Phase diagram and dependence of the critical temperature $T_c$ on the pressure for

$$Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$$

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Abstract

Using a mean-field BCS-like approach on the bidimensional extended Hubbard Hamiltonian we calculate the superconducting transition temperature $T_c$ as a function of the hole content $n_h$. This method can be used to determine the critical temperatures $T_c$ either for the extended $s$ wave or $d$ wave symmetry. We can also describe the pressure effects on $T_c$ by introducing the assumption that it induces a change in the magnitude $V$ of the attractive potential. This assumption yields an explanation for the intrinsic term, and together with the well known change in $n_h$, we set the critical temperature as $T_c = T_c(n_h(P), V(P))$. Then, we obtain a general expansion of $T_c$ in terms of the pressure $P$ and the hole content $n_h$. We apply this expansion to the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ system ($0.0 \leq x \leq 0.35$) and our results provide a good fitting for the experimental data for the variation of $T_c$ with the pressure $P$ and $n_h$.

Key words: BCS Model, Hubbard Hamiltonian, Phase Diagram, Pressure Effects

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1 Introduction

In spite of the advance attained in the research of the high temperature superconductors (HTSC), a great number of questions related to them remain to be answered. In order to obtain a better understanding of these new materials many experiments were performed, but the different experiments were interpreted by different theories. One of the most fundamental evidence that these experiments showed was the interplay among critical temperature $T_c$, hole content $n_h$, and pressure $P$, since one of the effects of the application of external pressure is a change in the hole content $n_h$ in the CuO$_2$ planes [1], which results in a large change in $T_c$. The large increase of $T_c$ by the application of pressure [2] has been the motivation for a vast number of works on the study of the effects of pressure on the critical temperature $T_c$ of the high temperature superconductors [3–6], not only to achieve higher $T_c$ but also to obtain a hint for chemical substitution which originates new materials and yields a better understanding of their physical properties.

Thus, in the detailed study of the dependence of the critical temperature $T_c$ of the HTSC on the pressure $P$, it has been suggested that the derivate $dT_c/dP$ may be strongly influenced by a pressure-induced alteration in the density of hole-like charge carriers $n_h$ on the CuO$_2$ planes [7]. This proposal was also supported by experimental observations of Hall constant’s pressure dependence [1] that confirmed the existence of a growth in $n_h$ in the CuO$_2$ planes when the pressure is applied [8]. Therefore, there is a pressure induced charge transfer (PICT) from the block layers into the CuO$_2$ planes, that is, $n_h = n_h(P)$. Since one expects $dT_c/dP = 0$ at the optimum doping, and $T_c(n_{op})$ generally increases with $P$, it is well accepted that the pressure also increases $T_c$ by a different mechanism of “intrinsic” origin [3,5,9], and such intrinsic term is a characteristic of each family of compounds. Therefore, we can separate these two effects by considering [3,5,9,10]:

$$\frac{dT_c}{dP} = \frac{dT_c^i}{dP} + \frac{\partial T_c}{\partial n_h} \frac{\partial n_h}{\partial P}. \quad (1)$$

Here the first term, $dT_c^i/dP$, represents the intrinsic contribution, not related to the charge transfer induced by pressure $\partial n_h/\partial P$. Thus, the change of $T_c$ with the hole content is given by $\partial T_c/\partial n_h$.

In this paper we consider the intrinsic contribution as originated from a variation of the magnitude $V$, of the attractive potential that forms the Cooper pairs in the superconducting phase with the applied pressure $P$, in such a way that $V = V(P)$. Similar proposition was previously made by Angilella et al. [9] and de Mello et al [3,5]. As discussed in Ref. [3,4], as $V$ increases with the applied pressure, the zero temperature superconductor gap also in-
creases. This hypothesis has been indirectly verified in the experimental study of polycrystallines samples of $Hg_{0.82}Re_{0.18}Ba_2Ca_2Cu_3O_{8+\delta}$ \[11\].

2 The Method

In order to study the dynamics of the hole-type carriers in the superconducting phase as well as the normal phase with correlations and the basic attractive interaction, we consider a two dimension extended Hubbard Hamiltonian $[3,5,9]$

$$H = -\sum_{\langle ij \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{<ij>_{\sigma\sigma'}} V_{ij} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{j\sigma'} c_{i\sigma}, \quad (2)$$

where $t_{ij}$ is the hopping integral between the nearest-neighbour and next-nearest-neighbour sites $i$ and $j$; $U$ is the on-site correlated repulsion and $V_{ij}$ describes the attractive interaction between nearest-neighbour sites $i$ and $j$.

In the superconducting phase the paired states form a condensate separated from the single-particle states by a “gap” (order parameter). Using a BCS-type mean-field approximation \[12\] the self-consistent gap equation, at finite temperatures, is given by

$$\Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \frac{E_{k'}}{2k_B T}, \quad (3)$$

with

$$E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}. \quad (4)$$

Here, $V_{kk'}$ is the interaction potential which contains the repulsive and attractive potential, and may be written in a separable form $[9,13]$

$$V_{kk'} = U + 2V \cos(k_x a) \cos(k'_x a) + 2V \cos(k_y a) \cos(k'_y a), \quad (5)$$

where it was considered a square lattice of lattice parameter $a$ and equal coupling constants $V$ along both directions in the Cu-O planes, in the context of mean field approximation.

A tight-binding approximation may be employed to dispersion relation in Eq.4, which yields

$$\varepsilon_k = -2t(\cos(k_x a) + \cos(k_y a)) + 4t_{xy} \cos(k_x a) \cos(k_y a) - \mu. \quad (6)$$
This equation has been previously considered [3,5,9,13], but here it was considered identical hopping integrals along both directions in the Cu-O planes for the nearest-neighbour \((t_x = t_y = t)\) and a different one for the next-nearest-neighbour \((t_{xy})\); \(\mu\) is the chemical potential.

Also, using the same BCS-type mean-field approximation applied to the gap (Eq.3), we obtain the hole-content equation [14]

\[
n_h(\mu, T) = \frac{1}{2} \sum_k \left(1 - \frac{\varepsilon_k}{E_k} \tanh \frac{E_k}{2k_BT} \right),
\]

(7)

where \(0 \leq n_h \leq 1\).

Following the steps of Ref [9], one observes that the substitution of the potential (Eq.5) in the gap equation (Eq.3) leads to the appearance of a gap with two different symmetries

\[
\Delta_k(\mu, T) = \Delta^{\text{max}}(\mu, T)[\cos(k_xa) \pm \cos(k_ya)],
\]

(8)

where the plus sign is for extended \(-s\) wave and the minus sign, for \(d\) wave symmetry. The anisotropy of the gap is one of the characteristic distinctions between the usual low temperatures superconductors and the HTSC. Many experiments and theoretical calculations suggest that the HTSC exhibit a pairing symmetry different than the usual superconductors [15], and in some cases even a mixture of different symmetries must be considered [16]. Thus, the determination of the symmetry of the gap is the first step in the identification of the pairing mechanism of the charge carriers and the subsequent development of a microscopic theory for the HTSC.

To obtain the phase diagram, the gap equations are solved numerically, in the limit \(T \longrightarrow T_c\), together and self-consistently with the density of hole carriers \(n_h\) (Eq.7). In these calculations it was considered that there were no symmetry mixture near the critical point [9,16].

The values of the hopping integrals \(t\) and \(t_{xy}\) used in the calculation of the phase diagram of the \(Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7\) series are taken from A.R.P. E.S. measurements for the Bi2212 [9], since it is a HTSC with similar structure, having two \(CuO_2\) identical layers per unit cell [17], although this does not guarantee that the real \(t\) and \(t_{xy}\) have this values and that is why we have tried a small variation around the A.R.P.E.S results. The chemical potential \(\mu\) is calculated self-consistently. The values of \(U\) and \(V\) are considered adjustable parameters, in order to reproduce the \(T_c \times n_h\) curve close to the experimental data. Our method to derive the phase diagrams is similar to the approach based on a change in the zero temperature gap [18]. On Fig. 1 we show the phase diagram with the theoretical curves from the numerical calculation for
the *extended* — *s* and *d* wave symmetries, together with the experimental data for the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ [19].

![Phase Diagram](image)

Fig. 1. Phase diagram showing the numerical calculation for the *extended* — *s* and *d* wave symmetry together with the experimental data of the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ series taken from Ref. [19].

Fig. 2 illustrates the behavior of the phase diagram, for the *extended* — *s* symmetry, when $V$ is varied. Both symmetries exhibit a similar dependence on the potential $V$.

Notice that although there is a strong tendency toward a *d*-wave symmetry on many experiments the HTSC, our results, with the parameters $t$ and $t_{xy}$ fixed, show that the *extended* — *s* symmetry seems to reproduce well the phase diagram of the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ series in a better agreement with the experimental points than the *d* wave one. This is in accordance with the results of Schneider et al. [13].
Fig. 2. Phase diagram of the $Tl_{0.5}Pb_{0.5}Sr_{2}Ca_{1-x}Y_{x}Cu_{2}O_{7}$ series showing the effect of a change in the magnitude $V$ of the attractive potential.

Thus, the study of the phase diagram yields the best values $t=0.05eV$, $t_{xy}=0.023eV$, $U=0.052eV$ and $V=-0.0875eV$ for the extended $s$ symmetry, and $t=0.05eV$, $t_{xy}=0.0275eV$, $U=0.052eV$ and $V=-0.057eV$ for the $d$ wave symmetry, which will be used in the next section.

3 The Pressure Effects

On Fig. 2 we show that $T_c$ is quite sensible with respect to a change in the magnitude $V$ of the attractive potential. Therefore, as it was previous mentioned, we suppose that the pressure induces a change in the attractive potential, in such a way that $V = V(P)$. In the absence of informations of how $V$ effective behaves with respect to the pressure $P$, we assume a linear depen-
dence [3,5,20], which should be the case since the pressure causes very small structural changes in the lattice constants [9]. Therefore
\[ V(P) = V + \Delta V(P). \] (9)

In the same way, for the density of carriers, we have
\[ n_h(P) = n_h + \Delta n_h(P). \] (10)

Here, \( V \) and \( n_h \) are the \( P = 0 \) values of \( V(P) \) and \( n_h(P) \). The pressure dependence is defined as
\[ \Delta V(P) = c_1 P, \quad \Delta n_h(P) = c_2 P \] (11)

where \( c_1 = (\partial V/\partial P) \) and \( c_2 = (\partial n_h/\partial P) \) are parameters usually determined from the experimental data.

Our previous discussion leads to \( T_c(n_h, P) = T_c(n_h(P), V(P)) \). Thus, we can estimate \( T_c \) for a compound with a certain value \( n_h \), and under pressure \( P \), using an expansion of \( T_c(n_h, P) \) in terms of \( P \). Consequently, we have
\[ T_c(n_h, P) = T_c(n_h, 0) + \left( \frac{dT_c}{dP} \right)_{P=0} P + \frac{1}{2!} \left( \frac{d^2T_c}{dP^2} \right)_{P=0} P^2 + \frac{1}{3!} \left( \frac{d^3T_c}{dP^3} \right)_{P=0} P^3 + \cdots, \] (12)

where
\[ \frac{d^2T_c}{dP^2} = \left( c_1 \frac{\partial}{\partial V} + c_2 \frac{\partial}{\partial n_h} \right)^2 T_c(n_h(P), V(P)). \] (13)

\( T_c(n_h, 0) \) is the critical temperature for \( P=0 \). The Eq. (12) can be written as
\[ T_c(n_h, P) = \sum_z \alpha_z \frac{P^z}{z!}, \] (14)

with
\[ \alpha_z = \left( c_1 \frac{\partial}{\partial V} + c_2 \frac{\partial}{\partial n_h} \right)^z T_c(n_h(P), V(P)). \] (15)
One can see by considering the case \( z = 1 \) in the above equation, and comparing with Eq.(1), that

\[
\frac{dT^i_c}{dP} = \frac{\partial V}{\partial P} \frac{\partial T_c}{\partial V},
\]

which clearly shows that, in our model, the intrinsic contribution is related to the variation of the magnitude \( V \) of the attractive potential with the pressure \( P \). Now, the analytical expressions for the coefficients \( \alpha_z \) will be derived below as a function of the parameters \( c_1 \) and \( c_2 \), for the values of \( n_h \) and \( P \).

The first coefficient \((z = 1)\) for the above expression is given by

\[
\alpha_1 = \left( c_1 \frac{\partial T_c}{\partial V} + c_2 \frac{\partial T_c}{\partial n_h} \right).
\]

Restricting ourselves to small changes in \( V \), we may approximate

\[
\frac{\partial T_c}{\partial V} \approx \frac{\Delta T_c}{\Delta V},
\]

where the horizontal bar denotes a “mean” over the values of \( T_c \) obtained direct from the phase diagram as a function of \( V \), as it is shown in Fig. 2. This “mean” is realized for each value of \( n \). To estimate \( \partial T_c/\partial n_h \) we may either use an experimental value, or use directly the curves of Fig. 2 or a phenomenological universal parabolic curve [19]:

\[
T_c = T_c^{\text{max}}[1 - 4\beta(n_{op} - n_h)^2],
\]

and, therefore, an analytical expression for \( \partial T_c/\partial n_h \) is obtained. Thus, we derive the following expression for the coefficient \( \alpha_1 \)

\[
\alpha_1 = c_1 \frac{\Delta T_c}{\Delta V} + c_2 2(4\beta)T_c^{\text{max}}(n_{op} - n_h),
\]

and \( \alpha_2 \), which is given by

\[
\alpha_2 = \left( c_1 \frac{\partial}{\partial V} + c_2 \frac{\partial}{\partial n_h} \right) \left( c_1 \frac{\partial T_c}{\partial V} + c_2 \frac{\partial T_c}{\partial n_h} \right),
\]

and results in

\[
\alpha_2 = 2(4\beta)\frac{\Delta T_c^{\text{max}}}{\Delta V}(n_{op} - n_h)c_1c_2 - 2(4\beta)T_c^{\text{max}}c_2^2,
\]
where \( \frac{\Delta T_{\text{max}}}{\Delta V} \) is an empirical mean derived numerically by inspection on Fig. 2 at the optimum doping compound \( n_{\text{op}} \). Following along the same procedure, the third coefficient becomes

\[
\alpha_3 = -4(4\beta) \frac{\Delta T_{\text{max}}}{\Delta V} c_1 c_2^2. \tag{23}
\]

As one can notice the coefficients \( \alpha_z \), for \( z \geq 4 \), are all nulls.

4 Comparison with experimental data

In order to study the effects of the pressure on the critical temperature of any given family of compounds, we need first to calculate the constants \( c_1 \) and \( c_2 \), which yield the coefficients \( \alpha_z \). Thus, we can see that the constants \( c_1 \) and \( c_2 \) are determined by how \( V \) and \( n_h \) changes with the pressure (Eq (11)). Hall effects can give directly \( \frac{\partial n_h}{\partial P} \) as in the case of Bi2212 [8] and therefore \( c_2 \) [4–6]. Since these measurements are not available for the \( T_{l0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7 \), we can obtain \( c_1 \) and \( c_2 \) by comparing with the curves of \( T_c \times P \) for two values of \( n_h \). In fact Wijngaarden et al. [17] also estimate the value of \( c_2 \) from their experimental data for the \( T_{l0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7 \).

Since at low pressures only the linear term comes into play, the higher order coefficients can be ignored. Thus, \( \alpha_1 \) becomes the slope of a linear approximation from the initial points of the \( T_c \times P \) curve, for a given \( n_h \) compound. Starting with \( n_h = n_{\text{op}} \), in spite of not being strictly necessary, we determine \( c_1 \) using the estimated \( \alpha_1 \) in Eq.(20), as long as at \( n_{\text{op}} \) the charge transfer term vanishes. To determine \( c_2 \) we estimate \( \alpha_1 \) from the \( T_c \times P \) curve of an \( n_h \neq n_{\text{op}} \) compound, and use again Eq.(20). Once these two constants are determined, the \( \alpha_z \) coefficients for any \( n_h \) value can be calculated (Eq.(15)).

For the \( Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7 \) [17,19] series we used the experimental values for the \( n_h = n_{\text{op}} = 0.15 \) and \( n_h = 0.20 \) compounds to calculate \( c_1 \) and \( c_2 \). The estimated \( \alpha_1 \) were 1.5K/GPa and 0.41K/GPa for \( n_{\text{op}} \) and \( n_h = 0.20 \), respectively. The phase diagram parameters \( \frac{\Delta T_{\text{max}}}{\Delta V} \) taken from Fig. 1 and 2 and used in the calculations were 2900K/eV for the extended – s wave and 2300K/eV for the \( d \) wave symmetry for the \( n_{\text{op}} \) compound and 2700K/eV for the extended – s wave and 2600K/eV for the \( d \) wave symmetry for the \( n_h = 0.20 \) compound. The parameters of the parabolic curve (Eq.19) used were \( \beta = 3.5 \) and \( T_c^{\text{max}} = 105.1\text{K} \). Therefore, the resulting constants were \( c_1^s = 5.17 \times 10^{-4}\text{eV/GPa} \) and \( c_2^s = 6.7 \times 10^{-3}\text{GPa}^{-1} \) for the extended – s wave and \( c_1^d = 6.52 \times 10^{-4}\text{eV/GPa} \) and \( c_2^d = 8.7 \times 10^{-3}\text{GPa}^{-1} \) for the \( d \) wave symmetry.
On Fig. 3 and 4 we present our results in comparison with the experimental data. One observes that, for the optimum doping, and the compounds near the optimum doping, we have a rather good result. For the optimum compound \( n_h=0.15 \) in particular, we had the better result, for both symmetries, with very good agreement with the experimental data [17,19]. For \( n_h=0.075, 0.20 \) and 0.25 we can reproduce well the low temperature data and obtain a qualitative agreement on the high pressure region.

![Graph](image)

**Overdoped Region**

Fig. 3. Numerical calculation for the extended – s (filled lines) and d wave (dashed lines) symmetries, in the overdoped region, together with the pressure experimental data of the \( Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7 \) series taken from Ref. [19].

The value of the constant \( c_2 \left( = 6.7 \times 10^{-3} GPa^{-1} \right) \), which means the rate of charge transfer by the pressure \( \left( \frac{\partial n_h}{\partial P} \right) \), for the extended – s symmetry is close to the experimental results for the \( YBCO \) compounds [10], and is smaller than the experimental Hall coefficient value for the Bi2212 [8]. The value estimated experimentally by Wijngaarden et al. [17,19] for the \( Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7 \) series was \( \frac{\partial n_h}{\partial P_{exp}} = 3.9 \times 10^{-4} GPa^{-1} \). This discrepancy can be at-
Fig. 4. Numerical calculation for the extended $s$ (filled lines) and $d$ wave (dashed lines) symmetries, in the underdoped region, together with the pressure experimental data of the $Tl_{0.5}Pb_{0.5}Sr_{2}Ca_{1-x}Y_{x}Cu_{2}O_{7}$ series taken from Ref. [19]

dtributed to the parameters $\Delta T_{c}/\Delta V$, which are difficult to be estimated with the very few experimental points, what introduces some uncertainties in the calculated phase diagrams. This discrepancy is also the reason why our curves is in good agreement with the experimental data up to 10GPa, but starts to deviate above this value. Another evidence that our main source of error comes from $\partial n_{h}/\partial P$ is the fact that the optimum compound, with $n_{h}=0.15$, which is the one with $\partial n_{h}/\partial P=0$, is in much better agreement with the experimental results than the others, with different $n_{h}$. 
5 Conclusions

In conclusion, to relate the pressure $P$, the density of holes $n_h$ and the attractive potential $V$ we used in the calculation a BCS-type mean-field approach on the bidimensional extended Hubbard Hamiltonian with the potential $V$ as an adjustable parameter. Our method has general application, and can therefore be used in any compound under pressure. We showed that these calculations can describe reasonably well the pressure effects on the critical temperature $T_c$ for the series $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1−x}Y_xCu_2O_7$, for the four measured doping values.

Our results for the extended $−s$ wave symmetry give a better quantitative agreement with the experimental data. But the $d$-wave calculations are also in qualitative agreement with the experimental data, showing that the order parameter symmetry is not decisive to study the pressure effects.

Thus, our method provides a very interesting novel explanation to the intrinsic term, which is related with the change in the potential $V$, in agreement with a previous hypothesis that the pressure increases the zero temperature superconducting gap [3,4] and with some experimental results [11].
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