EFFECT OF A PSEUDOGAP ON $T_c$ AND ON THE SUPERCONDUCTING ORDER PARAMETER

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Abstract

We further develop the pseudogap model proposed by J.L. Tallon and J.W. Loram, Physica C 349, 53–68 (2001). For the pseudogap order parameter we choose a particular form which reproduces the main features of the high temperature superconductor (HTSC) phase diagram which depends on carrier number, \( n \). For fitting the key features of the cuprate oxides we have sensible parameters at our disposal, namely, \( a \), which fixes the density where the pseudogap order parameter is maximum, \( \alpha' \) which allows us to display the \( T_c \) vs \( n \) curve and \( E_{go} \) which gives us the value of the pseudogap. We have reproduced in a qualitative fashion the main details of the experimental data given in the work of Suryadijaya, T. Sasaqawa, and H. Takagi, Physica C 426–431, 402–406 (2005). Our main results are the following:

1. To have decreased the value of \( T_c \) with respect to the “free” case, namely, \( E_{go} = 0 \), namely, when the pseudogap order parameter is not present.

2. To have obtained the maximum of \( T_c \) by choosing \( \alpha' \neq 0 \).

3. To have chosen the minimum value of \( T_c \) inside the pseudogap region, namely, in the region where the pseudogap parameter is a maximum.

4. To have bounded the region of the superconducting dome by choosing the value of \( E_{go} \).

In short, we have proposed a phenomenological form for the pseudogap energy, which depends on carrier number and which reproduces in a qualitative way the results of Suryadijaya, T. Sasaqawa and H. Takagi, Physica C 426–431, 402–406 (2005). Consequently, we conclude that the pseudogap is necessary for HTSC.
I. INTRODUCTION

Since their discovery [1], the copper–oxide high–$T_c$ superconductors have become one of the most investigated materials in solid state physics [2–25]. Sixteen years has passed since their discovery and we still do not know its physical origin. This is most likely due to the fact that we do not understand the state of matter from which the superconductor state comes[26]. In optimally and low doped materials, the superconducting state exhibits a pseudogap with temperatures, $T^*$, which are larger than $T_c$, namely, $T^* \geq T_c$. Consequently, one of the most puzzling ingredients in the area of high temperature superconductivity (HTSC), besides its mechanism, is the identification of the energy scales associated with abnormal properties of these compounds for $T \geq T_c$. $T_c$ represents the onset of a coherent condensate of superconducting quasi–particles. $T^*$ is an energy scale where the HTSC materials show anomalous behavior. As pointed out by S. Häfner, Hossain, Damascelli, and Sawatzky[3], in the superconducting cuprates there are two fundamental energy scales coexisting over the whole superconducting dome. These two energy scales are the pseudogap order parameter and the superconducting order scale.

In this work we propose a phenomenological pseudogap density of states which agrees with Fig. 1(b) of the above paper[3], namely, that the superconducting order parameter and the pseudogap order parameter coexist below $T_c$. By assuming this, we solve our self–consistent equations and we find $T_c$ vs $n$, where $n$ is the number of carrier/site in the system. By postulating that the superconducting order parameter, $E_{PG}(\vec{k})$, depends on $n$ in a particular way, we derive the $T_c$ vs $n$ which are similar to the experimental curves, by a proper choice of the parameters of our model.

The paper is organized as follows. In Section II we present the self–consistent equations at $T = T_c$ and $T = 0 \ K$. In Section III we show the numerical results of solving the self–consistent equations presented in Section II. In Section IV we present our conclusions and state some directions of future work.

II. THE BCS SELF–CONSISTENT EQUATIONS AND THE PSEUDOGAP MODEL

We assume that superconductivity is governed by mean–field equations[27] and that “correlations” can be taken into account at the level of the density of states. In this way, we can use “modified” self–consistent BCS equations.

At $T = T_c$ the “modified” self–consistent BCS equations are:

$$\frac{1}{V} = \frac{1}{2} \int N_{PG}(\omega) \tanh \left( \frac{\omega - \mu}{2k_BT_c} \right) \frac{d\omega}{(\omega - \mu)}$$

$$n = 1 - \int \bar{N}(\omega) \tanh \left( \frac{\omega - \mu}{2k_BT_c} \right) d\omega ,$$

(1)
where $\mu$ is the chemical potential, $V$ is the absolute value of the pairing interaction, $N_{PG}(\omega)$ is the density of states in the presence of a phenomenological pseudogap as given in Ref.[28] and $T_c$ is the superconducting critical temperature. $n$ is the number of carriers per site. These two self–consistent equations have to be solved numerically. We refer as “modified” BCS equations due to the presence of the carrier number self–consistent equation.

Similarly at $T = 0$ K the “modified” self–consistent BCS equations are:

$$\frac{1}{V} = \frac{1}{2} \int N_{PG}(\omega) \frac{d\omega}{\sqrt{(\omega - \mu) + \Delta_0^2}}$$

$$n = 1 - \int N(\omega) \frac{\omega - \mu}{\sqrt{((\omega - \mu)^2 + \Delta_0^2)}} d\omega . \quad (2)$$

In Eqs. (1)-(2) the density of states in the presence of a pseudogap, $N_{PG}(\omega)$, and the free density of states, $N(\omega)$, are given, respectively, by:

$$N_{PG}(\omega) = \frac{N_0 |\omega - \mu|}{E_{PG}(n)} \text{ if } |\omega - \mu| < E_{PG}(n)$$

$$= N_0 \text{ if } |\omega - \mu| > E_{PG}(n) \quad (3)$$

$$\overline{N}(\omega) = \frac{1}{2\pi^2 t \sqrt{1 + \alpha' \omega/t}} \times K \left( \frac{1 - (\alpha' - \omega/t)^2}{1 + \alpha' \omega/t} \right) , \quad (4)$$

where $\alpha'$ is the next nearest neighbor hopping matrix element, namely, $t' = \alpha' \times t$; and $K(x)$ is the elliptical integral of the first kind[29]. $t$ is the nearest hopping matrix element. The density of states in the presence of a pseudogap order parameter, namely, Eq. (3) has been proposed by Tallon and Loram[28]. The pseudogap model we adopted for the density of states, $N_{PG}(\omega)$, is similar to the one studied by [30] and co–workers. See also Ref. [31].

The free band structure is given by

$$\varepsilon(\vec{k}) = -2 t \left[ \cos(k_x) + \cos(k_y) \right] + 4 t \alpha' \cos(k_x) \times \cos(k_y) \quad . \quad (5)$$

In what follows we choose the nearest hopping matrix element, $t = 1$. We have taken a pseudogap order parameter density of states in the equation for $T_c$ or $\Delta_0$ assuming that this order parameter also appears at the Fermi level, namely, around $\mu$.

The density of states, $N_{PG}(\omega)$ and $\overline{N}(\omega)$, are shown in Figs. 1 and 2 respectively. We have used an approximation for the $PG$ energy ($E_{PG}(n)$) as follows:

$$E_{PG}(n) = (E_{go} - E_0) \ast exp(-((n - 1/a)/s)^2)) + E_0 \quad (6)$$

where $E_{go}$, $E_0$, $a$ and $s$ (Fig. 3) which give a constant pseudogap energy scale as function of $n$, except in a small carrier number interval. Here we have fixed $a = 1/0.7$, $E_{go} = 0.37$, $E_0 = 0.35$ and $s = 0.05$. We have
adopted these parameters Eq. (6) with the purpose of reproducing the experimental results of Suryadijawa, Sasaqawa and Takagi[32], in particular their Fig. 3b. Eq. (6) is the key element of this paper. The physical interpretation of it is that the pseudogap energy scale might be due to a local electronic interaction which is almost constant as function of \( n \) (or doping), except in a small carrier number.

III. NUMERICAL RESULTS

We present our numerical results as follows:

1. \( a = 0 \) and \( \alpha' = 0 \) (Figs. 4, 5, 6 and 7).
2. \( a \neq 0 \) and \( \alpha' = 0 \) (Figs. 8 and 9).
3. \( a = 0 \) and \( \alpha' \neq 0 \) (Figs. 10 and 11).
4. \( a \neq 0 \) and \( \alpha' \neq 0 \) (Figs. 12 and 13).
5. We present in Fig. 14 our best choice to reproduce in a qualitative way the experimental results of the system LSCO (\( T_{c,\text{max}} = 36K \)) [35]. Please notice that in our model our final free parameter is \( D \) related to the effective band–width of the model. So, by adjusting the value of \( D \) we can fit the generic curves of the cuprates, namely, \( T_c \) vs \( n \).

![FIG. 1: Approximation to the pseudogap density of states, \( N_{PG} \), with different values of \( a \), namely, \( a = 0.88 \) and 0.90 (see Eq. (3) and text for details).](image)

In Fig. 1 we present a density of states with a pseudogap order parameter[28] which looks like a \( d \)-wave superconductor density of states, namely, a “triangular” shape near the chemical potential, \( \mu \). The density of states is normalized, namely, the integral of the density of states is unity for any value of \( a \). The condition that \( \int_{-\infty}^{+\infty} N(\omega) \, d\omega = 1 \) is a requirement which produces a relation between \( N_o \) and \( D \), where \( N_o \) is the strength of the DOS and \( D \) defines where we have to integrate, namely, the interval \([-D, +D]\).

In Fig. 2 we present the free density of states, \( N(\omega) \) vs \( \omega \), for different values of the nearest neighbor parameter, \( \alpha' \). From this figure we observe that the van Hove singularity is moving to the right or to the left depending on the sign of \( \alpha' \).
In Fig. 3 we show the approximation we have adopted for the pseudogap order parameter as given in Eq. (6), which has to be inserted in the density of states, $N_{PG}$, advanced by Tallon and Loram[28]. The physical meaning of this approximation is the following: the high-temperature superconductors (HTSC) are strongly correlated materials and this correlation appears in the so-called pseudogap density of states, $N_{PG}(\omega)$. Our approximation looks like a Coulomb interaction which depends on carrier number in a certain region of the carrier number. However, the reason of choosing this type of approximation for the pseudogap energy scale is to reproduce the general phase diagram of the cuprate high-temperature superconductors. A similar approach to ours, namely, a phenomenologically one, has been taken by Loram and Tallon[28]. In addition, Storey, Tallon, Williams and Loram[33] have used an energy dispersion and a model for the normal state pseudogap, both based on ARPES results, to show that the shrinking Fermi arc picture is inconsistent with Raman data below $T_c$ and thermodynamic data for $T \approx T^*$. Consequently, this creates some excitement in the area of the Fermi arc interpretation of the cuprate superconductors[34].

Specifically, we have adopted this approximation because of the following:

1. To limit the carrier interval where the superconducting critical temperature is different from zero,
namely, $T_c \neq 0$. This is obtained by using the constant part of the pseudogap energy;

2. To gain the dip of $T_c$ vs $n$ in the underdoped regime, around $x \approx 1/8$.

In Figs. (4–5) we present $T_c/t$ vs $n$ and $\Delta_o/t$ vs $n$, respectively, for the pseudogap density of states given by Tallon and Loram[28], with our choice of the pseudogap order parameter, $E_{PG}(n)$, given in Eq. (6). See also Fig. 3. From these two figures we immediately observe that the pseudogap order parameter is detrimental to both $T_c/t$ and $\Delta_o/t$. Or, in other words, these two coexisting order parameters are competing. We see that the chemical potential does not depend on the value of $E_{go}$. This is due to the fact that $\mu$ is a global quantity: it is used to fix the number of carriers.

![Graph](image)

FIG. 4: $T_c$ vs $n$ for different values of $E_{go}/t$ (upper part of the figure). In the lower part of the figure we have $\mu/t$ vs $n$ for the same values of $a$ chosen in the upper part of the figure. In particular, $E_{go}/t = 0.20, 0.30, 0.40$ and 0.50. In this figure the additional parameters are $V/t = 0.95, a = 0$, $\alpha' = 0$ and $t = 1$.

In Fig. 6 we plot $\Delta_o/T_c$ vs $n$ for different values of $E_{go}$ ($E_{go}/t = 0.30, 0.40$ and 0.50). Other parameters are $V/t = 0.95$, $a = 0$ and $\alpha' = 0$. We observe that as a function of $n$ this ratio does not change too much, namely, it stays around the value of 1.5. However, it does not reproduce exactly the BCS value $\approx 1.7$. However, we can safely say that the approach we are using is a mean field one.

In Fig. 7 we plot $T_c$ vs $E_{go}$ for different values of $V/t$, namely, $V/t = 0.95$, and 0.80. In this figure, $a = 0$ and $\alpha' = 0$. $n$ is chosen at half–filling, namely, $n = 1$. We observe that $T_c/t$ decreases with the value of the pseudogap parameter. This is equivalent to say that the presence of the pseudogap order parameter is detrimental to $T_c/t$. Also, we observe the sensibility of $T_c(n = 1)$ to slightly different values of $V/t$. 

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FIG. 5: $\Delta_n$ vs $n$ for different values of $E_{go}/t$ (upper part of the figure). In the lower part of the figure we have $\mu/t$ vs $n$ for the same values of $a$ chosen in the upper part of the figure. In particular, $E_{go}/t = 0.20, 0.30, 0.40$ and 0.50. In this figure the additional parameters are $V/t = 0.95$, $a = 0.0$, $\alpha' = 0$ and $t = 1$.

FIG. 6: $T_c/t$ vs $E_{go}$ for $n = 1$. Refer to the text for more details.

In Fig. 8 we plot $T_c/t$ vs $n$ for different values of $E_{go}$ ($E_{go}/t = 0.31, 0.32$ and 0.33, when $a \neq 0$. Here $\alpha' = 0$. We immediately see that the experimental feature of the high temperature superconductors, namely, the depletion of $T_c/t$ around some value of $n$ is present. This, in our view, is basically due to the chosen form of the $PG$ order parameter, given in Eq. (6). To compare with experimental results, we refer the reader to Ref. [35].
FIG. 7: $T_c$ vs $E_{go}$ for different values of $V/t$. In this figure, $a = 0$ and $\alpha' = 0$. $n$ is chosen at half–filling, namely, $n = 1$. Refer to the text for a discussion of these results.

FIG. 8: $T_c/t$ vs $n$ for different values of $E_{go}$, when $\alpha' \neq 0$. Because $\alpha' = 0$ $T_{c,max}$ is exactly at half–filling, namely, $n = 1$. See the text for additional discussion.

In Fig. 9 we plot $\Delta_o/t$ vs $n$ for different values of $E_{go}$, when $a \neq 0$. Here $\alpha' = 0$. The features found in Fig. 9, namely, the depletion of $\Delta_o/t$ around some value of $n$ are found here.

All previous results were obtained when $\alpha' = 0$. Now we relax this condition and study the effect of this parameter on the superconducting properties of our model. For example, in Fig. 10, we observe that the maximum value of $T_c/t$ is displaced with respect to $n = 1$ and the figure is deformed around its maximum. In other words, as it is always the case, the parameter $\alpha' \neq 0$ breaks down the symmetry.
FIG. 9: $\Delta_n/t$ vs $n$ for different values of $E_{go}$, when $a \neq 0$. Because $\alpha' = 0$ $T_{c,\text{max}}$ is exactly at half–filling, namely, $n = 1$. See the text for additional discussion.

around half–filling.

The same kind of conclusions (obtained for Fig. 10) are valid when we plot $\Delta_n/t$ vs $n$, for different values of $E_{go}/t$, selecting $\alpha' \neq 0$. For this case, we refer the reader to Fig. 11. Due to the fact that $a = 0$ we do not observe the depletion of $T_c$ at maximum carrier number.

In Fig. 12 we present $T_c$ vs $n$ for several values of $E_{go}/t$, namely, $E_{go} = 0.36, 0.37$ and 0.38, and for $V/t = 0.85$, $a = 1/7$ and $\alpha' = -0.41$.

In Fig. 14 ($T_c/t$ vs $n$), we observe that the maximum value of $T_c/t$ is displaced with respect to $n = 1$ and the figure is deformed around its maximum. In other words, as it is always the case, the parameter $\alpha' \neq 0$ breaks down the symmetry around half–filling. As $a = 0.7$ the minima of the curve $T_c/t$ vs $\mu/t$ are located at a particular value of $n$, related to $a$. And precisely this is what we have been looking for, namely, to distort the parabolic shape of $T_c$ vs $n$ for $x \approx 1/8$ or $n \approx 0.875$.

IV. CONCLUSIONS AND OUTLOOK

We have calculated the superconducting critical temperature, $T_c$, and the superconducting order parameter at zero temperature, $\Delta_n$, as a function of the number of carriers, $n$, or equivalently, to the chemical potential, $\mu$. In order to solve the self–consistent equations we have postulated a pseudogap order parameter, which looks like as a Coulomb interaction with carrier number dependence. This choice has been made based on phenomenological grounds, namely, we may associate the pseudogap energy scale with an
FIG. 10: $T_c/t$ vs $n$ for different values of $E_{pg}/t$ ($E_{pg}/t = 0.30$, 0.35 and 0.40), when $\alpha' = -0.4 \neq 0$ and $a = 0.0$. We see that the maximum of this figure is displaced to lower carrier numbers with respect to the one when $\alpha' = 0$.

The electronic energy coming from the Hubbard model in the limit of strong correlations.

Our results show that the presence of the pseudogap opens a “triangular” gap at the chemical potential, allowing us to describe the effective density of states as done in the work of Tifrea et al.[30]. Our contribution is to have approximated the pseudogap order parameter in the way done by Tallon and Loram[28] to solve the two self-consistent equations.

With respect to the questions stated previously by Hufner et al.[3] we arrive to the following conclusions:

- The pseudogap is a necessary ingredient for HTSC. In our interpretation, they are independent, since $E_{PG}$ is probably due to another mechanism. However, if we stick to a mean-field approach for the BCS equations, the pseudogap energy scale puts some constraints on the BCS parameters to reproduce the generic phase diagram of the cuprate superconductors and, because of this, it is a necessary element in the description of these superconducting materials.

- There is an order parameter associated with the pseudogap, which coexists with the superconducting order parameter for $T \leq T_c$. The PG order parameter in our model is given by $E_{PG}(n)$ (see Eq. (6)).

- The correct phase diagram of the cuprate superconductors is given by the superconducting dome with the pseudogap line coexisting inside this superconducting dome.
FIG. 11: $\Delta_\alpha/t$ vs $n$ for different values of $E_{go}/t$ ($E_{go}/t = 0.30, 0.35$ and $0.40$), when $\alpha' = -0.40 \neq 0$ and $a = 0.0$, when $\alpha' = -0.40 \neq 0$ and $a = 0.0$. We see that the maximum of this figure is displaced with respect to the one when $\alpha' = 0$.

- It is not possible to answer the nature of the electronic states in the superconducting phase with our phenomenological model, because we do not have a microscopic model for $E_{PG}(n)$. However, the electronic one–particle Green function is composed of four peaks, two for the SC quasi–particles and two for the pseudogap order parameter. Every pair of peaks in the Green function are symmetric.

By choosing our free parameters in a reasonable way we have been able to reproduce the experimental curves of $T_c$ vs $n$. Namely, we have been able to obtain the following features:

1. To decrease the value of $T_c$ with respect to the “free” case, namely, $E_{go} = 0$.
2. To display the maximum of $T_c$ by choosing $\alpha' \neq 0$.
3. To choose the minimum value of $T_c$ inside the pseudogap region, namely, in the region where the pseudogap parameter is a maximum.
4. To bound the region of the superconducting dome by choosing the value of $E_{go}$.

We would like to place our work in perspective with respect to relevant literature on the subject. For example,

1. We have considered a single SC order parameter and a correlated $d$–wave one. However, Khasanov et al.[36] concluded from their experiments the existence of two order parameters, namely, one $s$–wave
FIG. 12: $T_c/t$ vs $n$ for several values of $E_{go}/t$, namely, $E_{go} = 0.36, 0.37$ and 0.38. See text for additional information.

like along the $c$–axis and one $s+d$ wave like in–plane in bulk $YBa_2Cu_3O_6$. They think that these features are generic and universal for the bulk cuprates. Also, Udomsamutharum[37] has postulated the existence of two parameters in order to explain the phase diagram of the cuprate superconductors.

2. 3–D structure is important as proven in the $YBa_2Cu_3O_6+x$ phase diagram[38]. We have considered a two–dimensional structure, but the inclusion of the third dimension is not a problem, from a numerical point of view.

3. The lattice is important for having bound states as discussed by Bak[39]. The presence of the parameter $\alpha'$ in our calculations has played an important role to locate the maximum of $T_c$.

4. Our sample is completely homogeneous. However, Kashiwaya et al.[40] have discussed the effect of impurities in the quasi–particle lifetime effect on local tunneling spectra in HTSC’s.

5. Our simple model is valid for low energy, namely, close to the chemical potential. However, to explain all the dynamical properties of the cuprates HTSC’s we should include the high energy features in single–particle spectra of hole–doped SC’s.

6. Our approach has been phenomenological. However, there are microscopic approaches to explain the origin of the pseudogap. For example, Kaneshita et al.[41] consider that the HTSC cuprates at $x \approx 1/8$ are explained by a transition of a phase stripe. Additionally, Trunin[42] concludes that
FIG. 13: $\Delta_o/t$ vs $n$ for several values of $E_{go}/t$, namely, $E_{go} = 0.36, 0.37$ and 0.38. See text for additional information.

FIG. 14: $T_c/t$ vs $\mu/t$ for $V/t = 8.1; a = 1/0.7$ and $\alpha' = -0.4$.

his experiments are best explained with a $d$–density wave pseudogap. Furthermore, Lee et al.[43] consider that the $SC$ state emerges from the Mott insulator under doping.

7. Just recently, Harrison et al.[44] have included the effect of short–range antiferromagnetic order on the cuprate Fermi orbits and Fermi arcs. In particular, they showed that a reduced coherent length gives an asymmetric broadening of the quasi–particle dispersion, resulting in simulated ARPES data very similar to those observed in experiments[45].

8. Aimi and Imada[46] have recently asked the question whether the simple two–dimensional Hubbard
model accounts for High–$T_c$ superconductivity in copper oxides. They have performed numerical results using pre–projected Gaussian–basis Monte Carlo method and studied superconducting correlations of $d_{x^2−y^2}$ wave symmetry. They conclude that these correlations are too weak for the realistic account of the cuprate high–$T_c$ superconductivity. This is in agreement with our feeling that some extra–ingredient has to be taken into account to explain superconductivity in the first place. In addition, we have included the pseudogap order parameter to explain the rich phase diagram of the cuprate superconductors away from half–filling.

We have to calculate the isotope exponent[47], $\alpha$ which is defined by $T_c = M^{−\alpha}$, where $M$ is the isotope ionic mass. In order to calculate it we have to impose a certain kind of cut–off frequency, $\omega_c$, around the chemical potential. We leave this for the future. However, before concluding, we would like to mention that the depletion of $T_c$ for $x \approx 1/8$, is going to give a lot of structure to the isotope exponent in this region of doping due to the fact that this exponent depends on derivatives of $T_c$.

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