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Study of the Phase Diagram and the T_c Pressure Dependence for $HgBa_2CuO_{4-\delta}$ Superconductors

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We apply a method recently derived based on the extended Hubbard Hamiltonian to obtain the superconducting critical temperature dependence with carrier density of $HgBa_2CuO_{4-\delta}$. We show that this approach can be used to study the effects of pressure and reproduces for the first time the experimental data for the whole doping regime and their high and low pressure dependence.

One of the effects of the pressure on high T_c superconductors (HTSs) which is generally accepted is an increase of the carrier concentration on the CuO_2 planes transferred from the reservoir layers. Such pressure induced charge transfer (PICT) has been confirmed by Hall effect and thermoeletric power measurements in several compounds[1]. Therefore this effect was largely explored to account for the quantitative relation between T_c and the pressure P and gave origin to several models[2-4]. Some of these models also invoked that several HTSs have a T_c versus carrier density n (per CuO_2) diagram which satisfies a phenomenological universal parabolic curve, i.e., $T_c = T_c^{max}[1-\eta(n-n_{op})^2]$ where n_{op} is the optimum n. Following along these lines we can write $T_c = T_c(n,P)$ and easily derive an expansion in powers of P, namely

$$T_c(n,P) = T_c(n,0) + \alpha_1(n)P + \alpha_2(n)P^2 \qquad (1)$$

where the coefficients are,

$$\alpha_1(n) = \partial T_c(n)/\partial P - 2\eta T_c^{\max}(n-n_{op})\partial n/\partial P (2)$$

in which the first term is known as the intrinsic term and $\alpha_2(n) = -\eta T_c^{\max}(\partial n/\partial P)^2$. This simple method was very successful in describing the data in the vicinity of n_{op}[3] but fails to describe more recently set of data with a large variation of n values from underdoped to overdoped regime[1,5]. Futhermore this phenomenological approach does not give any indication of the physical origin of the intrinsic term.

We propose in this work some new ideas to interpret the effects of pressure. We apply a recently introduced method[7] based on a BCS type mean field analysis which uses the extended Hubbard Hamiltonian (t-U-V) on a square lattice.

In connection with this method we are led to propose that the effects of pressure are two-fold: (i)- The well accepted PICT; (ii)- The relation $2\Delta_0 = \gamma K_B T_c^{max}$ ($\gamma = 3.5$ for weakly BCS and $\gamma \approx 4.3$ for the method mentioned above) suggests a very definite effect of the pressure on Δ_0. This is equivalent to say that the structural modifications due to the applied pressure cause a variation on the attractive potential V (which is the most influencial parameter on the value of Δ_0).

The above assumptions can be simple written as $T_c = T_c(n,\Delta_0)$ and $\Delta_0 = \Delta_0(P)$. On Fig.1 we plot two curves to study how T_c changes with Δ_0. If we now perform an expansion of T_C in terms of P, we obtain terms up to the third order and each coefficient is given by

$$\alpha_Z = \left(\frac{\partial}{\partial\Delta_0}\frac{\partial\Delta_0}{\partial P} + \frac{\partial}{\partial n}\frac{\partial n}{\partial P}\right)^Z T_(n,\Delta_0) \qquad (3)$$

where $Z = 0,1,2$ and 3 is the order of the corresponding coefficient. We can derive simple analytical expressions for each coefficient in an approximate way, using the universal parabolic fitting and with $T_c^{\max}(P) = 2\Delta_0(P)/\gamma$ which explicits the T_c dependency on P (assumption ii). This procedure gives an intrinsic term which is radically different than that derived on the basis

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of the PICT alone as well as a new third order term.

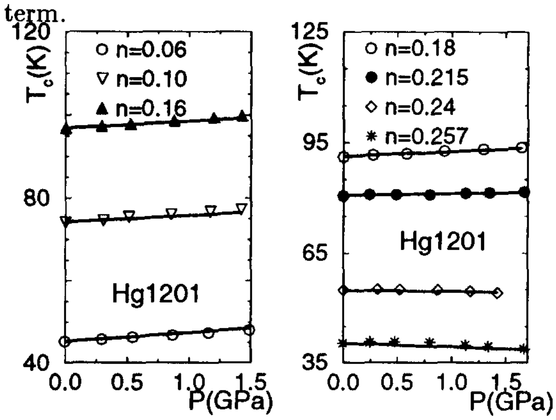

Fig.2a

Fig.2b

Figure 1. a) The lines are our calculations for the underdoped region in comparison with the experimental points of Ref.6. b) The same calculations for the overdoped region in comparison with the points of Ref.6.

We apply now the above general procedure to the low pressure results of Cao et al[5] for the Hg1201. Thus to compare with their data we fix the linear term at $n_{op} = 0.16$, $\alpha_1 = 1.85$K/GPa (which is equal to the intrinsic term and from this we determine $\partial\Delta_0/\partial P$) and at $n = 0.06$ we take $\alpha_1 = 2.6$K/GPa (the intrinsic term is then 0.9K/GPa and the charge transfer is equal 1.7K/GPa what gives $\partial n/\partial P = 1.8\mathrm{x}10^{-3}$). Thus the value that we obtain to $\partial n/\partial P$ is very close to other calculations [2,4] and in this way all the coefficients of Eq. (3) are determined. Far from n_{op} the charge transfer term dominates over the intrinsic one and the linear term decreases up to -1.0K/GPa (at $n = 0.26$) in the overdoped region. Our results for all densities n are in excellent agreement with the experimental data in both the underdoped and overdoped region, as shown on Figs.1a and 1b.

In Fig.2 we show the results for the high pressures measurements for the three family of compounds of mercury [10] at n_{op}. At the high pressures the quadratic and the cubic terms in the pressure expansion become important (for $P > 20$ GPa) and the agreement with the data is also remarkable. It is very interesting that the values obtained above at the low pressures yielded results with the maxima around 30GPa which is the value of highest T_c for a HTSs [10]. For the first time a simple theory is capable to describe successfully all this ensemble of data.

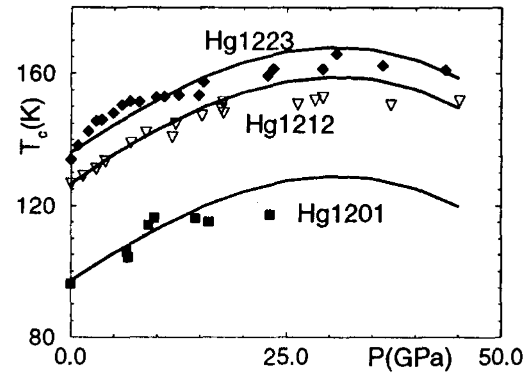

Fig.3

Figure 2. a) The high pressures data of Ref. 11 and our calculations (the continuous lines).

Thus, we conclude pointing out that our novel calculations (based on a BCS type mean field with the extended Hubbard Hamiltonian and $\Delta_0 = \Delta_0(P)$) demonstrate to be highly successful to describe the effects of the pressure with just two simple assumptions.

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