Physica B 403 (2008) 4209–4212

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Doped high-T_c superconductors under pressure

S. Orozco [a], M.A. Ortiz [a,*], R.M. Méndez-Moreno [a], M. Moreno [b,1]

[a] Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Apartado Postal 21-092, 04021 México, D.F., México
[b] Departamento de Física, Cinvestav, Av. IPN 2508, Col. San Pedro Zacatenco, 07360 México, D.F., México

ARTICLE INFO

Article history:
Received 7 June 2007
Received in revised form
8 April 2008
Accepted 9 September 2008

PACS:
74.20.Fg
74.62.-c
74.72.Jt
74.72.-h

Keywords:
High-T_c
Cuprate
Charge carrier
Pressure

ABSTRACT

Within the BCS framework generalized Fermi surface topologies, modeled with band overlapping, are proposed as a mechanism to enhance the electronic density of states at the Fermi level. This band overlapping allows the high-T_c values observed in cuprate superconductors at different pressures. With this approach the correlation between the critical temperature, the charge carrier density and the pressure is obtained in terms of the coupling constant and the band overlapping parameter. In order to obtain numerical results the model is applied to a Tl-based superconductor.

1. Introduction

At present it seems well established that the superconducting and normal state properties of high-T_c cuprates and other related ceramic compounds depend strongly on the charge carrier density. It is commonly believed that the charge carriers responsible for the superconducting pairing of many high-T_c cuprates are holes mainly confined to the CuO_2 layers [1]. The charge carrier density n_h is defined as the number of holes per CuO_2 layer. Taking this property into account a two-dimensional (2D) fermion gas is a good model for high-T_c cuprates.

The principal experimental results in cuprates related to the charge carrier density can be summarized with the following points [2]: at atmospherical pressure, the concentration of charge carriers in the CuO_2 planes can be changed either by changing the oxygen concentration or by substituting some suitable element in the charge reservoir layers which lie between the CuO_2 planes. Experimentally, n_h can be changed by preparing various samples with different doping. The critical temperature T_c depends on the carrier concentration and for most cuprates it is generally accepted that it obeys an inverse parabolic relation with the hole concentration n_h. The maximum T_c (T_{cmax}) appears at the optimal carrier concentration, n_{hop}. Compounds with lower n_h are said to be underdoped while compounds with higher n_h are said to be overdoped.

On the other hand, the high-T_c cuprate superconductors (HTSC) have been extensively studied under high pressures [3,4]. The pressure is an important parameter capable of increasing the T_c of several HTSC. However, this is not a general trend for all HTSC. It is known both from experiments and calculations that the application of high pressures is a useful mechanism to modify the charge carrier concentration n_h. $T_c(p)$ is expected to follow a parabolic curve, which is indeed observed for a number of compounds [5]. This parabolic behavior can be different in some high-T_c superconductors in which nonequivalent superconducting layers are present due to the peculiarities of the crystallographic structure. Nevertheless, pressure can increase T_{cmax} to a value higher than the one obtained at any doping under atmospheric pressure, implying that there exists an intrinsic enhancement of T_c due to pressure. The resulting $T_c(p)$ of every compound is determined by the combination of these effects, which provide important clues to the existence of superconductivity at higher temperatures.

High-pressure experiments can be done to find new materials and to test theoretical models, since the pressure dependence of T_c must be predicted correctly by the theory. The hydrostatic pressure modifies the lattice parameters taking into account the

* Corresponding author. Tel.: +52 5556224855; fax: +52 5556224854.
E-mail address: maof@fciencias.unam.mx (M.A. Ortiz).
[1] On sabbatical leave from: Instituto de Física. Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México, D.F., Mexico.

0921-4526/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2008.09.005

specific compressibility of each HTSC under pressure: it is widely noted that these parameters are intimately related to the nature of the electronic band structure of the superconducting cuprates. Additionally, first principle calculations show overlapping energy bands at the Fermi level [6]. The short coherence length observed in high T_c superconductors has been also related to the presence of overlapping energy bands [7].

The predominant dependence of T_c on the electronic density of states (DOS) on the proximity and at the Fermi level is supported by numerous experiments. An increase in DOS favors higher T_c values. In order to increase the DOS for the 2D system at the Fermi level, a generalized Fermi surface with two overlapping bands is proposed as a prototype to describe multiband HTSC [8]. The energy band overlapping modifies the DOS near the Fermi level allowing the high T_c values observed. A similar effect can also be obtained with other mechanisms as a van Hove singularity in the DOS [9].

In this work, a simple schematic form of these generalized surface structures is proposed for a 2D fermion system. Within the BCS framework, a generalized Fermi surface with two overlapping bands is proposed. This model is applied to study the behavior of HTSC with equivalent CuO_2 layers, i.e. with only one kind of charge carriers, in order to separate doping and intrinsic effects on T_c under pressure. Different doping and high pressures are considered. An important issue to address is how the variation of pressure affects the bands overlapping so that T_c increases.

2. Theory

A generalized Fermi sea of concentric *shells* of occupied orbitals is considered. The basic hypothesis of the model with two overlapping bands is introduced by the following particular distribution in momentum space:

$$n_k = \Theta(\gamma k_F - k) + \Theta(\gamma k_F - k)\Theta(k - \beta k_F), \tag{1}$$

with k_F the Fermi momentum, and $0<\beta<\gamma<1$. The distribution in momentum space induces one in energy, $E_\beta = \beta^2 E_F < E_\gamma = \gamma^2 E_F$ [8]. E_F is the Fermi energy. There is only one independent parameter because they must satisfy $2\gamma^2 - \beta^2 = 1$ to keep the average number of electron states constant. Then γ^2 is the overlapping parameter, if $\gamma^2 = 1$ the distribution in momentum space reduces to the normal one.

The gap equation at $T = T_c$ is the starting point. In this approach, an integral related to each band is obtained.

$$1 = \frac{\lambda}{2}\int_{\gamma^2 E_F - E_D}^{\gamma^2 E_F + E_D} \tanh\left(\frac{E - E_F}{2k_B T_c}\right)\frac{dE}{E - E_F} + \frac{\lambda}{2}\int_{(2\gamma^2-1)E_F}^{E_F} \tanh\left(\frac{E - E_F}{2k_B T_c}\right)\frac{dE}{E - E_F}, \tag{2}$$

where $\lambda = V_0 D(E)$ is the coupling parameter, with $D(E)$ the DOS of a bidimensional system. k_B is the Boltzmann constant, $E_F = (\hbar^2\pi/m)n_{2D}$, with n_{2D} the number of carriers per CuO_2 layer. The phonon-mediated effective interaction is considered to be a constant $V = V_0$ within a range of the order $E_D = \hbar\omega_D$ at E_γ, and zero elsewhere. Here E_D and ω_D are the Debye energy and the cutoff frequency for phonon-mediated superconductivity, respectively.

The integration in the surface at E_γ in the first band is restricted to states in the interval $E_\gamma - E_D \leqslant E_k \leqslant E_\gamma + E_D$. In the second band, in order to conserve the particle number, the integration is restricted to the interval $E_\beta = (2\gamma^2 - 1)E_F \leqslant E_k \leqslant E_F$, if $E_\gamma + E_D > E_F$, while $E_F - E_\gamma \leqslant E_D$ implies that the energy difference between the anomalously occupied states must be provided by the material itself. Then the overlapping parameter γ^2 must be in the range $\gamma_D^2 \leqslant \gamma^2 < 1$ where the minimum overlapping parameter $\gamma_D^2 = 1 - E_D/E_F$ is determined by the Debye limit. It means that the maximum overlapping is given by $1 - \gamma_D^2$.

After the integration, a relationship between λ and the characteristic parameters γ^2, T_c and T_F can be obtained for high-T_c compounds. It is possible to obtain a numerical exact solution or an approximate analytical expression for these integrals [10]. In any case a specific material must be selected to introduce the available experimental data. Ranges for the coupling parameter λ, and the overlapping parameter γ^2, consistent with the model and the experimental data, can be obtained for each material.

3. Results

In this work, characteristic properties of HTSC are evaluated. The two overlapping band model has been applied to describe HTSC with different number of layers [10]: however, in order to separate doping and intrinsic effects on T_c under pressure a system with only one kind of charge carriers in the CuO_2 layers must be considered, $n_{2D} = n_h$.

A systematic investigation of $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ was carried out by Liu [11]. They changed the charge carrier density n_h of the CuO_2 layers by adjusting the doping x. This system exhibits superconductivity over the entire range from $x = 0$ to 0.6. The maximum T_c is obtained at $x = 0.21$. Thus, samples at atmospheric pressure were available at different points on the $T_c(x)$ curve. Initially, the model proposed here is applied to study the behavior of this material with different doping.

The possible T_c values for this cuprate, from Eq. (2), that the model with two overlapping bands can predict at atmospherical pressure are calculated. In Fig. 1, T_c as function of λ in the weak coupling regime $\lambda \leqslant 0.58$ is shown. Different γ^2 values in the range $1 < \gamma^2 \leqslant \gamma_D^2$, for $n_{2D} = n_{hop} = 0.16$ [12], were considered. The continuous curve shows the relationship between T_c and λ, with maximum overlap, $\gamma^2 = \gamma_D^2 = 0.88$, for this carrier density. The other curves are calculated at intermediate overlaps, the small dashed curve with $\gamma^2 = 0.94$ and the large dashed one with $\gamma^2 = 0.96$. Consistent with the maximum experimental T_c value for $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$ obtained at atmospheric pressure we obtain, with all these overlapping parameters, a $T_c = 105$ K at $\lambda = 0.5, 0.52$ and 0.56, respectively. All the curves are strictly increasing with T_c: then for a given overlap the system requires bigger λ values to reproduce higher T_c values. From this figure it is

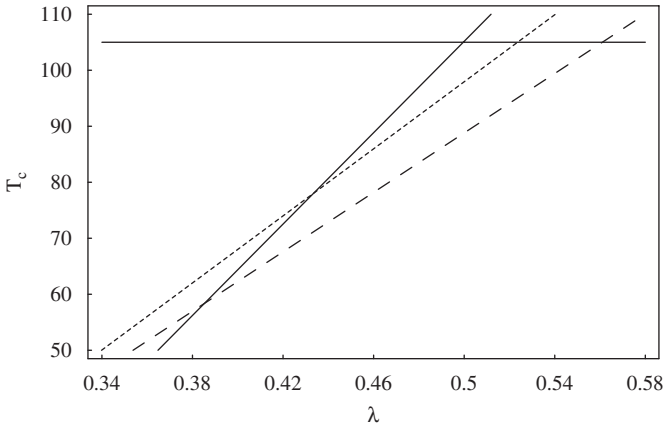

Fig. 1. T_c as a function of the coupling parameter λ, with $n_{2D} = 0.16$ for $Tl_{0.5}Pb_{0.5}Sr_2Ca_{1-x}Y_xCu_2O_7$. The continuous curve shows the results with $\gamma^2 = \gamma_D^2$. $T_c = 105$ K is obtained at $\lambda = 0.5$, consistent with the maximum experimental T_c value for this cuprate. The other curves, from top to bottom, are calculated with $\gamma^2 = 0.94$ and 0.96.