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Extended Hubbard model applied to study the pressure effects in high-temperature superconductors

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We make use of a BCS-type approach based on the extended Hubbard Hamiltonian to study the superconductor transition and to give a microscopic interpretation of the pressure effects on T_c in high-temperature superconductors. This method suggests that the applied pressure causes an increase of the superconducting gap and this effect is explored in order to explain the variations of T_c. Our approach is therefore beyond the scope of previous phenomenological models which basically postulate a pressure-induced charge transfer and an intrinsic term linear in pressure. We obtain a microscopic interpretation of this intrinsic term and a general expansion of T_c in terms of the pressure. To demonstrate the efficiency of the method we apply it to the experimental data of the Hg-based superconductors. [S0163-1829(97)07925-3]

I. INTRODUCTION

After the discovey of high-temperature superconductors (HTS's) it was realized that the critical temperature (T_c) could be substantially enhanced by applying high pressures. This very interesting effect attracted a lot of attention as it is summarized by several review articles which have been written on the subject.[1–3] The motivation for all this effort is not only the quest for higher temperatures but also to understand which are the parameters which optimize T_c besides the possibility of following the structural changes induced by pressure by means of x rays and neutron diffraction techniques. It is hoped that these investigations lead to the preparation of new materials by chemical substitution as well as some better insights into these highly complex systems.

One of the effects of the pressure which is generally accepted and well documented in certain materials[1–3] 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.[2] Therefore this effect combined with an assumption of an intrinsic variation of T_c (linear on the pressure) independent of the charge transfer was largely explored to account for the quantitative relation between T_c and the pressure P and gave the origin of many models.[4–8] Some of these models also invoked the fact that several HTS's have a T_c versus carrier density n (per CuO_2) diagram which satisfies a phenomenological universal parabolic curve, i.e., $T_c = T_c^{\max}[1-\eta(n-n_{\mathrm{op}})^2]$ where n_{op} is the optimum n. Following along these lines we can write $n(P)=n+\Delta n(P)$, $T_c=T_c(n,P)$ and derive an expansion in powers of P, namely,

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

where the coefficients are

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

and

$$\alpha_2(n)=-\eta T_c^{\max}(\partial n/\partial P)^2, \tag{2b}$$

where the first term in α_1 is known as the intrinsic term and it was estimated to be constant.[4–9] This approach was largely used in describing the data in the vicinity of n_{op},[2,6] but fails to describe more recently measurements on different compounds with a large variation on the initial n values from the underdoped to overdoped regime.[2,10] Furthermore, this phenomenological method does not provide any physical insight into the origin of the (charge-transfer-independent) intrinsic term.

II. METHOD AND APPROACH

We propose in this work some ideas which are general enough to be applied to any family of compounds and which provide some microscopic interpretation on the effects of pressure. We use as starting point a recently introduced approach[11] based on a BCS-type mean-field analysis which uses the extended Hubbard Hamiltonian (t-U-V) on a square lattice (of lattice parameter a),

$$H=-\sum_{\langle ij\rangle,\sigma} t(c_{i\sigma}^{\dagger}c_{j\sigma}+\mathrm{H.c.})+U\sum_i n_{i\downarrow}n_{i\uparrow}-V\sum_{\langle ij\rangle} n_i n_j\,. \tag{3}$$

For the sake of completeness we briefly outline the method. A gap equation at zero temperature is derived which has the same form as in the usual BCS theory, i.e.,

$$\Delta_{\vec{k}}=-\sum_{\vec{l}} V_{\vec{k}\vec{l}}\frac{\Delta_{\vec{l}}}{2(\xi^2_{\vec{l}}+\Delta^2_{\vec{l}})^{1/2}}, \tag{4}$$

where $\xi_{\vec{k}}=-4t[\cos(k_xa)+\cos(k_ya)]-\mu$, $V_{\vec{k}\vec{l}}$ is the Fourier transform of the potential of Eq. (3), which is approximately given by

$$V_{\vec{k}\vec{l}}\approx U-4V[\cos(k_x-l_x)a+\cos(k_y-l_y)a]. \tag{5}$$

As in the BCS mean-field method[11] the gap has the same functional form of the potential, namely, $\Delta_{\vec{k}}=\Delta_0[\cos(k_xa)$

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$\pm\cos(k_y a)]/2$, where the plus sign is for the s-wave and the minus sign is for d-wave channel. The chemical potential μ must be calculated self-consistently but as it concerns the superconducting phase boundary it suffices to approximate it by the value of the maximum energy (concentration dependent) in a tight-binding band. One then derives a finite-temperature analog of Eq. (4) and in order to determine the phase boundary we take $T=T_c$ at the limit where $\Delta_0=0$ is applied. The zero temperature and the finite temperature with $T=T_c$ gap equations are solved numerically and one matches T_c with Δ_0 for a given carrier concentration n. Thus one obtains a phase diagram $T_c\times n$ for a given Δ_0 which was found to reproduce well the experimental phase diagrams for the HTS's when the position of the attractive potential V was changed from the original nearest-neighbor position and became an adjustable parameter.[11] The ratio of U/V is not relevant to determine the phase diagram boundary as long as $U \gg V$, but on the other hand, it determines the value of Δ_0. The exact calculations of Δ_0 in terms of U and V are not easy to be performed in a many-body system and thus it becomes a second parameter to be determined by comparison with the experimental $T_c\times n$ phase diagrams. It was shown[11] that the chosen values for Δ_0 that reproduce the phase diagrams of the lanthanum and yttrium family of compounds are also in excellent agreement with the gap measurements taken from tunneling experiments and the specific heat. As concerns the ratio of the positions of V used for these families, it was also shown *a posteriori* that their values match their ratio of the coherence length (as discussed in Ref. 11, these are strongly coupled systems and the bound states are confined which is not the case with weakly coupled systems), thus providing a possible physical explanation for this quantity and why they are so different for the La and Y families of compounds.

In connection with the above discussion we are led to propose that the effects of pressure are twofold: (i) The well-accepted PICT and (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 that if $T_c^{\max}$ is a linear function of the pressure P (as assumed for the behavior of the intrinsic term[5–7]), then Δ_0 must also be a linear function of P. As concerns the Hamiltonian of Eq. (3) this is equivalent to saying that the structural modifications due to the applied pressure induce a variation on the attractive potential V (which is the most influencial parameter on the value of Δ_0). In fact the real effect of the structural changes can only be estimate by electronic band calculations,[2,3,12,13] but they are not adequate to be performed in the context of the strong correlations of the t-U-V Hamiltonian.

Thus the PICT (i) implies that $n(P)=n+\Delta n(P)$ and the assumption of a pressure dependent gap (ii) implies $\Delta_0(P)=\Delta_0+\Delta\Delta_0(P)$ which can be simple written as $T_c=T_c(n(P),\Delta_0(P))$. In Fig. 1 we plot two curves calculated with two differents values of Δ_0 to study how $T_c(n)$ change if the pressure induces a change in Δ_0. Therefore to estimate T_c of a compound with an initial given value of n and under a given pressure P, we perform an expansion of $T_c(n)$ in terms of P. With the assumption of linear variation of n and $T_c^{\max}$ (or Δ_0) on the pressure, we obtain only terms up to third order, that is,

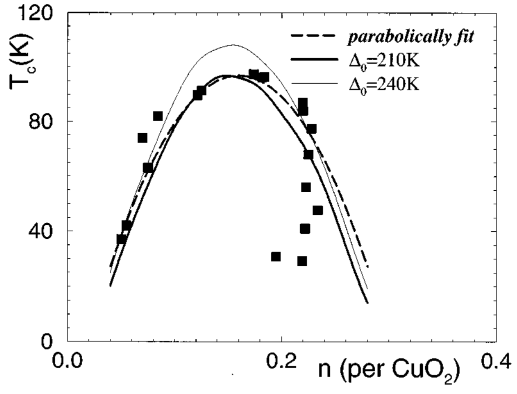

FIG. 1. The phase diagram for HgBa$_2$CuO$_{4-\delta}$. The squares are the experimental points of Ref. 6. Our best fitting with $\Delta_0=210$ K and the results with $\Delta_0=240$ K to illustrate the effect of changing this parameter.

$$T_c(n,P)=\sum_{Z=0}^{3}\alpha_Z P^Z, \tag{6a}$$

with

$$\alpha_Z=\left(\frac{\partial}{\partial\Delta_0}\frac{\partial\Delta_0}{\partial P}+\frac{\partial}{\partial n}\frac{\partial n}{\partial P}\right)^Z T_c(n(P),\Delta_0(P)). \tag{6b}$$

Furthermore, one 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 makes explicit the T_c dependence on P [assumption (ii)]. This procedure gives an intrinsic term which is radically different than that used before[4–8] as well as a new third-order term.

III. COMPARISON WITH THE EXPERIMENTS

To illustrate the entire method we will apply it to the mercury system. The mercury family of compounds represents a real challenge to any theory for the following reasons: (a) The highest transition temperatures obtained up to date have been measured on Hg1223 at 25–30 GPa,[14–17] reaching values up to 164 K. (b) The various pressure data for the underdoped and overdoped compounds of HgBa$_2$CuO$_{4-\delta}$ (Hg1201) could not be interpreted[10] by the models described in the Introduction. (c) The largest pressure effect on T_c with a change of almost 50 K over a span of 20 GPa has been recently measured by one of us[18] in Hg2212.

As a preliminary step and also in order to determine the initial parameters, we need to study the $T_c\times n$ phase diagram at zero pressure. Thus we perform a calculation using the method of de Mello[11] to obtain a Hg1201 phase diagram which is in agreement with the experimental results.[10] As discussed above this method of calculation involves two parameters; our best result is obtained with $\Delta_0=210$ K and the position of the attractive potential V at the sixth neighbor. Our results are plotted in Fig. 1 and, just for comparison and for future use, the phenomenological parabolic fitting with $\eta=50$ and $T_c^{\max}=97$ K as used by Cao *et al.*[10] Thus the calculation for the Hg family phase diagram is our first step and it is independent of the pressure studies which we will deal next.

To study the effects of the pressure we also plotted in Fig. 1 our calculation for the phase diagram with $\Delta_0 = 240$ K. We see that near $n_{\mathrm{op}} = 0.16$ the variations of T_c with respect to Δ_0 are almost twice as those at the extremes (low T_c), and since this is the origin of the intrinsic term, it also varies in the same way and this behavior will be discussed below. It is important to notice that the two partial derivatives that appear in Eq. (6b) become two parameters to be determined by comparing with the $T_c \times P$ measurements for two compounds with different charge density n. At low pressures only the linear terms α_1 comes into play since the higher-order coefficients are negligible. It is desirable (but not crucial) to start with $n = n_{\mathrm{op}}$ to determine $\partial \Delta_0 / \partial P$ since at n_{op} the charge transfer term vanishes. So with other sets of $T_c \times P$ data at another value of $n \neq n_0 p$, we determine $\partial n / \partial P$. After these two parameters being determined we can apply the expansion Eq. (6a) to any other compound with different value of n.

To illustrate the above general procedure, we will apply it to the low-pressure results of Cao *et al.*[10] for Hg1201 and those of higher pressures of Gao *et al.*[16] Our purpose is to show that we can describe all their results with a single choice of parameters. Thus to obtain the value of the two partial derivatives of Eq. (6b) pertinent to their measurements we do the following: We start with the set of data taken with the compound with $n_{\mathrm{op}} = 0.16$, which has a $T_c \times P$ curve at low pressures that is a straight line and from which we can infer that the linear term $\alpha_1 = 1.85$ K/GPa, which at n_{op} is equal to the intrinsic term, and from this we determine $\partial \Delta_0 / \partial P$. To determine the other partial derivative we study the $T_c \times P$ plot made with the sample with $n = 0.06$. We see that the low-pressure slope (α_1) can be taken as $\alpha_1 = 2.6$ K/GPa. At $n = 0.06$ the intrinsic term is half of that at n_{op} according to the discussion in the above paragraph, and therefore the intrinsic term is 0.9 K/GPa and then the charge transfer must be equal to 1.7 K/GPa since the sum of both terms is equal to α_1. Using now the explicit expression for α_1 with the parabolic fitting with $T_c^{\max} = 97$ K and $\eta = 50$ we can derive that $\partial n / \partial P = 1.8 \times 10^{-3}$ holes/GPa. We notice that this value that we obtain for $\partial n / \partial P$ is very close to other estimations.[5,7,18,9] Thus with this procedure the two derivatives which are derived in the calculations of the coefficients of Eq. (6b) are determined and we are set now to apply Eq. (6a) to any Hg compound. Far from n_{op} the charge transfer term dominates over the intrinsic one and thus the linear term α_1 varies from the 2.6 K/GPa chosen above at $n = 0.06$ up to -1.0 K/GPa (at $n = 0.26$) in the overdoped region. The results of our calculations for all other compounds with different densities n are in excellent agreement with the low-pressure experimental data in both the underdoped and overdoped regimes and are plotted on Figs. 2(a) and 2(b). In Fig. 3 we show the results for the high pressure measurements for the three families of mercury[16] at n_{op}. As one can see in Fig. 3 at 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 parameters obtained above at the low pressure yielded results with the maxima around 30 GPa which is the value of highest T_c for a HTS's.[16] Our results can also be applied to other measurements on differents families and compounds of Hg which, at n_{op}, also yielded the T_c maxima around 30 GPa.[17] This simple theory is capable of describing successfully entire this ensemble of low- and high-pressure data and furthermore provides some insight into the microscopic effects of the pressure.

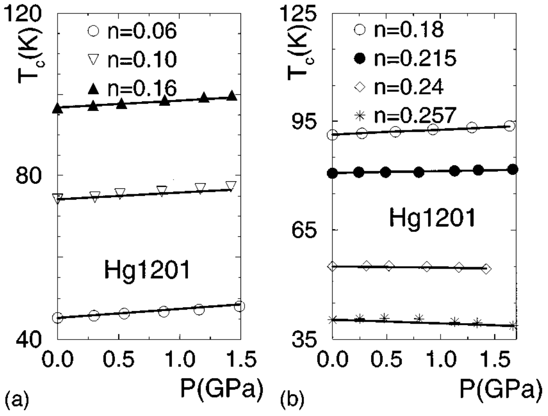

FIG. 2. (a) The lines are our calculations for the underdoped region in comparison of the experimental points of Ref. 10. (b) The same calculations for the overdoped region in comparison of the experimental points of Ref. 10.

IV. CONCLUSIONS

Thus, we conclude by pointing out that our calculations (based on a BCS-type mean field with the extended Hubbard Hamiltonian) are demonstrated to be highly successful to describe the effects of pressure with just two simple assumptions. The PICT which is well accepted and that of the pressure-induced variation of the superconductor gap which was introduced, to our knowledge, in this work. We hope that this assumption can be confirmed in the future by *in situ* experiments like specific heat and tunneling measurements. We recently learned about the work of Angilella *et al.*[19] which also uses the extended Hubbard model within a BCS-type approach. Furthermore they estimate the effects of the

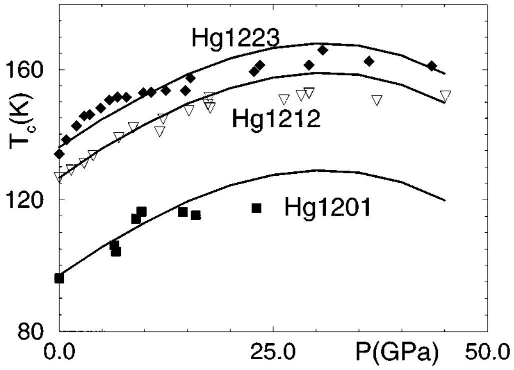

FIG. 3. The high-pressure data of Ref. 16 and our calculations (solid lines) described in the text.

pressure on the attractive potential V which goes along with the lines of our assumption over Δ_0. They also obtained very good results for the effects of pressure in the Bi2212 family, given more support to the BCS mean-field calculations with the extended Hubbard calculation as a model for the physics of the charge carriers in the HTS's.

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