implies that the essentially nontrivial cosine dispersion law for motion in the third direction is correctly treated.

Now we discuss the features of the BKT transition in our model. In contrast to the Hamiltonian (9) the field \( \theta \) is also depend on the imaginary time \( \tau \), and therefore by Fourier decomposition, one can write

\[
\theta(\tau, \mathbf{r}) = \sum_{n=-\infty}^{\infty} \exp(i2\pi n T \tau) \theta_n(\mathbf{r}) \tag{17}
\]
From Eq. (12) we can see that the nonzero mode $\theta_n(r)$ $n \neq 0$ has a mass $m_n^2 \sim (2\pi n T)^2 K$, and only the massless component $\theta_0(r)$ is relevant in the low-energy region. In terms of the $\theta_n$ fields, the effective classical action is expressed by

$$
\Omega_{kin} = \frac{1}{2d} \int dr \left[ J(\nabla_\perp \theta_0)^2 + J_z(\nabla_z \theta_0)^2 + \sum_{n \neq 0} \left\{ J(\nabla_\perp \theta_{-n})(\nabla_\perp \theta_n) + J_z(\nabla_z \theta_{-n})(\nabla_z \theta_n) + m_n^2 \theta_{-n} \theta_n \right\} \right].
$$

(18)

Recalling that $\theta$ is an angular variable, we see that the $\theta_0$-part of the effective classical action (18) is nothing but the Hamiltonian of the quasi-2D XY model (9). This makes it possible to write the equation for $T_{BKT}^q$:

$$
T_{BKT}^q = \frac{\pi}{2} J(\mu, T_{BKT}^q, \rho) \left[ 1 + \frac{8\pi}{\ln^2 \alpha(\mu, T_{BKT}^q, \rho)} \right],
$$

(19)

where $\alpha(\mu, T, \rho) = J_z(\mu, T, \rho)/J(\mu, T, \rho)$ is a function of $\mu$, $T$ and $\rho(\mu, T)$. Recall that equation (13) is only correct in the limit $\alpha \ll 1$. Thus after the calculation of $T_{BKT}^q$ one must check that the condition $\alpha \ll 1$ is satisfied.

$\theta_0$ has non-trivial dynamics described by the correlation function

$$
\langle e^{i\theta_0(r)} e^{-i\theta_0(0)} \rangle \to \alpha^{T/4\pi J} \quad r \to \infty,
$$

(20)

which is identical to (11) but with $\theta$ replaced by $\theta_0$. However the gauge-invariant correlation function, $\langle \Phi^\ast(\tau = 0, r) \Phi(0) \rangle$, has an additional factor from the massive modes $\theta_n, n \neq 0$ and, regardless of the correlator for $\theta_0$ (20), one has

$$
\langle \Phi^\ast(\tau = 0, r) \Phi(0) \rangle \to 0 \quad r \to \infty
$$

(21)

for any $T > T_c$ (see the details in [10]) which is consistent with the assumption that LRO is absent.

Although mathematically the problem reduces to a known problem, the analogy is incomplete. Indeed, in the XY model the vector (spin) subject to ordering is assumed to be a unit vector with no dependence on $T$. In our model this is not the case, and a self-consistent calculation of $T_{BKT}$ as a function of $n_f$ requires additional equations for $\rho$ and $\mu$, which together with (19) form a complete system.
Using the definition (8), one obtains (see e.g. [5])

$$\Omega_{\text{pot}}(v, \mu, T, \rho) = v \left[ \frac{\rho^2}{V} - \int \frac{d \mathbf{k}}{(2\pi)^3} \left\{ 2T \ln \cosh \frac{\sqrt{\xi^2(\mathbf{k}) + \rho^2}}{2T} - \xi(\mathbf{k}) \right\} \right],$$  \hspace{1cm} (22)

where \(\xi(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu\) with \(\varepsilon(\mathbf{k}) = k_\perp^2/2m_\perp - w \cos k_z d\). Then the missing equations are the condition \(\partial \Omega_{\text{pot}}(\rho)/\partial \rho = 0\) and the equality \(v^{-1} \partial \Omega_{\text{pot}}/\partial \mu = -n_f\), which fixes \(n_f\):

$$\frac{1}{V} = \int \frac{d \mathbf{k}}{(2\pi)^3} \frac{1}{2\sqrt{\xi^2(\mathbf{k}) + \rho^2}} \tanh \frac{\sqrt{\xi^2(\mathbf{k}) + \rho^2}}{2T},$$  \hspace{1cm} (23)

$$n_F(\mu, T, \rho) = n_f.$$  \hspace{1cm} (24)

The equations (23) and (24) obtained above comprise a self-consistent system for determining the modulus \(\rho\) of the order parameter and the chemical potential \(\mu\) in the mean-field approximation for fixed \(T\) and \(n_f\). In the phase where \(\rho \neq 0\) the mean-field approximation for \(\rho\) describes the system well due to the nonperturbative character of the Hubbard-Stratonovich method and the character of the perturbation theory in the modulus-phase variables.

To simplify the problem one can take the limit \(m_z \to \infty\) in the expressions (13), (16) assuming that \(m_z/m_\perp \gg 1\) and \(w = m_z^{-1} d^{-2} \ll T_{\text{BKT}}^q\). This is indeed the case in real HTSC compounds e.g. for \(m_z \approx 10^2 m_e\) and \(d = 10 \AA\) the value of \(\hbar^2/(m_z d^2 k_B) \sim 10\text{K}\) is far less than the critical temperature. This simplification is useful but not essential since the numerical results are practically unchanged by this approximation.

The energy of two-particle bound states in vacuum \(\varepsilon_b = -2W \exp(-4\pi d/m_\perp V)\) (see e.g. [22]) where \(W\) is the bandwidth in the plane, is more convenient than the four-fermion constant \(V\). For example, one can easily take the limits \(W \to \infty\) and \(V \to 0\) in the equation (23), which after this renormalization becomes (in the limit \(m_z \to \infty\))

$$\ln \frac{|\varepsilon_b|}{\sqrt{\mu^2 + \rho^2} - \mu} = 2 \int_{-\mu/T}^{\infty} \frac{du}{u^2 + \left(\frac{\rho}{T}\right)^2} \left[ \frac{1}{\exp \sqrt{u^2 + \left(\frac{\rho}{T}\right)^2} + 1} \right].$$  \hspace{1cm} (25)

Thus, in practice, we will solve numerically the system of equations (19), (23) and (24) to study \(T_{\text{BKT}}^q\) as a function of \(n_f\).

Setting \(\rho = 0\) in the equations (23) and (24), we arrive (in the same approximation) at the equations for the critical temperature \(T_\rho\) above which \(\rho = 0\) and the corresponding value
of $\mu$:
\[
\ln \left| \frac{\varepsilon_b}{T_\rho} \right| \frac{\gamma}{\pi} = - \int_0^{\mu/2T_\rho} du \frac{\tanh u}{u} \quad (\gamma = 1.781),
\]
(26)
\[
T_\rho \ln \left[ 1 + \exp \left( \frac{\mu}{T_\rho} \right) \right] = \epsilon_F,
\]
(27)
where $\epsilon_F = \pi n_f d/m_\perp$ is the Fermi energy [23]. Note once more that these equations coincide with the system which determines the mean-field temperature $T_{c(2D)}^{MF}$ and $\mu(T_{c(2D)}^{MF})$ (see [22, 3]). This is evidently related to the mean-field approximation used here and the limit $m_z \to \infty$.

Certainly in the simplest Landau theory one appears to have a phase transition since $\rho$ takes on a non-zero value only below $T_\rho$. In fact the parameter $\rho$ describes a gap only in the spectrum of the neutral fermion field $\chi_\sigma(x)$. In describing the charged (physical) fermion field $\psi_\sigma(x)$, $\rho$ only appears in conjunction with $\theta$ in every correlation function. At zero temperature in closely related four-Fermi models [8, 24] the pole in the neutral fermion Green’s function associated with the gap in the neutral fermion spectrum is converted by the phase fluctuations into a branch cut in the Green’s function for charged fermions and we strongly suspect that similar behaviour is present at finite temperature.

In the present approximation the neutral fermion Green’s function $\mathcal{G}(k, \omega)$ [4] is identical to the BCS Green’s function but with energy gap $\rho$ rather than $\Delta$. As such the spectral density of the neutral fermion Green’s function, $\mathcal{G}$, is the sum of two delta functions centered on the isolated poles of $\mathcal{G}$, $\omega = \pm E(k)$ where $E(k) = \sqrt{\xi^2(k) + \rho^2}$ and one has zero density of states inside the gap $\rho$ [22]. In the case of a branch cut (as postulated for the charged fermion Green’s function) the spectral density is non-zero for $\omega$ in the entire range $-E(k) \leq \omega \leq E(k)$. Thus the spectral density is smeared and one expects a corresponding smearing of the gap. An illustrative example where a branch cut does lead to pseudogap behaviour is given in [24].

We believe that (see also discussion in [3]) the expected smearing of the neutral fermion gap in the present model may well describe the observed pseudogap behaviour. Furthermore the fluctuations in $\theta$ are expected to convert the sharp phase transition to a smooth crossover.
4 Results and Conclusions

The analytical and numerical investigation of the systems (21), (25), (24) and (26), (27) yield the following results.

One can show that at large densities ($\epsilon_F \gg |\epsilon_b| \gg T$) when $\mu \simeq \epsilon_F$

\[
J(\epsilon_F, T, \rho) = \frac{1}{\pi} \epsilon_F \left[ 1 - \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{1}{\cosh^2 \sqrt{x^2 + \frac{\rho^2}{4T^2}}} \right]
\]

(28)

and

\[
J_z(\epsilon_F, T, \rho) = \frac{1}{2\pi} \frac{m_\perp}{m_z} w \left[ 1 - \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{1}{\cosh^2 \sqrt{x^2 + \frac{\rho^2}{4T^2}}} \right]
\]

(29)

which yields

\[
\alpha(\epsilon_F) = \frac{J_z}{J} = \frac{m_\perp}{m_z} \frac{w}{2\epsilon_F}
\]

(30)

which is independent of both $\rho$ and $T$. Thus even for a modest anisotropy in the initial fermion Hamiltonian one expects to obtain a large anisotropy (or equivalently a low value of $\alpha$) in the effective quasi-2D XY model Hamiltonian. Indeed at all densities we find small values for $\alpha$. Surprisingly $\alpha$ even decreases as the carrier density increases. For this reason one can indeed use the equation (21) to determine $T_{BKT}^q$. Therefore one expects the results obtained for the pure 2D model to persist to the quasi-2D case.

Indeed for modest carrier densities ($\epsilon_F \lesssim 10^2 |\epsilon_b|$ or the underdoped case) the PP (see Fig. 1) in the present model is roughly equal in size to the superconducting region i.e. $(T_\rho - T_{BKT}^q)/T_{BKT}^q \sim 1$. This allows us to believe that in spite of the oversimplified character of the model proposed in [5] this approach may explain some of the observed normal state anomalies of HTSC. For these densities we argue that the temperature $T_c$ for true LRO is probably roughly equal to $T_{BKT}^q$. For very low densities we find a large region between $T_c$ and $T_{BKT}^q$ where the system is superconducting but one has two-dimensional and not three-dimensional order. It is difficult to say whether such behaviour can be observed experimentally because the densities are so low that the Fermi surface is absent [6, 13].
The model considered here is also a simple one. Certainly at sufficiently large densities the BKT and PP region will disappear due to a direct transition to the state with long-range order particularly for low anisotropy. For example, in the case of an indirect interaction in 2D, it has already been shown [13] that the PP region only exists at low carrier density.

The other results obtained in [5] remain valid. In particular one obtains a linear dependence of the critical superconducting temperature \( T_{\text{BKT}}^\rho \) on the carrier density over a wide range of densities as is seen in experiment.

For instance the kink in \( \mu \) at \( T = T_\rho \), (discussed in reference [27]) occurs at the NP-PP boundary or before superconductivity appears. The ratio \( 2\Delta/T_{\text{BKT}}^\rho \) is also always greater than the standard BCS value [28]. The concentration behaviour of this ratio is consistent with experiment, namely it decreases with increasing \( \epsilon_F \).

It is also interesting to note that the qualitative difference between the temperature dependence of the spin and charge correlations in the normal state of the 2D attractive Hubbard model which was found in [29] acquires a natural explanation in the framework of the approach used here. Indeed, while the neutral (with spin, but chargeless) fermions have the gap \( \rho \) in the PP, this gap should be smeared out for the initial charged fermions due to the phase fluctuations.

To summarize, the presence of interlayer tunneling does not destroy the pseudogap phase above the critical superconducting temperature since the effective anisotropy (see (30)) is far larger than the simple estimate of \( m_z/m_\perp \).

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References

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[1] V.M. Loktev, Fiz. Nizk. Temp. 22 (1996) 3 [Engl. Trans.: Low Temp. Phys. 22 (1996) 1].

[2] D. Pines, Tr.J. of Physics 20 (1996) 535.

[3] B.G. Levi, Physics Today 49 (1996) 17.

[4] H. Ding, T. Yokoya, J.C. Campuzano, T. Takahashi, M. Randeria, M.R. Norman, T. Mochiki, A. Kadowaki, J. Giapintzakis, Nature 382 (1996) 51.

[5] V.P. Gusynin, V.M. Loktev, S.G. Sharapov, Pis’ma Zh. Eksp. Teor. Phys. 65 (1997) 170 [Engl. Trans.: JETP Lett. 65 (1997) 182]; Fiz. Nizk. Temp. 23 (1997) 816 [Engl. Trans.: Low Temp. Phys. 23 (1997) 612]; Preprint cond-mat/9709034.

[6] V.M. Loktev, S.G. Sharapov, Preprint cond-mat/9706285, to be published in Cond.Mat.Phys. (Lviv) No.11 (1997) 131.

[7] R. MacKenzie, P.K. Panigrahi, S. Sakhi, Int. J. Mod. Phys. A 9 (1994) 3603.

[8] E. Witten, Nucl. Phys. B 145 (1978) 110.

[9] V. Emery, S.A. Kivelson, Nature 374 (1995) 434; Phys. Rev. Lett. 74 (1995) 3253.

[10] H. Yamamoto, I. Ichinose, Nucl. Phys. B 370 (1992) 695.

[11] P.C.E. Stamp, L. Forro and C. Ayache, Phys. Rev. B 38 (1988) 2847.

[12] E.V. Gorbar, V.M. Loktev, S.G. Sharapov, Physica C 257 (1996) 355.

[13] V.M. Loktev, S.G. Sharapov, V.M. Turkowski, Preprint cond-mat/9703070, Physica C 295 No. 3-4 (1998).

[14] I.E. Dzyaloshinskii and E.I. Kats, Zh. Eksp. Teor. Fiz. 55 (1968) 2373.
[15] J. Shützman, H.S. Somal, A.A. Tsvetkov, D. van der Marel, G.E.J. Koops, N. Kolesnikov, Z.F. Ren, J.H. Wang, E. Brück and A.A. Menovsky, Phys. Rev. B 55 (1997) 11118.

[16] M.R. Cimberle, C. Ferdeghini, E. Giannini, D. Marré, M. Putti, A. Siri, F. Federici and A. Varlamov, Phys. Rev. B 55 (1997) 14745.

[17] T. Watanabe, T. Fujii, A. Matsuda, Phys. Rev. Lett. 79 (1997) 2113.

[18] I.J.R. Aitchison, P. Ao, D.J. Thouless, X.-M. Zhu, Phys. Rev. B 51 (1995) 6531.

[19] M. Capezzali, D. Ariosa, H. Beck, Physica B 230-232 (1997) 962.

[20] S. Hikami, T. Tsuneto, Progr. Theor. Phys. 63 (1980) 387.

[21] A.M.J. Schakel, Mod. Phys. Lett. B 4 (1990) 927.

[22] E.V. Gorbar, V.P. Gusynin, V.M. Loktev, Fiz. Nizk. Temp. 19 (1993) 1171 [Engl. Trans.: Low Temp. Phys. 19 (1993) 832]; Preprint ITP-92-54E (1992).

[23] The Fermi energy for the quasi-2D system \( \epsilon_F = \epsilon_F^{2D} d \), where \( \epsilon_F^{2D} = \pi n_f / m_\perp \) is the Fermi energy for the 2D system with the quadratic dispersion law.

[24] A.J. da Silva, M. Gomez and R. Köberle, Phys. Rev. D 20 (1979) 895.

[25] J.R. Schrieffer, Theory of superconductivity (Benjamin, New-York, 1964).

[26] O. Tchernyshyov, Phys. Rev. B 56 (1997) 3372.

[27] D. van der Marel, Physica C 165 (1990) 35.

[28] The large size of this ratio in the strongly underdoped cuprates was recently interpreted using the BKT scenario: A.A. Abrikosov, Phys. Rev. B 55 (1997) 6149.

[29] N. Trivedi, M. Randeria, Phys. Rev. Lett. 75 (1995) 312.
Figure 1: $T_{\text{BKT}}^q$, $T_{\text{BKT}}$ (dots) and $T_\rho$ versus the noninteracting fermion density. The regions of the normal phase (NP), pseudogap phase (PP) and BKT phase are indicated. Note that in the approximation used the value of $T_\rho$ is the same for the 2D and quasi-2D models. We assumed that $m_z/m_\perp = 100$ and $(m_z d^2 |\varepsilon_b|)^{-1} = 0.1$. 