The Hubbard model applied to the phase diagram and pressure effects in $YBa_2Cu_3O_{7-\delta}$ superconductors

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We apply a method based on a BCS-type approach to the extended Hubbard model on a square lattice to deal with the $YBa_2Cu_3O_{7-\delta}$ family of superconductors under pressure. The parameters of the tight-binding band are taken from experiments, and the coupling strength $U$ and $V$ are estimated by the zero pressure phase diagram ($T_c \times n_h$). This scheme yields the nontrivial dependence of the superconductor critical temperature $T_c$ as a function of the hole concentration $n_h$ in the CuO$_2$ plane. With the assumption that the pressure $P$ modifies the potential $V$ and the on plane hole content $n_h$, we can distinguish the charge transfer and the intrinsic contribution to $T_c(P)$. We show that the changes on $T_c(P)$ for the $YBa_2Cu_3O_7$ optimally doped compound at low pressures are almost entirely due to the intrinsic term.

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I. INTRODUCTION

Pressure experiments have played an important role in understanding high-$T_c$ superconductors (HTSC). Several review papers have been written on this subject. In short, the pressure investigation is a helpful tool to display the potential effects of the chemical pressure, thereby providing useful information for synthesis of related compounds and, more important to the present work, to understand which are the structural parameters that influence the microscopic superconducting mechanism responsible for the HTSC.

It is well known that the pressure effects are twofold: (1) It is documented that the applied pressure $P$ increases the hole concentration $n_h$ on the CuO$_2$ planes with a maximum rate of charge transfer approximately given by $\partial n_h/\partial P = 0.02 GPa^{-1}$. This is called the pressure induced charge transfer (PICT) term. (2) Another pressure effect is the increase of $T_c$ for the optimum doped compound ($n_{op}$) above the zero pressure value, which indicates another mechanism independent of the PICT, known as the “intrinsic” contribution term. Recently, a very large intrinsic term of $\partial T_c/\partial P = 6.8 K GPa^{-1}$ has been measured, however, its origin is still a matter of research. Usually these two effects, the PICT and the intrinsic term, have to be combined in order to account for the experimental data on a given family of compounds. It is very convenient to separate both contribution because the PICT can be measured independently by thermal measurements, like the Hall coefficient. Some earlier works have estimated the magnitude of both effects through a phenomenological pressure expansion applied to the $YBa_2Cu_3O_{7-\delta}$ family of compounds.

A method using a BCS-type mean field approach with an extended Hubbard Hamiltonian was introduced to derive the phase diagram $T_c \times n_h$. This procedure was used to deal with the pressure effects and it was assumed that, besides the hole content $n_h$, the pressure also changes the magnitude $V$ of the attractive potential, and ultimately changes the zero temperature superconducting gap $\Delta(0)$. Thus, the critical temperature $T_c(n_h, P)$ was obtained as an expansion in powers of $P$, for a determined $n_h$ value, and each contribution was singled out, which is very convenient to interpret the experimental results. This method was applied to the experimental results of Hg 1201 and Hg 1223, with a fixed set of parameters, with excellent agreement with the underdoped and overdoped compounds. In a similar approach, also using the BCS method and the extended Hubbard Hamiltonian, Anglella et al. used the isothermal compressibility tensor to estimate the change of $n_h$ with the pressure and, through the derived $T_c \times n_h$, they obtained the variation of the attractive potential $V$ with the pressure $P$. In their calculations they have also taken into account pressure dependence for the lattice parameter $a_c$, so that the hopping integrals $t_i$ depends on the pressure too ($t_i = t_i(a(P))$). In this way, they could separate the charge transfer and the intrinsic contribution. Their calculations for the intrinsic term were in good agreement with the measurements of the Bi 2212.

Calculations based on the extended Hubbard Hamiltonian provide a possible microscopic interpretation for the intrinsic term since it is related with the superconducting interaction $V$. Through such calculations, one may extract some clues to the behavior of the fundamental microscopic mechanism under the structural changes provided by the applied pressure, and some hints for the mechanism itself.

Recently, we have combined both approaches of Ref. in order to study the measured $T_c \times P$ curves of the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1+x}Y_xCu_2O_{7}$ series. A characteristic of this method is that, if the phase diagram is experimentally known, $T_c(P)$ can be calculated for the entire family of different $n_h$ compounds, and the value of $\partial n_h/\partial P$ calculated for this specific family. Our calculated $T_c(n_h, P)$ for the $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1+x}Y_xCu_2O_{7}$ series agreed well...
with the experiments for the extended-$s$ wave symmetry.

In a recently letter, Chen et al. have calculated the pressure effects on the nearly optimum doped \(YBa_2Cu_3O_7\) and underdoped \(YBa_2Cu_4O_8\), using a BCS-type method. Using values of \(\partial n_h/\partial P\) averaged from different results of several groups, they obtained very good agreement with the experimental data. However, calculating \(\partial T_c/\partial P\) for different \(n_h\) compounds of the \(YBa_2Cu_3O_{7-\delta}\) family, they found almost the same values for different parameter potentials, which led them to conclude that the main contribution to the critical temperature \(T_c(n_h, P)\) was from the PICT term. To check whether the \(YBa_2Cu_3O_7\) compound has an intrinsic contribution term or not we have performed calculations on the YBCO system using our method.

In our method we use a BCS approach with the extended Hubbard model to calculate the phase diagram of the \(YBa_2Cu_3O_{7-\delta}\) system, which is compared with the experimental data. Then we take into account the effects produced by the pressure through a change in the intersite potential: as first order approximation we write \(V(P) = V + \Delta V(P)\). Here \(\Delta V(P) = c_1 P\), with \(c_1\) being a constant independent of \(P\) that will be defined later. Since the structural changes for typical pressures are small, we neglect its effect on the hopping integrals. For the density of hole carriers we use the well know dependence of \(n_h\) with \(P\). From this we estimate the critical temperature \(T_c(n_h(P), V(P))\) as an expansion in terms of the pressure \(P\). Our results showed good agreement with the experimental data.

II. THE PHASE DIAGRAM

To develop the dynamics of the hole-type carriers in the Cu-O planes, we adopt a two dimension extended Hubbard Hamiltonian in a square lattice of lattice parameter \(a\)

\[
H = - \sum_{<ij>\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{<ij>\sigma\sigma'} V_{ij} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{j\sigma'} c_{i\sigma},
\]

(1)

where \(t_{ij}\) is the nearest-neighbor and next-nearest-neighbor hopping integral between sites \(i\) and \(j\); \(U\) is the Coulomb on-site correlated repulsion and \(V_{ij}\) is the attractive interaction between nearest-neighbor sites \(i\) and \(j\).

The transformation of Eq. (1) to the momentum space leads to the appearance of the dispersion relation. In order to compare with YBCO system, we used a dispersion relation within a tight-binding approximation, which may be compared with the one estimated from ARPES measurements. Thus,

\[
\varepsilon_k = -2t_1(\cos(k_x a) + \cos(k_y a)) + 4t_2 \cos(k_x a) \cos(k_y a)
+ 2t_3(\cos(k_x a) + \cos(2k_y a))
+ 4t_4 \cos(2k_x a) \cos(k_y a)
- 4t_5 \cos(2k_x a) \cos(k_y a) + \cos(2k_y a) \cos(k_x a) - \mu,
\]

(2)

where it was considered identical hopping integrals along both directions in the Cu-O planes for the nearest-neighbor \((t_x=t_y=t_1)\), a different one for the next-nearest-neighbor \((t_2)\), and so on. Here it was considered a hopping from the first to the fifth neighbor. Equation (2) is in agreement with the one given by Schabel et al., \(\mu\) is the chemical potential which controls the hole concentration. 

Like the low temperature superconductors, the HTSC exhibit an energy “gap” (order parameter) in the superconducting phase which separates the paired states from the single-particle states. Using a BCS-type mean-field approximation to develop Eq. (1) in the momentum space, one obtains the self-consistent gap equation, at finite temperatures,

\[
\Delta_k = - \sum_{k'} V_{kk'} \frac{\Delta_k}{2E_{k'}} \tanh \frac{E_{k'}}{2k_B T},
\]

(3)

with

\[
E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2},
\]

(4)

which contains the interaction potential \(V_{kk'}\) that comes from the transformation to the momentum space of Eq. (1).

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

(5)

![FIG. 1. Phase diagram $T_c \times n_h$ for the $d$ wave and extended-$s$ wave symmetries, with the experimental data of the $YBa_2Cu_3O_{7-\delta}$ taken from Ref. [1] (open squares).](image)
The substitution of Eq. (6) into Eq. (3) leads to appearance of a gap with two distinct symmetries:

\[ \Delta_{\mathbf{k}}(\mu, T) = \Delta_{\text{max}}(\mu, T)[\cos(k_x a) \pm \cos(k_y a)], \] (6)

where the plus sign is for extended-\( s \) wave and the minus sign, for \( d \) wave symmetry. In accordance with Ref. [1], one observes that the \( d \) wave part of the gap does not depend on the coupling constant \( U \), depending only on \( V \). The extended-\( s \) symmetry depends on both \( U \) and \( V \). As it is well known, at the critical temperature there is no symmetry mixture, and the gap might be in the extended-\( s \) or \( d \) wave state when \( T \rightarrow T_c \).

Using the same BCS-type mean-field approximation used in the gap equation one obtains the hole-content equation [2]

\[ n_h(\mu, T) = \frac{1}{2} \sum_{\mathbf{k}} \left( 1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh \frac{E_{\mathbf{k}}}{2k_B T} \right), \] (7)

where \( 0 \leq n_h \leq 1 \). This equation, together with the gap equation and the dispersion relation, are solved numerically self-consistently, in the limit of \( T \rightarrow T_c \), to obtain the phase diagrams for both gap symmetry.

To compare with the experimental results for the Y123 system, we perform our calculations with the hopping integrals: \( t_1=0.32eV \) as the nearest-neighbor value; for \( t_2 \) it was adopted the ratio \( t_2/t_1=0.50 \) for the \( d \)-wave symmetry and \( t_2/t_1=0.57 \) for the extended-\( s \); the remaining band parameters followed: \( t_3/t_1=0.16 \), \( t_4/t_1=0.11 \), and \( t_5/t_1=0.031 \). All these values are close to the ARPES measurements on Y123 system [4].

Using these band parameters we first estimated the coupling constant \( V \), using the \( d \)-wave gap symmetry, reproducing the experimental phase diagram of Ref. [2]. The best value obtained was \( V=-0.1152eV \). For the case of the extended-\( s \) gap symmetry, the value \( U=0.0096eV \) was obtained, using the same coupling constant \( V \) of the \( d \)-wave. The chemical potential \( \mu \) is calculated self-consistently. Fig.1 shows the results of our numerical calculations together with the experimental data of Ref. [3] for the \( YBa_2Cu_3O_{7-\delta} \) series.

### III. THE METHOD

To calculate the variations of \( T_c \) for a given compound with a certain value \( n_h \), and under pressure \( P \), we may use an expansion of \( T_c(n_h, P) \) in powers of \( P \). Therefore,

\[ T_c(n_h, P) = T_c(n_h, 0) + \left( \frac{dT_c}{dP} \right)_{P=0} P + \frac{1}{2!} \left( \frac{d^2T_c}{dP^2} \right)_{P=0} P^2 + \cdots, \] (8)

where

\[ \frac{d^2T_c}{dP^2} = \left( c_1 \frac{\partial}{\partial V} + c_2 \frac{\partial}{\partial n_h} \right)^z T_c(n_h(P), V(P)). \] (9)

Here, \( c_1 = (\partial V/\partial P) \) and \( c_2 = (\partial n_h/\partial P) \) are constant parameters, which are determined fitting the experimental data for a given system. \( T_c(n_h, 0) \) is the critical temperature for \( P=0 \). Equation (8) can be written in a compact form, as

\[ T_c(n_h, P) = \sum_z \alpha_z \frac{P^z}{z!}. \] (10)

with

\[ \alpha_z = \left( c_1 \frac{\partial T_c}{\partial V} + c_2 \frac{\partial T_c}{\partial n_h} \right)^z T_c(n_h(P), V(P)). \] (11)

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

\[ \alpha_1 = \left( c_1 \frac{\partial T_c}{\partial V} + c_2 \frac{\partial T_c}{\partial n_h} \right). \] (12)

It is important to stress that the first term in \( \alpha_1 \) is the intrinsic contribution, and the second one is the PICT contribution. Therefore, both contributions can be singled out. Restricting ourselves to small changes \( V \), we may approximate

\[ \frac{\partial T_c}{\partial V} \approx \frac{\Delta T_c}{\Delta V}. \] (13)

![Phase Diagram](33563d703/phase_diagram.png)

FIG. 2. Phase diagram \( T_c \times n_h \) for the \( d \)-wave showing the effect of a change on the coupling constant \( V \), together with the experimental data of the \( YBa_2Cu_3O_{7-\delta} \) taken from Ref. [2] (open squares).
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 $n_h$. To obtain $\partial T_c/\partial n_h$, we may either use an experimental value, or use directly the curves of Fig.2, as done here. One can also use a phenomenological universal parabolic relation between $T_c$ and $n_h$ \cite{2,13}.

For the coefficient $\alpha_2$ we have

$$\alpha_2 = \left(c_1 \frac{\partial}{\partial V} + c_2 \frac{\partial}{\partial n_h}\right) \left(c_1 \frac{\partial T_c}{\partial V} + c_2 \frac{\partial T_c}{\partial n_h}\right). \quad (14)$$

Thus, $\alpha_2$ becomes

$$\alpha_2 \approx c_2^2 \frac{\partial^2 T_c}{\partial n_h^2}. \quad (15)$$

The other coefficients of the expansion can be obtained using the same procedure.

IV. THE PRESSURE EXPERIMENTAL DATA

First of all, one observes that, at low pressures only the linear term ($\alpha_1$) of the expansion $T_c(n_h, P)$ comes into play. Therefore, we can approximate $\alpha_1$ as the slope of the initial points of the $T_c \times P$ curve, for a given $n_h$ compound. Starting with $n_h = n_{op}$, we determine $c_1$ using the estimated $\alpha_1$ in Eq.(12), as long as at $n_{op}$ the charge transfer term vanishes. To determine $c_2$ we obtain $\alpha_1$ from the $T_c \times P$ curve of an $n_h \neq n_{op}$ compound, and use again Eq.(12). Once these two constants are determined, the $\alpha_2$ coefficients for any $n_h$ value can be calculated (Eq.(14)).

For the $YBa_2Cu_3O_{7-\delta}$ system we only have the non zero pressure data for the $n_h = n_{op} = 0.165$ ($\delta \approx 0$) and $n_h = 0.15$ ($\delta \approx 0.15$) compounds \cite{2,13}. Thus, from the $T_c \times P$ curves of Ref.2\cite{2} we estimate $\alpha_1 = 0.75 K/GPa$ and $1.4 K/GPa$ for $n_{op}$ and $n_{15}=0.15$, respectively. The phase diagram parameters (2\cite{2}) taken from Fig.2 and used in the calculations were 1652K/eV and 1475K/eV for the $d$-wave and 1164K/eV and 1099K/eV for the extended-$s$ wave for $n_{op}$ and $n_{15}=0.165$ compounds, respectively. Therefore, the resulting constants for the $d$-wave were $c_1 = 4.54 \times 10^{-4} eV/GPa$ which furnishes an intrinsic contribution of $0.8K/GPa$, and $c_2 = 3.15 \times 10^{-3} GPa^{-1}$ which is the charge transfer term ($c_2 = \frac{\partial n_h}{\partial P}$). For the extended-$s$ wave we obtained $c_1 = 6.4 \times 10^{-4} eV/GPa$ and $c_2 = 2.2 \times 10^{-3} GPa^{-1}$. It is important to mention that our values for $\partial T_c/\partial P$ (the intrinsic contribution; see Eq.(12)) were in the same order of magnitude of Neumeier and Zimmermann\cite{13}, despite the difference in the approaches.

![FIG. 3. Numerical results: the solid and dashed lines are the $d$-wave results, while the long-dashed lines are the extended-$s$ wave results. The open squares and filled squares are experimental data of $YBa_2Cu_3O_{7-\delta}$ taken from Ref.2\cite{2} and Ref.3\cite{3}, respectively.](image)

On Fig.3 we compare the $T_c(n_h, P)$ expansion with the experimental data. We observe a very good agreement for both compounds, specially for $n_{op}$, using the $d$-wave gap symmetry, where the data can be fitted up to 20 GPa. The increase of $n_{op}$ with the pressure is attributed to the intrinsic contribution in our theory, and the maximum $T_c$ at $P \approx 7 GPa$ and subsequent decrease is due to the negative second order term of the expansion, which reflects the effect of the PICT. The extended-$s$ wave results did not show good results indicating a preference for the $d$-wave pairing mechanism for the Y-123 system.

V. CONCLUSIONS

We conclude this letter emphasizing that our method based on the BCS approach with the extended Hubbard model, with both the attractive potential $V$ and the density of carriers $n_h$ depending on the pressure $P$, predicted an intrinsic term and a PICT contribution similar to those predicted earlier \cite{2}. In our method we propose a direct pressure dependence for the attractive potential $V$, which is different from other works\cite{2} that use $V$ as an adjustable parameter in order to fit the known experimental dependence of $T_c$ on $P$. Our results for the $d$-wave are in excellent agreement with the Y-123 pressure data and, the intrinsic term being the most important contribution to the low pressure data on the optimum compound. Concerning the underdoped compound the intrinsic and PICT contribution are both present and must, as previously known by several experiments and theories\cite{2}, be taken into account. Such results support the $d$-wave symmetry in these compounds.

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