Interplay among critical temperature, hole content, and pressure in the cuprate superconductors

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Within a BCS-type mean-field approach to the extended Hubbard model, a nontrivial dependence of T_c on the hole content per unit CuO_2 is recovered, in good agreement with the celebrated nonmonotonic universal behavior at normal pressure. Evaluation of T_c at higher pressures is then made possible by the introduction of an explicit dependence of the tight-binding band and of the carrier concentration on pressure P. Comparison with the known experimental data for underdoped Bi2212 allows us to single out an ''intrinsic'' contribution to dT_c/dP from that due to the carrier concentration, and provides a remarkable estimate of the dependence of the intersite coupling strength on the lattice scale. [S0163-1829(96)02445-9]

I. INTRODUCTION

The comparison between superconductive and normal state properties of the high-temperature superconductors often unveils quite remarkable features in their phenomenology, thus helping in establishing most of the known universal behaviors. Among them, the nontrivial dependence of the critical temperature T_c on the hole content ρ per unit CuO_2 is probably the most celebrated.[1,2]

To that purpose, high-pressure data provide a natural tool to investigate the correlations existing between the main superconductive properties and the structural properties, such as the relevant lattice anisotropy, thus allowing one to single out the role of the carrier concentration.[3–5]

Unfortunately, earlier experimental works did not help in setting up a homogeneous picture of the problem, possibly due to an uncareful analysis of the data coming up from samples, often characterized by uneasily reproducible features, such as the hole content, when even a slight presence of impurities has been proved to influence dramatically the behaviour under pressure.[6]

Nowadays there is a general conviction that pressure P may affect T_c, both changing the hole content ρ, which is evidenced by Hall resistance measurements,[7,8] and in an ''intrinsic'' way, mainly due to a lattice rearrangement induced by pressure. Quantitatively, the latter statement can be summarized by assuming $\rho=\rho(P)$ and $T_c=T_c(\rho,P)$, which yields[9,10]

$$\frac{dT_c}{dP}=\frac{\partial T_c}{\partial P}+\frac{\partial T_c}{\partial \rho}\frac{d\rho}{dP}. \tag{1}$$

Since, for the majority of the compounds, Hall resistance measurements under pressure suggest that $d\rho/dP>0$,[11] the different signs in dT_c/dP observed in different compounds may be explained as the result of a competition between the intrinsic contribution $\partial T_c/\partial P$ and the known dependence of T_c on ρ, through its pressure-induced change $\partial T_c/\partial \rho$, which may be negative or positive for underdoped or overdoped samples at normal pressure, respectively. Different trends of T_c as a function of P have been actually reported for several cuprate superconductors.[5] In particular, high pressure can improve T_c up to an ''optimal'' value ($dT_c/dP\geqslant 0$) and then decrease it down to lower values ($dT_c/dP<0$). By the way, possible extrinsic microscopic mechanisms have been recently devised, in order to describe the pressure dependence of the carrier concentration, especially due to oxygen-ordering effects, e.g., in Tl-based cuprates.[12–14]

The theoretical implications of such a pressure-dependent T_c and of such a wide range in the values of dT_c/dP have been often considered mainly as checks to known theories,[15–17] though they are still inconclusive both on the nature of the condensate pairs and on the nature and strength of their coupling interaction.[18]

In this paper, we shall address our attention to the generalization at high pressures of a mean-field approach to a system of interacting fermions. In Sec. II, we shall outline the model and the mean-field approach at normal pressure ($P=0$). The choice of a well-established tight-binding dispersion relation for the carriers will make us able to reproduce the observed dependence of T_c on ρ, allowing a direct comparison, e.g., with the experimental data available for Bi2212.[19] In Sec. III, we shall generalize such an approach to the case of an applied external pressure ($P\neq 0$). Reasonable pressure dependences will be obtained both for the band parameters and for the carrier concentration. A comparison with available experimental data for T_c under pressures $P\leqslant 1.6$ GPa in underdoped Bi2212 (Ref. 20) will be presented, which will permit us to separate the two contributions to dT_c/dP in Eq. (1). Besides, a nontrivial dependence on pressure (and therefore on the lattice scale) will be derived for the intersite coupling strength, thus suggesting a non-negligible lattice influence on the superconductive properties of the electronic system. We shall eventually summarize and address our conclusions in Sec. IV.

II. MEAN-FIELD APPROACH AT NORMAL PRESSURE

A. Model

At normal pressure ($P=0$), in order to describe the interacting Fermi liquid of the hole-type carriers in an anisotropic lattice, we adopt an extended Hubbard Hamiltonian

TABLE I. Lattice parameters (Ref. 21) isothermal compressibilities (Ref. 37); and band parameters (Refs. 29 and 30) for Bi2212 at normal pressure ($P=0$).

a_x	a_y	a_z	[Å]
5.414	5.418	30.89	
κ_x	κ_y	κ_z	κ_V	$[10^{-3}\ \mathrm{GPa}^{-1}]$
4.3	4.3	8.3	16.6	
t_x	t_y	t_z	t_{xy}	$[e\mathrm{V}]$
0.05	0.05	0.005	0.0225	

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

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is a fermionic creation (annihilation) operator on the lattice site i, with spin projection $\sigma\in\{\uparrow,\downarrow\}$ along a specified direction, and $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ is the density operator on site i. In Eq. (2), t_{ij} denotes the hopping integral between the lattice sites $\langle\langle ij\rangle\rangle$, located at the positions $\boldsymbol{R}_i$ and $\boldsymbol{R}_j=\boldsymbol{R}_i+\boldsymbol{\delta}_2$, respectively, with $\boldsymbol{\delta}_2$ spanning over the vectors connecting a given site i to its nearest-neighbor and in-plane next-nearest-neighbor sites j ($t_{ij}\equiv t_{\boldsymbol{\delta}_2}$, for translational invariance), and U measures the on-site interaction, while V_{ij} describes the interaction between in-plane nearest-neighbor sites $\langle ij\rangle$, separated by the vectors $\boldsymbol{\delta}_1$ ($V_{ij}\equiv V_{\boldsymbol{\delta}_1}$).

Using the standard transformation to the momentum representation

$$c^{\dagger}_{\boldsymbol{k}\sigma}=\frac{1}{\sqrt{N}}\sum_{i} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}c^{\dagger}_{i\sigma}, \quad (3)$$

N being the total number of lattice sites, the Hamiltonian (2) takes the form

$$H=\sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}+\frac{U}{N}\sum_{\substack{\boldsymbol{kpq}\\ n}} c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{\boldsymbol{p}\downarrow}c_{\boldsymbol{p}-\boldsymbol{q}\uparrow}c_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{G}_n\downarrow} + \frac{1}{N}\sum_{\substack{\boldsymbol{kpq}\\ \sigma\sigma' n}} \widetilde{V}_{\boldsymbol{q}}c^{\dagger}_{\boldsymbol{k}\sigma}c^{\dagger}_{\boldsymbol{p}\sigma'}c_{\boldsymbol{p}-\boldsymbol{q}\sigma'}c_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{G}_n\sigma}, \quad (4)$$

where

$$\varepsilon_{\boldsymbol{k}}=\sum_{\boldsymbol{\delta}_2} t_{\boldsymbol{\delta}_2}e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_2} \quad (5)$$

is the dispersion relation for the free carriers, in the tight-binding approximation, and

$$\widetilde{V}_{\boldsymbol{q}}=\sum_{\boldsymbol{\delta}_1} V_{\boldsymbol{\delta}_1}e^{i\boldsymbol{q}\cdot\boldsymbol{\delta}_1} \quad (6)$$

is the Fourier transform of the nearest-neighbors intersite interaction potential V_{ij}. In Eq. (4), the sums over momenta run over the first Brillouin zone [i.e., $-\pi\leqslant k_i a_i<\pi$, $i=x,y,z$, for the momentum $\boldsymbol{k}$, a_i being the spacings of an orthorhombic (nearly tetragonal) lattice (Table I for Bi2212) (Ref. 21)], and momentum conservation is enforced up to a vector $\boldsymbol{G}_n$ of the reciprocal lattice.

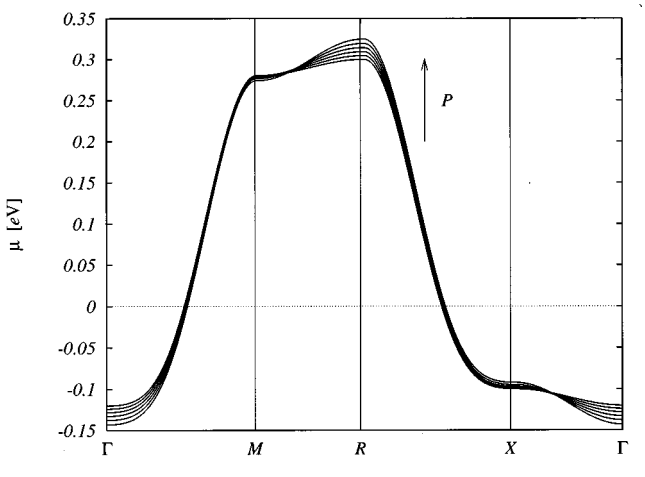

FIG. 1. Band dispersion, Eq. (7), along a symmetry contour of the first Brillouin zone of a simple cubic lattice. The different solid lines refer to increasing pressure, $P=0-20$ GPa. Due to the lattice anisotropic structure, a weaker dispersion is recognized along the directions M-R, X-Γ, parallel to the z axis, which remarkably increases by increasing pressure.

A few comments are now in order about the free dispersion relation, Eq. (5), and the interaction terms in the Hamiltonian, Eq. (4).

Detailed band structure calculations indicate that the layered pattern of the cuprate oxides is reflected in the charge density surrounding their lattice sites.[21–23] Such density exhibits a quasibidimensional arrangement, which closely follows the rich orbital structure of the Cu and O ions.[24] This behavior suggests a strong degree of hybridization along the bond directions. The intermediate oxygens therefore provide suitable bridgings between two nearest-neighbor coppers, thus favoring directional charge transport. A quite complex band structure results, almost dispersionless in the symmetry direction orthogonal to the Cu-O planes (Fig. 1). Such a band structure gives rise to exotic Fermi surfaces, which exhibit quasicylindrical shapes, at typical fillings.[25]

A tight-binding approximation to the band dispersion relation can be employed up to an arbitrary degree of accuracy, by including a suitable number of $\boldsymbol{k}$ harmonics.[26,27] Equation (5) restricts to the lowest orders and yields the model dispersion relation[25,28–30]

$$\varepsilon_{\boldsymbol{k}}=-2t_x\cos(k_xa_x)-2t_y\cos(k_ya_y) +4t_{xy}\cos(k_xa_x)\cos(k_ya_y)-2t_z\cos(k_za_z)-\mu, \quad (7)$$

where μ denotes the Fermi level. The hopping parameters t_x, t_y, t_z, and t_{xy} have been evaluated by comparison with the available angle-resolved photoemission spectra[31,32] (ARPES) for the observed dispersion and Fermi surface (Refs. 21,27,29,30) and (Table I). In particular, providing t_z with a nonzero, though small ($t_z\ll t_x,t_y$) value, i.e., assuming a true, three-dimensional dispersion function $\varepsilon_{\boldsymbol{k}}$, ensures against the awkward occurrence of van Hove singulari-

ties. Figure 1 displays Eq. (7) along a symmetry contour of the first Brillouin zone for increasing pressure P (cf. *infra*).

Since only states next to the Fermi surface do significantly contribute to the sums in the interaction terms of Eq. (4), only the terms with $\boldsymbol{G}_n=0$, $\boldsymbol{k}+\boldsymbol{p}=0$ can be safely retained. This eventually simplifies the Hamiltonian, Eq. (4), as

$$H=\sum_{k\sigma}\ \varepsilon_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}+\frac{1}{N}\sum_{\boldsymbol{k}\boldsymbol{k}'}\ V_{\boldsymbol{k}\boldsymbol{k}'}c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{-\boldsymbol{k}\downarrow}c_{-\boldsymbol{k}'\downarrow}c_{\boldsymbol{k}'\uparrow}, \tag{8}$$

where $V_{\boldsymbol{k}\boldsymbol{k}'}$ includes the on-site interaction term and the restriction to the singlet channel only of the intersite interaction,[33]

$$V_{\boldsymbol{k}\boldsymbol{k}'}=U+\tfrac{1}{2}(\widetilde{V}_{\boldsymbol{k}-\boldsymbol{k}'}+\widetilde{V}_{\boldsymbol{k}+\boldsymbol{k}'}), \tag{9}$$

which takes on the ''separable'' form

$$V_{\boldsymbol{k}\boldsymbol{k}'}=U+2V\cos(k_xa_x)\cos(k'_xa_x)+2V\cos(k_ya_y)\cos(k'_ya_y), \tag{10}$$

where a symmetric intersite coupling constant V has been assumed along both directions in the Cu-O planes.

Such an interaction does not refer to any particular pairing mechanism, and therefore does not require any particular nature of the couples. However, experimental indications on the momentum dependence of the gap function, although still questioned, clearly suggest an intermediate range for the effective (renormalized) interaction between the carriers in the cuprate planes. In particular, at least an intersite attractive term is required, in order to allow for a gap which displays the observed nodes in the $\boldsymbol{k}$ space. Besides, the competition between an attractive effective intersite V and a repulsive effective on-site U is expected to rule on the actual onset of superconductivity and the opening of a gap. For our purposes, it is safe to retain only the on-site and intersite terms in the interaction, although other phenomenological properties of the cuprates may suggest different functional forms for $\widetilde{V}_{\boldsymbol{q}}$.[34]

B. Approach

In order to study the possibility for the Hamiltonian, Eq. (8), to give rise to a superconducting instability, a BCS-type mean-field approximation can be employed. The superconducting condensate is then characterized by an auxiliary gap field, which at finite temperature T obeys the BCS-type self-consistent, nonlinear equation

$$\Delta_{\boldsymbol{k}}=-\frac{1}{N}\sum_{\boldsymbol{k}'}\ V_{\boldsymbol{k}\boldsymbol{k}'}F_{\boldsymbol{k}'}, \tag{11}$$

where

$$F_{\boldsymbol{k}}=\frac{\Delta_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}}\tanh\frac{E_{\boldsymbol{k}}}{2T},\quad E_{\boldsymbol{k}}=\sqrt{\varepsilon^2_{\boldsymbol{k}}+\Delta^2_{\boldsymbol{k}}}, \tag{12}$$

and where we set Boltzmann's constant $k_B=1$. At the same degree of approximation, the density of carriers ρ is correspondingly given by[33]

$$\rho(\mu,T)=\frac{1}{2N}\sum_{\boldsymbol{k}}\ \left(1-\frac{\varepsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\tanh\frac{E_{\boldsymbol{k}}}{2T}\right), \tag{13}$$

with $0\leqslant\rho\leqslant1$. Although a mean-field approach could be generally questioned, since it does not take into account the ''correlations,'' nonetheless it proved itself a very useful approximation even in the case of non separable potentials.[34] Besides, standard diagrammatic techniques (though perturbative in nature) have been recently employed in order to evaluate the corrections to the gap due to the correlations in a simplified version of the model here employed.[35] Such corrections, however, show up to be negligible in the strong coupling limit.

Due to the separable form of the potential, Eq. (10), direct inspection yields

$$\Delta_{\boldsymbol{k}}=\Delta_0+2\Delta_x\cos(k_xa_x)+2\Delta_y\cos(k_ya_y), \tag{14}$$

Δ_0, Δ_x, and Δ_y being real constants satisfying the following set of nonlinear, coupled equations:

$$\Delta_0+U\langle\Delta_{\boldsymbol{k}}\rangle=0, \tag{15a}$$

$$\Delta_x+V\langle\Delta_{\boldsymbol{k}}\cos(k_xa_x)\rangle=0, \tag{15b}$$

$$\Delta_y+V\langle\Delta_{\boldsymbol{k}}\cos(k_ya_y)\rangle=0, \tag{15c}$$

where

$$\langle f_{\boldsymbol{k}}\rangle=\frac{1}{N}\sum_{\boldsymbol{k}}\ \frac{f_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}}\tanh\frac{E_{\boldsymbol{k}}}{2T}. \tag{16}$$

The invariance property $\Delta_{\boldsymbol{k}}=\Delta_{-\boldsymbol{k}}$ follows again from the restriction of the intersite interaction Eq. (10) to the singlet channel only.

Setting

$$\Delta_{\pm}=\tfrac{1}{2}(\Delta_x\pm\Delta_y), \tag{17}$$

and forming the linear combinations

$$S_{\boldsymbol{k}}=\cos(k_xa_x)+\cos(k_ya_y), \tag{18a}$$

$$D_{\boldsymbol{k}}=\cos(k_xa_x)-\cos(k_ya_y), \tag{18b}$$

the gap function can be reexpressed as

$$\Delta_{\boldsymbol{k}}=\Delta_0+2\Delta_+S_{\boldsymbol{k}}+2\Delta_-D_{\boldsymbol{k}}. \tag{19}$$

One may observe that the two sets of $\boldsymbol{k}$ functions $\{1,\ S_{\boldsymbol{k}}\}$ and $\{D_{\boldsymbol{k}}\}$ belong to two irreducible representations of the group of rotations in the (k_x,k_y) plane. In other words, one has $\Delta_{\boldsymbol{k}}=\Delta^s_{\boldsymbol{k}}+\Delta^d_{\boldsymbol{k}}$ where $\Delta^s_{\boldsymbol{k}}=\Delta_0+2\Delta_+S_{\boldsymbol{k}}$ and $\Delta^d_{\boldsymbol{k}}=2\Delta_-D_{\boldsymbol{k}}$, which explicitly display s-wave and d-wave symmetry character, respectively. Besides, all the dependence of $\Delta_{\boldsymbol{k}}$ on temperature T and on the chemical potential μ is given by the set of the three parameters Δ_0, $\Delta_\pm$, whose relative value fix the overall symmetry pattern.

At zero temperature, and in the limiting case of $U=0$ ($\Delta_0=0$), Spathis *et al.*[36] found that Eqs. (15) can account for s ($\Delta_x=\Delta_y$) and d ($\Delta_x=-\Delta_y$), as well as mixed s-d ($|\Delta_x|\neq|\Delta_y|$) gap symmetry, depending on the position of the Fermi level within the band. However, at the critical point ($T=T_c$), no symmetry mixing is allowed,[25] and two cases are possible: (i) $\Delta_-=0$, and $\Delta_0,\Delta_+\to0$ as $T\to T_c$ (s wave); (ii) $\Delta_0,\Delta_+=0$, and $\Delta_-\to0$ as $T\to T_c$ (d wave). Therefore, if one lowers T at a fixed chemical potential, one expects to observe first a transition towards a superconducting state,

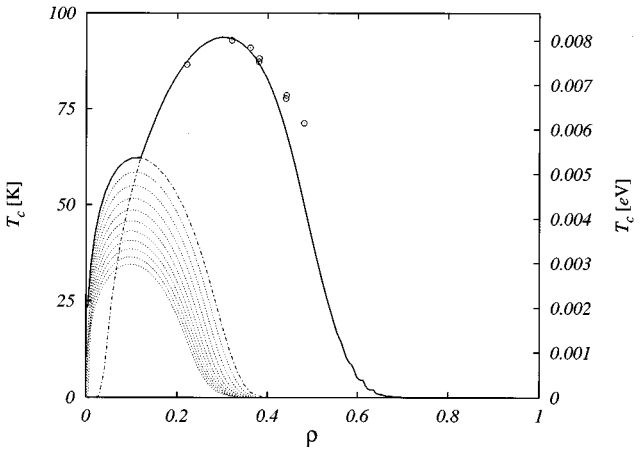

FIG. 2. Critical temperature T_c (solid line) and crossover temperature towards gap symmetry mixing (dashed-dotted line) vs hole content ρ at $P=0$. The effect of increasing $U=0.0$ to $-V$ is also shown on the T_c corresponding to s-wave gap (dotted lines). By increasing U, one observes a decrease of T_c at fixed ρ. The circles are experimental data obtained by Allgeier and Schilling (Ref. 19) for Bi2212.

characterized by a gap function of definite symmetry, which can eventually evolve towards a mixed symmetry state, as T lowers down to zero.

In either case, at $T=T_c$, it is possible to linearize Eqs. (15) with respect to Δ_0, $\Delta_\pm$. A condition for the existence of a nontrivial solution is then easily found to be

$$(1+V\langle D_{\boldsymbol{k}}^2\rangle_c)[(1+U\langle 1\rangle_c)(1+U\langle S_{\boldsymbol{k}}^2\rangle_c)-UV\langle S_{\boldsymbol{k}}\rangle_c^2]=0, \tag{20}$$

where

$$\langle f_{\boldsymbol{k}}\rangle_c=\lim_{T\to T_c}\langle f_{\boldsymbol{k}}\rangle=\frac{1}{N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}}}{2\varepsilon_{\boldsymbol{k}}}\tanh\frac{\varepsilon_{\boldsymbol{k}}}{2T_c}. \tag{21}$$

For fixed values of the coupling constants U, V and of the chemical potential μ, Eq. (20) yields, in general, two solutions for T_c. The larger one is easily interpreted as the temperature below which a superconductive gap opens (with definite symmetry), and the other as the temperature below which the gap symmetry mixing occurs. Moreover, one of the two temperatures is clearly not affected by the presence of a nonzero on-site coupling, U.

Figure 2 displays T_c vs ρ, consistently obtained through Eq. (13), corresponding to the values $V\approx -0.052$ eV and $U=0.0$ to $-V$ of the coupling parameters, obtained by comparison with the available experimental data for Bi2212.[19]

As can be seen, an s-wave gap opens at very low values of the hole content ρ, corresponding to low critical temperatures, whereas a d-wave gap is preferred near the optimal doping and beyond. As expected, the on-site repulsion acts against the intersite attraction with respect to the onset of superconductivity: By increasing U at constant V, one observes a decrease of T_c (Fig. 2), although the influence of U is restricted only to the solution of Eq. (20) corresponding to an s-wave gap. As a consequence of symmetry, the on-site interaction U does not affect the d-wave solution for the gap (see also Ref. 25 for a full discussion). However, as Fig. 2 clearly shows, the comparison with the experimental results obtained by Allgeier and Schilling in Ref. 19 is reasonable only for the solution of Eq. (20), which corresponds to the opening of a d-wave gap. We can therefore safely restrict ourselves to that case in the following.

The nontrivial dependence of T_c on the holelike carrier concentration is clearly nonmonotonic, and correctly reproduces the qualitative universal behavior experimentally observed in the cuprates.[1,2]

III. GENERALIZATION TO NONZERO PRESSURE

The mean-field approach thus far described can be straightforwardly generalized when a nonzero pressure P is applied. The effect of a pressure increase is threefold, involving both the lattice and the carriers, either directly or indirectly: (i) It decreases the lattice spacings and may distort the lattice itself, resulting in structural phase transitions; (ii) it increases the carrier concentration ρ; (iii) in oxygen-doped cuprates, it may induce oxygen ordering, through a rearrangement of the excess ions into and from the Cu-O planes.[12–14]

At a given pressure P, the following nonzero (positive) components of the isothermal compressibility tensor and of the isothermal volume compressibility may be defined:

$$\kappa_i=-\frac{1}{a_i}\left(\frac{\partial a_i}{\partial P}\right)_T, \quad \kappa_V=-\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T \tag{22}$$

$(i=x,y,z)$, $V=a_xa_ya_z$ being the volume of an elementary cell. Experimental values for κ_i and κ_V are listed in Table I for Bi2212.[37] Since they are almost constant over a quite wide range of pressure, and since $\kappa_x\simeq\kappa_y$ (within the experimental error), we may neglect transitions from the tetragonal to the orthorhombic structure. Under such assumptions, at the lowest order in P the lattice parameters are seen to obey a linear law

$$a_i(P)=a_i(0)[1-\kappa_iP], \tag{23}$$

which will be later used to parametrize the dependence of the lattice spacings on pressure P.

Since $\kappa_i\approx 10^{-3}$ GPa^{-1} (Table I), the lattice spacings keep their magnitude of several angstroms, typical of the cuprates, even at high pressures, so that one may neglect the contribution to the band structure given by the ionic core orbitals also at high pressures. We may therefore keep unchanged the $\boldsymbol{k}$ dependence of the tight-binding approximation to the dispersion relation, Eq. (7), provided that a pressure dependence is attributed to the hopping parameters t_i and t_{xy}. Charge density calculations at normal pressure suggest a very simple linear combination of atomic orbitals (LCAO) picture,[21–23] in which the hopping parameters are simply proportional to the overlap integrals between the main atomic orbitals involved in the formation of the bonds between copper and oxygen sites. The latter integrals can be easily worked out analytically as functions of the lattice separations (see the Appendix for details). Normalizing their values to those established at normal pressure, Table I, and making use of Eq. (23), we eventually obtain a pressure-dependent band dispersion relation. Figure 1 displays the dispersion relation $\varepsilon_{\boldsymbol{k}}$, Eq. (7), along a symmetry contour of the first Brillouin zone,

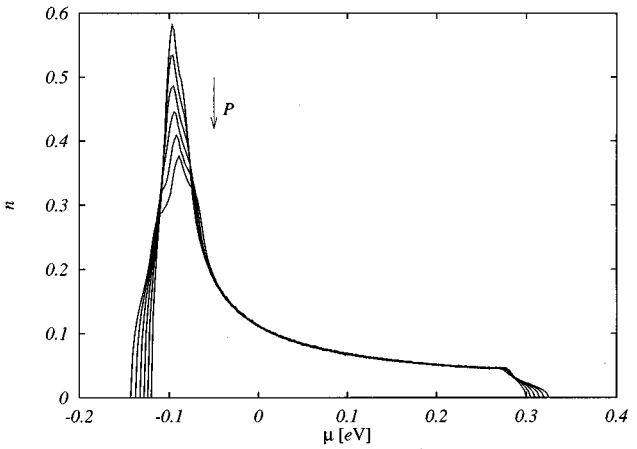

FIG. 3. Density of states as a function of the Fermi level μ, $\mu_\perp \leqslant \mu \leqslant \mu_\top$. By increasing pressure $P=0.0$ –20.0 GPa, the band widens, while the DOS peak lowers.

showing an increasing dispersive behavior in the direction orthogonal to the Cu-O planes as P increases. Figure 3 shows the densities of states (DOS)

$$n(\mu)=\sum_{\boldsymbol{k}} \delta(\varepsilon_{\boldsymbol{k}}-\mu), \tag{24}$$

computed correspondingly as functions of the Fermi level. As can be seen, within this simple model, an applied pressure widens the band extension, decreasing its bottom $\mu_\perp$ and increasing its top $\mu_\top$, and therefore lowers the height of what would have been a true van Hove singularity, so to keep n normalized to unity,

$$\int_{\mu_\perp}^{\mu_\top} n(\mu)d\mu=1. \tag{25}$$

The presence of such a large peak is mainly due to the quasibidimensional character of the perovskite compounds, and it is confirmed both by ARPES measurements[31,32] and by band structure calculations.[29,30] Its relevance with respect to the phenomenological properties of the high-T_c superconductors has been recently underlined.[38] In particular, an antiferromagnetic–van Hove (AFvH) theoretical picture[39,40] suggests a link between the presence of a large peak in the DOS and the existence of an optimal value of T_c at a small hole content.[41] Since pressure decreases the height of the DOS peak, that optimal hole content is expected to increase, which is actually what we observed plotting T_c vs ρ, for increasing values of pressure.

Let us now turn to the pressure dependence of the hole content. Making the usual assumption that all the charge carriers are localized within the Cu-O planes, one may identify the Hall resistance as $R_H=V/(ze\rho)$, where e is the elementary charge and z the number of Cu ions within a unit cell of volume V. Equations (22) then promptly yield

$$\kappa_\rho=\frac{1}{\rho}\left(\frac{\partial\rho}{\partial P}\right)_T=\kappa_H-\kappa_V, \tag{26}$$

where

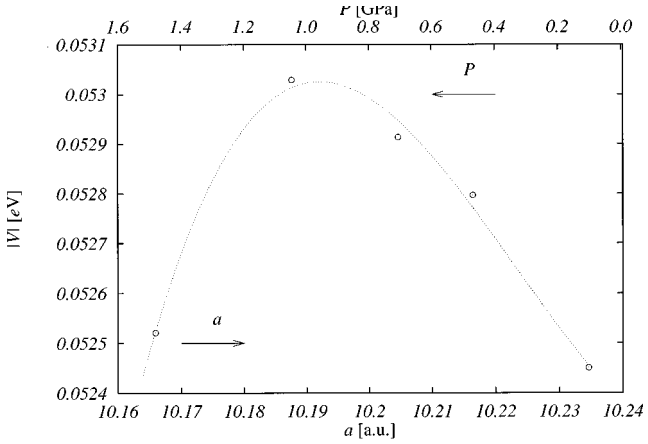

FIG. 4. The absolute value of the intersite coupling strength, $|V|$, as a function of the in-plane lattice spacing $a=a_x\simeq a_y$ (bottom scale) and of pressure P (top scale). The circles make directly reference to the experimental values (P,T_c) given by Huang *et al.*, (Ref. 20) while the dashed line has been evaluated by a standard best-fit procedure. (cf. also Fig. 5).

$$\kappa_H=-\frac{1}{R_H}\left(\frac{dR_H}{dP}\right)_T. \tag{27}$$

Therefore, at the lowest order in P,

$$\rho(P)=\rho(0)[1+\kappa_\rho P]. \tag{28}$$

However, one usually finds $\kappa_H>\kappa_V$, so that $\kappa_\rho>0$ for the majority of compounds. For underdoped Bi2212, Huang *et al.*[20] find $\kappa_H=+0.08$ GPa^{-1}, so that $\kappa_\rho=+0.0634$ GPa^{-1}.

In summary, Eq. (28) fixes the hole content ρ at the pressure P, given its value $\rho(0)$ at normal pressure $(P=0)$. The knowledge of the lattice spacings, Eq. (23), and of the band parameters as a function of P yields a model P-dependent band dispersion, giving rise to a flattened DOS (Fig. 3). The inversion of Eq. (13) then allows one to evaluate the corresponding chemical potential μ, while Eq. (20) eventually yields the critical temperature T_c as a function of the coupling parameters U and V. At this stage, we may leave the latter as free, and determine it in order to fit the known experimental dependence of T_c on P. Restricting to d-wave symmetry, Eq. (20) yields

$$V=-\frac{1}{\langle D_{\boldsymbol{k}}^2\rangle_c} \tag{29}$$

as a function of the critical temperature T_c. Of course, nothing can be said about U, since its value does not affect the d-wave solution for the gap.

Figure 4 displays V, Eq. (29), vs a_x, Eq. (23), evaluated in correspondence to the five experimental couples (P,T_c) reported for underdoped Bi2212 by Huang *et al.*[20] The dashed line, which interpolates among these points, has been obtained by a standard best-fit procedure for $P=0-1.6$ GPa. Although the latter curve yields an overall trend, a nontrivial correlation is suggested between the interaction strength and the structural properties of the lattice, such as its in-plane spacing, which closely follows the dependence of T_c on P.[20] A similar conclusion has been derived by Neumeier,[6]

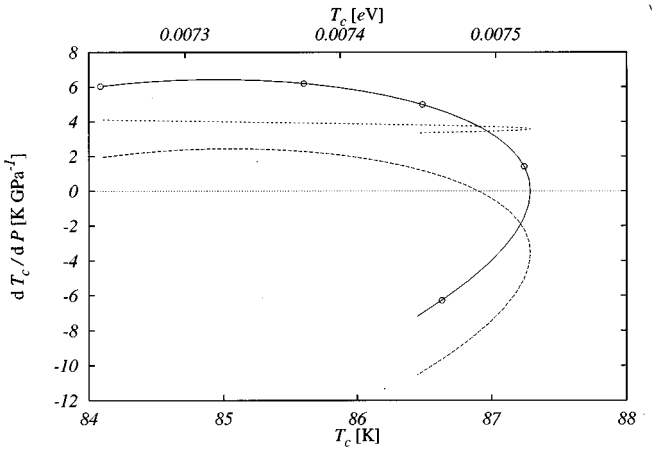

FIG. 5. The solid line best fits the experimental data of Huang *et al.*[20] for dT_c/dP vs T_c in Bi2212 under pressures $P=0-1.6$ GPa (circles). Our numerical estimates for the hole-induced (dashed line) and intrinsic (dotted line) contributions to the latter are also shown, according to Eq. (1).

using data for the pressure dependence of T_c in Y-Ba-Cu-O, and assuming a strong-coupling BCS expression in comparison with an improved McMillan expression for T_c. Even if the latter do not reliably account for the rich phenomenology of the cuprates (viz., the high values of their T_c), a satisfactory agreement was recognized with the observed trend in $d\ \ln T_c/dP$. Both results seem to support a nonspectator role of the lattice in the onset of an electronic instability towards superconductivity. Although the present analysis does not address the problem of the nature and origin of the attractive interaction, Fig. 4 suggests a nontrivial behavior of the intersite interaction V as a function of the cell spacing.

We are eventually in the position to distinguish between the two contributions to dT_c/dP in Eq. (1). The solid line in Fig. 5 is the best fit to the values of dT_c/dP vs T_c deduced from the experimental work by Huang *et al.*[20] on Bi2212 under pressures $P=0-1.6$ GPa. Figure 5 also displays

$$\frac{\partial T_c}{\partial \rho}\frac{d\rho}{dP}=\rho(0)\kappa_\rho\frac{\partial T_c}{\partial \rho}, \tag{30}$$

numerically evaluated on the basis of our results (Fig. 2), assuming $\rho(0)\simeq 0.2$ by comparison of the results of Huang *et al.*[20] with the known dependence of T_c on ρ at normal pressure.[19] The intrinsic contribution $\partial T_c/\partial P$ is eventually resolved as the difference between the previous two.

A non-negligible intrinsic term $\partial T_c/\partial P$ is recognized, thus suggesting an effective contribution of the lattice to the mechanism of high-T_c superconductivity against the role of carriers. However, since $\partial T_c/\partial P>0$ in the pressure region considered, the change of sign in the total dT_c/dP observed in underdoped Bi2212 is mainly due to the nonmonotonic dependence of T_c on ρ, via Eq. (1).

IV. CONCLUSIONS

In summary, we have employed a BCS-type mean-field approximation of the extended Hubbard model to describe a system of fermionic, holelike carriers, subjected to an intermediate-range interaction, in order to reproduce the observed universal behavior of T_c vs the hole content ρ in the high-T_c superconductors. A model tight-binding dispersion relation for the free carriers in the lattice has been adopted, as suggested by ARPES measurements and band structure calculations. A simplified, though accurate, LCAO approximation has been employed in order to provide the band parameters with a suitable dependence on the lattice steps, and therefore on pressure, through the known compressibilities. Due to the quasibidimensional lattice structure, an almost dispersionless character emerged for the carriers in the direction orthogonal to the planes, and a quite large van Hove–like peak in their DOS. As predicted within an AFvH picture, a pressure induced decrease in the DOS peak produces a shift in the optimal doping level towards higher values.

The comparison with known experimental data for T_c vs ρ (Ref. 19) and T_c vs P (Ref. 20) in Bi2212 allowed us to interpret in a quantitative way the interplay between T_c, ρ, and P. A strong contribution to dT_c/dP, given by an increase of the hole content through an applied pressure, evidenced by Hall resistance pressure measurements, has been resolved from a non-negligible intrinsic one, mainly due to the lattice rearrangement induced by pressure. On the basis of this result, we can argue that the lattice structure is not completely influent on the mechanism of high-T_c superconductivity. The latter statement has been supported by a quantitative estimate of a nontrivial correlation between the intersite coupling strength and the in-plane lattice spacings.

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APPENDIX: PRESSURE DEPENDENCE OF THE TIGHT-BINDING PARAMETERS

We here derive a convenient estimate of the dependence of the hopping parameters t_x, t_y, t_{xy}, and t_z which define the tight-binding model dispersion relation, Eq. (7), as a function of the lattice parameters, a_x, a_y, and a_z, and therefore of the pressure, through Eq. (23).

The parameters t_x and t_y measure the probability for a carrier to hop from one site to a nearest-neighbor site in the same Cu-O plane. In the tight-binding approximation, the dependence of t_x and t_y on the in-plane lattice spacings a_x and a_y may be approximated by the overlap integrals between the $2p_x$ and $2p_y$ hydrogenoid atomic orbitals, centered on the oxygen site, and the $3d_{x^2-y^2}$ one, centered on the copper site, distant $a_x/2$ and $a_y/2$ from the former, respectively. Such overlap integrals have been analytically evaluated employing elliptic coordinates, and they behave as $t_i\approx\exp(-5a_i/24a_0)$ for $a_i\gg a_0$, being a_0 the Bohr radius of the hydrogen atom.

In an analogous way, we take t_{xy} proportional to the overlap integral between the $2p_x$ and the $2p_y$ hydrogenoid atomic orbitals, centered on next-nearest-neighbors oxygen

sites, respectively, distant $a_i\sqrt{2}$ apart. t_z is assumed proportional to the overlap integral between the $3d_{3z^2-r^2}$ hydrogenoid atomic orbital centered on a copper site, and the $2p_z$ one, centered on the corresponding apical oxygen. One finds $t_{xy}\approx\exp(-a_{x,y}/2a_0)$ and $t_z\approx\exp(-5a_z/2a_0)$ for $a_i\gg a_0$. The proportionality constants are chosen so that Eq. (7) correctly fits the observed band dispersion at normal pressure (Fig. 1).

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