A PSEUDOGAP MODEL BEYOND BCS FOR THE CUPRATES:
THE EFFECT OF ORDER PARAMETER SYMMETRY,
DEBYE FREQUENCY AND BAND STRUCTURE

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One of the most intriguing aspects of high temperature superconductors (HTSC) is the presence of the pseudogap in the normal and the superconducting phases of the cuprate compounds. Several pseudogap models have been proposed to explain the abnormal properties of the cuprates. One of the recent models (J. J. Rodríguez–Núñez, A. A. Schmidt and H. Beck, J. Phys.: Condens. Matter 17, 323 (2005)) relies on the assumption that the self-energy is given by \( \Sigma_{PG}(i\omega_n) = -E_G^2(k) G_0(k, -i\omega_n) \) where \( G_0(k, i\omega_n) \) is the one–particle free Green function.

Going beyond this mean field model for the pseudogap we now take into account fluctuations of the pseudogap as \( \Sigma_{PG}(i\omega_n) = -E_G^2(k) G_{PG}(k, -i\omega_n) \) where \( G_{PG}(k, i\omega_n) \) is the one–particle full Green function. We study the combined effect of the band structure and the Debye frequency, \( \omega_D \), on the superconducting critical temperature, \( T_c \), as a function of the number of carriers per site, \( n \). Our conclusions are: 1) increasing the value of \( V/t \) increases the value of \( T_c/t \); 2) increasing the value of \( E_G/t \) decreases the value of \( T_c/t \). By the way, one needs some critical value of \( V/t \) to have finite values of \( T_c/t \). This is the reason we have taken high values of \( V/t \) to find superconductivity; 3) decreasing the value of \( \omega_D/t \) decreases the value of \( T_c/t \). This is reasonable since we have less available states around the Fermi; 4) the inclusion of \( \alpha' \), which we call the effect of the band structure, is important because it moves the center of curve of \( T_c/t \times n \). The center of this curve, with respect to half–filing \( (n = 1) \), is displaced to the left if \( \alpha' > 0 \); 5) the chemical potential is defined in the region where \( T_c/t \neq 0 \). However, in this region, it is almost identical for different values of \( V/t \). This is due to the fact that \( \mu \) is a global property; 6) our model always produces \( d \)–wave superconductivity around the Fermi level, independent whether \( E_G(\vec{k})/t \) is \( s \)– or \( d \)–wave symmetry.
I. INTRODUCTION

Originally discovered by Bednorz and Müller [1] in 1986, the high-temperature superconductors (HTSC) are still attracting a lot of interest due to their unusual physical properties, both in the normal and superconducting phases. Namely, the HTSC exhibit a pseudogap in the energy spectrum for temperatures in the interval $0 \leq T \leq T^*$. $T^*$ is defined by Maier et al. [2] as the crossover temperature where the spin susceptibility is a maximum. There is experimental evidence obtained by the group of Tallon and Loram [3] that the pseudogap exists below $T_c$, independently of the superconducting gap. This interpretation is in agreement with the experiment on energy gap evolution in the tunneling spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ performed by Dipasupil et al. [7]. They find that the pseudogap smoothly develops into the superconducting state gap with no tendency to close at $T_c$. However, a very important experimental identification that the pseudogap and the superconducting order parameters are independent of each other is given by Krasnov et al. [4–6] by intrinsic tunneling spectroscopy.

We assume that the normal state pseudogap self-energy is given by [8]

$$ \Sigma_{PG}(k, i\omega_n) = -E_g^2(k) G_{PG}(k, -i\omega_n) $$

where $E_g(k) \equiv E_g \phi(k)$ and $\phi(k) \equiv 1, \cos(k_x) - \cos(k_y)$ for $s, d$–wave order parameter symmetry. $E_g$ is the value of the pseudogap parameter. $G(k, i\omega_n)$ is the full one–particle Green function, $\omega_n = T \pi(2n+1)$ is the odd Matsubara frequency and $T$ is the absolute temperature. According to Ref. [8], $E_g$ can be calculated from superconducting fluctuations beyond a mean field approximation. In this paper, however, we adopt a phenomenological point of view where $E_g$ is a given parameter.

![FIG. 1: $N(\omega) \times \omega$ for $s$–wave symmetry (both for the pseudogap and the superconducting order parameters) with $\alpha' = 0.0$, and several values of $E_G/t$, namely, $E_G/t = 0.00, 0.50, 1.00, 2.00$ and $5.00$. We see that the symmetry around $\omega = 0$ is kept due to the fact that $\alpha' = 0$ and $\mu = 0$.](image)

This paper is organized as follows. Section I is devoted to an introduction and justification of the pseudogap energy scale. In Section II we justify our proposed self–energy (Eq. (1)) following the work of Kosuge et al. [8].
By the proposed self-energy Green function we derive the full one particle Green function, \( G(i\omega_n, \vec{k}) \). In Section III we present our numerical results and finally we conclude in Section IV.

II. THE PSEUDOGAP MODEL BEYOND MEAN FIELD

According to the perturbation theory of 2D superconducting fluctuations developed by Kosuge and co-workers [8] to second order in the attractive interaction, \( g \), the one–particle Green function to this order is given (we follow his notation):

\[
G^{(1)}(\vec{p}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon(\vec{p}) - \sum^{(1)}(\vec{p}, i\omega_n)}
\]

\[
\sum^{(1)}(\vec{p}, i\omega_n) = -\Delta_f^2 \times G^{(1)}(-\vec{p}, -i\omega_n)
\]

\[
\Delta_f^2 \equiv \frac{T}{N} \sum_{\vec{q}} K_1^{(1)}(\vec{q}, 0)
\]

\[
K_1^{(1)}(\vec{q}, i\omega_n) = \frac{g^2 \chi(\vec{q}, i\omega_n)}{1 + g \chi(\vec{q}, i\omega_n)}
\]

\[
\chi(\vec{q}, i\omega_n) \equiv \frac{T}{N} \sum_{\vec{p}, m} G^{(1)}(\vec{p}, i\Omega_m)
\]

\[
\times G^{(1)}(\vec{p}, i\omega_n - \Omega_m).
\]

FIG. 2: Same as Fig. 1 for \( d \)-wave symmetry.

In consequence, in the formalism of Kosuge et al. [8], one can, in principle, to calculate \( \Delta_f \) self-consistently. We recall the reader attention that for us \( E_g \equiv \Delta_f \). However, in order to simply matters we take \( E_g \) as a phenomenological parameter. In this case, we take Eq. (1) as our starting point.

By including the pseudogap self-energy (Eq. (1)) into the pseudogap Green function

\[
G_{PG}(k, i\omega_n) = [i\omega_n + \mu - \epsilon(k) - \Sigma_{PG}(k, i\omega_n)]^{-1}
\]

(2)
one obtains

\[ G_{PG}(k, \omega) = \left[ \frac{\omega + \epsilon(k) - \mu}{2E_g^2(k)} \right] \times \left[ 1 - \sqrt{1 - \frac{4E_g^2(k)}{\omega^2 - [\epsilon(k) - \mu]^2}} \right]^{-1}. \]  

(3)

We point out that the solution of the one particle renormalized Green function, \( G_{PG}(k, \omega) \), in the presence of the pseudogap, is obtained by solving a quadratic equation for \( G_{PG}(k, \omega) \). We have chosen one of the solutions in order to satisfy that the right limit is obtained for \( E_g \to \infty \), namely, \( \lim_{E_g \to \infty} G_{PG}(k, \omega) = G_0(k, \omega) \), the free one particle Green function.

According to experimental data in the HTSC, the pseudogap phase enters into the superconducting phase and becomes zero at a critical doping of \( x_c = 0.15 \) (with \( x = 1.0 - n \)), where \( n \) is the number of carriers per site. This leads to consider the effect of the PG energy scale on the superconducting properties, namely, \( T_c \) and the superconducting order parameter, \( \Delta(T) \).

**FIG. 3:** The superconducting critical temperature, \( T_c \times n \) (upper panel) and \( \mu \times n \) (lower panel) for a \( d \)-wave symmetry (for both order parameters) with \( \alpha' = 0 \), \( \omega_D/t = 0.50 \) and \( E_G/t = 0.50 \) and for several values of the pairing potential, namely, \( V/t = 4.50, 5.00, 5.50 \) and \( 6.00 \). From this figure it appears that for a fixed value of \( V/t \) we should have two regions of \( n \), to each side of half–filling, where we find superconductivity.

In the superconducting phase, in the presence of the pseudogap order parameter, we need to solve the Gorkov’s
\[
G_{PG}^{-1}(k, i\omega_n) G(k, i\omega_n) + \Delta(\vec{k}) F(k, i\omega_n) = 1 \tag{4}
\]
\[
G_{PG}^{-1}(k, -i\omega_n) F(k, i\omega_n) + \Delta(\vec{k}) G(k, i\omega_n) = 0 \tag{5}
\]

FIG. 4: The superconducting critical temperature, \( T_c \times \mu \) (upper panel) and \( n \times \mu \) (lower panel) for a \( d \)-wave symmetry (for both order parameters) with \( \alpha' = 0 \), \( \omega_D/t = 0.50 \), \( E_G/t = 0.40 \) and \( V/t = 6.25 \), \( 6.30 \), \( 6.35 \), \( 6.40 \), \( 6.45 \) and \( 6.50 \).

where \( G_{PG}^{-1}(k, i\omega_n) \equiv 1/G_{PG}(k, i\omega_n) \) and \( G_{PG}(k, i\omega_n) \) is the pseudogap one particle Green function, Eq. (3). \( G(k, i\omega_n) \) and \( F(k, i\omega_n) \) are the diagonal and off–diagonal one particle Green function in the superconducting phase, namely, for \( 0 \leq T \leq T_c \), in the Nambu formalism.

Now, taking into account the scenario where the pseudogap survives in the superconducting state, we obtain the superconducting critical temperature, \( T_c \), and the chemical potential, \( \mu \), from the two mean–field self–consistent equations

\[
\pi^2 = VT_c \int d^2k \phi^2(k) \psi(k) \times \sum_n G_{PG}(k, i\omega_n) G_{PG}(k, -i\omega_n) \tag{6}
\]
\[
n\pi^2 = T_c \int d^2k \sum_n G_{PG}(k, i\omega_n) \tag{7}
\]

where \( n \) is the number of carriers per site, \( \phi(k) = \cos(k_x) - \cos(k_y) \) and \( \psi(k) = 1 \) if \( |\epsilon(k) - \mu| \leq \omega_D \) (0 otherwise) where \( \omega_D \) is the Debye frequency. We adopt the following two–dimensional tight binding structure \( \epsilon(k) = -2t [\cos(k_x) + \cos(k_y)] + 4t \alpha' \cos(k_x) \cos(k_y) \) where \( t \) is the next nearest hopping and \( t' = \alpha' \times t \) is the second nearest hopping matrix element.
We have performed the Matsubara summation numerically, due to the fact that the pseudogap Green function, $G_{PG}(k, i\omega_n)$, does not have a simple pole structure dependence on $\omega_n$. However, we have expressed our $\vec{k}$-summation in a two dimensional integration in the usual way. In Section III, we present our results by solving the two coupled equations given previously, i.e., Eqs. (6–7).

III. NUMERICAL RESULTS

Due to the fact that our normal Green function has been approximated with a self-energy (Eq. (1)), which is beyond mean field theory, we expect that the normal density of states (NDOS) even in the presence of the pseudogap ($E_g \neq 0$) is going to produce a zero density of states only at $\omega = 0$. This result is independent whether we choose a $s$– or $d$–wave symmetry for the pseudogap order parameter. More specifically, the form of the density of states for both symmetries is $d$–type around the Fermi level.

![Graph showing $N(\omega) \times \omega$ for $s$–wave symmetry (both for the pseudogap and the superconducting order parameters) with $E_G/t = 2.0$, and several values of $(\alpha', \mu)$.](image)

FIG. 5: $N(\omega) \times \omega$ for $s$–wave symmetry (both for the pseudogap and the superconducting order parameters) with $E_G/t = 2.0$, and several pair values of $(\alpha', \mu)$.

Before presenting our numerical results, we define some quantities which are useful in photoemission experiments. They are the spectral function, $A(\vec{k}, \omega)$, and the density of states, $N(\omega)$. They are given by

$$A(\vec{k}, \omega) = \frac{1}{\pi} \lim_{\delta \to 0^+} \text{Im}[G(k, \omega + i\delta)]$$

$$N(\omega) = \frac{1}{\pi^2} \int_0^\pi d^2k A(\vec{k}, \omega). \quad (8)$$

In Fig. 1 we present the density of states, $N(\omega) \times \omega$, for $s$–wave symmetry, for both the pseudogap and the superconducting order parameters. In Fig. 2 we have chosen $\alpha' = 0$, and several values of the pseudogap parameter ratio, namely, $E_g/t = 0.00, 0.50, 1.00, 2.00$ and $5.00$. As we can see, as $\alpha' = 0$, the symmetry around half-filling, $n = 1.00$ or $\omega = 0.00$ is kept.
In Fig. 2 we present the density of states, $N(\omega) \times \omega$, for $d$–wave symmetry, for both the pseudogap and the superconducting order parameters. In Fig. 2 we have chosen $\alpha' = 0$, and several values of the pseudogap parameter ratio, namely, $E_g/t = 0.00, 0.50, 1.00, 2.00$ and 5.00. As we can see, as $\alpha' = 0$, the symmetry around half–filling, $n = 1.00$ or $\omega = 0.00$ is kept.

Comparing the two density of states of Figs. (1–2) we observe that, except by details in the high energy sector, for frequencies $\omega \approx 0.0$, we have $d$–type pseudogap behavior in that frequency range. For example, the density of states for $d$–wave symmetry is more extended somehow that the density of state for $s$–wave symmetry. Approximating the full density of states for a linear behavior around $\omega \approx 0$ is useful to perform analytical calculations, as done by Tifrea, Grosu and Crisan [11]. We recall that the pseudogap behavior has also been obtained by numerical simulations in the attractive Hubbard model [12–16].

To see the breaking of symmetry of $N(\omega) \times \omega$, around $\omega = 0$, we present the $s$–wave symmetry density of states for a set of parameters as given in Fig. 5. We have fixed the value of $E_G/t$ to 2.0, while we change the values of $(\alpha', \mu)$, as indicated in the figure.

In Fig. 3 we show the superconducting critical temperature, $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for a $d$–wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of the pairing potential, namely, $V/t = 4.50, 5.00, 5.50$ and 6.00. From this figure it is clear that for a fixed value of $V/t$ we should have two regions of $n$, to each side of half–filling, where we find superconductivity. That is the reason that we have decided to look more carefully in the parameter phase space (See Fig. 6).

In Fig. 4 we present the results of our search for the question posed after the results obtained in Fig. 3. Here, we plot $T_c \times \mu$ (upper panel) and $n \times \mu$ (lower panel) for a $d$–wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.40$ for several values of the pairing potential, namely, $V/t = 6.25, 6.30, 6.35, 6.40, 6.45$ and 6.50.

In Fig. 6 we show the superconducting critical temperature, $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for a $d$–wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of the pairing potential, namely, $V/t = 6.25, 6.30, 6.35, 6.40, 6.45$ and 6.50. After carefully searching the possible existence of two superconducting regions to both sides of half–filling we came to the conclusion that this is not the case. More precisely, we have found that for need reasonable large values of $V/t$ to have superconductivity in a certain region of carrier number and after some value of $V/t$ we have two regions with high values of $T_c/t$ (two bumps, let us say) and an intermediate region with small values of the superconducting critical temperature. As we can see, when all this structure appears, superconductivity exists in the whole region of carrier number.

Now we study the effect of second nearest hopping, i.e., $\alpha' \neq 0$. In Fig. 7 we show $T_c \times n$ for a $d$–wave symmetry, with $\alpha' = +0.20$, $\omega_D/t = 0.5$ and several values of the pairing potential, namely, $V/t = 3.00, 3.30, 4.00$, and 4.50. We see that the effect of a positive $\alpha'$ is to displace the curve of $T_c$ to the left, with respect to the one at half–filling.
FIG. 6: $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for $d$–wave symmetry (both for the pseudogap and the superconducting order parameters) with $\alpha' = 0.0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of $V/t$, namely, $V/t = 6.00, 6.50, 7.00$ and 7.50. The symmetry around half–filling ($n = 1$) is kept due to the fact that $\alpha' \equiv 0$.

IV. CONCLUSIONS AND OUTLOOK

Our conclusions have to be drawn from Figs. (1–7). The first thing to realize is that by adopting the approximation taken in this work, our normal state Green function produces always $d$–wave superconductivity (See Figs. (1–2)). Then it is sound to say that our pseudogap model is a $d$–wave model for the density of states around the Fermi level.

In Fig. (3) we present $T_c \times n$ and $\mu \times n$ for a $d$–wave symmetry, with $\alpha' = 0.0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of $V/t = 4.50, 5.00, 5.50$ and 6.00. ($t$ has been taken the energy unit). From this figure we observe that the symmetry around $n = 1$ is kept, since $\alpha' = 0$. We also observe that for some small values of $V/t$, there is not superconductivity, namely, $T_c/t = 0$, in a range of carrier concentration. From the lower panel of Figs. (3–7), we see that $\mu$ does not change appreciably with the considered values of $V/t$. In these figures (3–7), we see that the parameter controlling the symmetry around half–filling is $\alpha'$. Thus, $\alpha' = +0.20$ displaces the center of the $T_c \times n$ to the left of $n = 1.0$.

We have solved numerically our two coupled self–consistent equations (6–7) for $T_c$ and $\mu$ vs $n$ for several values of 1) the pseudogap parameter, $E_G/t$; 2) the second nearest hopping ratio, $\alpha'$; 3) the Debye frequency, $\omega_D/t$; and 4) the pairing interaction, $V/t$. The results we find are the following:

1. increasing the value of $V/t$ increases the value of $T_c/t$;
FIG. 7: Same as Fig. 6 for $d$–wave symmetry for $\alpha' = +0.20$ and $V/t = 3.00, 3.50, 4.00$ and 4.50. The symmetry around half–filling ($n = 1$) is broken due to the presence of the second nearest hopping term, namely, $\alpha' \neq 0$.

2. increasing the value of $E_G/t$ decreases the value of $T_c/t$. By the way, one needs some critical value of $V/t$ to have finite values of $T_c/t$. This is the reason we have taken high values of $V/t$ to find superconductivity. See Figs. (3–6);

3. decreasing the value of $\omega_D/t$ decreases the value of $T_c/t$. This is reasonable since we have less available states around the Fermi sea which contribute to the integral in Eq. 6;

4. the inclusion of $\alpha'$, which we call the effect of the band structure, is important because it moves the center of the curve $T_c/t \times n$. The center of this curve, with respect to half–filling ($n = 1$), is displaced to the left if $\alpha' > 0.0$;

5. the chemical potential is defined in the region where $T_c/t \neq 0$. However, in this region, it is almost identical for different values of $V/t$. This is due to the fact that $\mu$ is a global properties;

6. our model always produces $d$–wave superconductivity around the Fermi level.

Now, with respect to the outlook, we would like to do the following:

1. to calculate the isotope exponent, $\alpha$ as a function of $n$. $\alpha$ is given from the following expression $T_c \approx M^{-\alpha}$, where $M$ is the isotope mass of the ions. Naturally, all the kinks which appear in the curve of $T_c \times n$ are going to produce rapid changes in the isotope exponent [9];

2. $\Delta(T) \times T$, for fixed values of $n, V/t, E_G/t$ and $\alpha'$;
FIG. 8: The $s$–wave symmetry spectral density $A(\vec{k}, \omega) \times \omega$ for several values of $k_x$ and $k_y$: $\alpha' = 0$, $\mu = 0.0$, $E_G/t = 1.00$ and $\delta = 10^{-5}$.

3. to calculate the BCS–BEC crossover line as it was done in Ref. [9]. In particular, we would like to find the so–called metallicstatephase, which is characterized by $\Delta_0 = 0$ [9].

In order to go from the discrete version for $\omega_n$, the Matsubara frequency representation, we need to perform the spectral theorem for the Green function as follows

$$G(k, i\omega_n) = \sum_{-\infty}^{+\infty} \frac{A(k, z)dz}{z - i\omega_n}.$$ (9)

By performing the Matsubara frequency summation, Eq. (6) becomes

$$\pi^2 = V \int d^2k \phi^2(k) \psi(k) \int_{-\infty}^{+\infty} d\omega \sum_{-\infty}^{+\infty} d\omega'$$

$$\times \frac{A_{PG}(k, \omega) A_{PG}(k, \omega')(f(\omega) - f(\omega'))}{\omega - \omega'}$$

$$\times \frac{1}{\pi^2} = \int d^2k \int_{-\infty}^{+\infty} d\omega A_{PG}(k, \omega).$$ (10) (11)

While the spectral function, $A(\vec{k}, \omega)$, has very delicate structure, we prefer this form (Eq. 11) to the one given by Eq. (7), due to the fact that they are expressed by integrals and numerical quadrature routines to solve these equations quickly and with the desired accuracy. Also, we prefer integration over direct summation because
results will not depend on the number of Matsubara frequencies. In Figs. (8-9), we show the spectral function along $k_x$ and $k_y$ axes, for several parameters of the theory. As we can see the spectral function has properties of quasi–particle behavior (peak behavior) and non–coherent behavior (round behavior). These features are valid for both $s$– and $d$–wave symmetry.

In short, we have checked that the band structure parameters $\alpha'$ and $\omega_D$ influence the value of $T_c$. In particular, $\alpha' \neq 0$ breaks the symmetry around half filling and $\omega_D$ decreases the value of $T_c$. In our model of a pseudogap, beyond mean field theory, $E_g \neq 0$ also decreases the value of $T_c$. Also, for $E_g \neq 0$ we have $T_c(n) \neq 0$ in an interval of $n$. These global results are in qualitative agreement with the ones in Ref. [10]. However, the dynamical properties like the spectral function, the density of states (among others) are very different from the ones in Ref. [10], namely,

$$\Sigma_{PC}(k, i\omega_n) = -E_g^2(k) G_0(k, -i\omega_n),$$

(12)

with $G_0(k, i\omega_n)$ been the free one particle Green function. We should mention that the approximation given by Eq. (12) gives a semiconductor-type of gap for $E_G(\vec{k})/t = E_G/t = constant$. Only, for $E_G(\vec{k})/t = E_G/t(\cos(k_x) - \cos(k_y))$ the pseudogap produces a $d$–symmetry in the density of states. This was used in Ref. [11].
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