Possible phononic mechanism for $d_{x^2-y^2}$ superconductivity in the presence of short-range antiferromagnetic correlations

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(Received 8 September 1995; revised manuscript received 14 November 1995)

We discuss the high-temperature superconductors in a regime where the antiferromagnetic (AF) correlation length is only a couple of lattice spacings. In the model proposed here, these short-range AF fluctuations play an essential role in the dressing of the carriers, but the attraction needed for superconductivity arises from a transverse phonon oxygen mode with a finite buckling angle as it appears in $YBa_2Cu_3O_{7-\delta}$. A simple fermion-phonon model analog to the Holstein model is introduced to account for this effect. We argue that the model has a $d_{x^2-y^2}$-wave superconducting ground state. The critical temperature (T_c) and the O-isotope effect coefficient (α_O) versus hole density (x) are in qualitative agreement with experiments for the cuprates. The minimum (maximum) of α_O (T_c) at optimal doping is caused by a large peak in the density of states of holes dressed by AF fluctuations, as discussed in previous van Hove scenarios.

Since the discovery of high-temperature superconductors, the origin of their pairing mechanism has been controversial. Numerous studies have shown that normal-state properties deviate from a conventional Fermi liquid, and as a possible explanation several authors proposed the antiferromagnetic (AF) correlations as responsible for such nonstandard behavior. Theories based on AF pairing mechanisms analyzed using diagrammatic and numerical techniques predict $d_{x^2-y^2}$ superconductivity (SC).[1] Josephson junction experiments and angle-resolved photoemission (ARPES) data are consistent with such $d_{x^2-y^2}$ condensate.[2,3]

However, there are still some problems with this approach. For example, the AF correlation length ξ_{AF} in the normal state of the high-T_c cuprates at optimal doping, x_{opt}, may not be robust enough to induce SC. NMR measurements in $YBa_2Cu_3O_{7-\delta}$ suggest $\xi_{AF}/a \sim 2-3$ (Ref. 4) (a is the Cu-Cu lattice spacing). Inelastic neutron scattering studies for the same compound only show a broad peak at $\mathbf{q}=(\pi,\pi)$ in the dynamical spin structure factor.[5] Weak "shadow bands" in Bi2212 ARPES data at room temperature have been interpreted as produced by short-range AF correlations (although superlattice effects have not been ruled out).[6] Numerical studies[7] have shown that these weak AF-induced bands are quantitatively reproduced by the doped t-J model in a regime where $\xi_{AF}/a \sim 2-3$, in agreement with NMR. While many numerical studies suggest that this apparently small AF correlation can nevertheless substantially affect the quasiparticle (q.p.) dispersion (one-particle Green's function),[8] it has not been shown that it can also lead to pairing (two-particle Green's function, with hole Coulombic repulsion included) as it may occur in the regime $\xi_{AF}/a \gg 1$.[1]

A second problem for electronic mechanisms in general is the O-isotope effect observed in the cuprates. While experiments have shown that the coefficient α_O is very small at x_{opt}, it increases in the underdoped and overdoped regimes reaching values comparable to the BCS limit $\alpha_{BCS} = 0.5$.[9] It may be argued that this effect is caused by spurious changes in x after the replacement $O^{16} \rightarrow O^{18}$, but until a realistic calculation proves it, the experimental data cannot be simply neglected.

In this paper we *assume* that the normal-state ξ_{AF} at x_{opt} is not large enough to produce magnon mediated pairing, and thus we discuss possible alternative ideas that may explain SC in the cuprates. We argue that a small ξ_{AF} can still be important for the normal-state hole dispersion since carriers are much affected by the surrounding *local* spin environment. Short AF correlations can modify the hole dispersion reducing the bandwidth and producing anomalous "flat bands" as observed in the t-J and Hubbard models,[8] and in ARPES data.[3] The flat bands induce a robust *peak* in the density of states (DOS) at the top of the valence band that boost T_c and produce an "optimal doping" when the chemical potential μ reaches the peak, once a source of hole attraction exists. This combination of the AF and van Hove scenarios[10] is similar in spirit to previously discussed van Hove theories.[11] The key difference is the origin of the DOS large peak which in Ref. 10 was attributed to AF correlations. In the present paper, pairing is caused by a *phononic*-induced attraction supplemented by a hole dispersion modulated by short distance AF correlations that tend to prevent double occupancy and favor intrasublattice hopping. Thus concepts of both phononic and electronic theories are here mixed in a single scenario.

However, an immediate problem with this idea is the symmetry of the SC condensate. Evidence is accumulating in favor of $d_{x^2-y^2}$ SC which is natural in electronic AF theories, but seems unnatural in conventional phononic theories. For example, the Holstein model couples electrons to on-site oscillators[12] leading to a uniform s-wave condensate. To obtain d-wave phononic SC, we introduce a modification of the Holstein model with oscillators located at the oxygens of a two-dimensional (2D) square lattice rather than at the copper sites [Fig. 1(a,b)]. While this modification seems "*ad hoc*," physical realizations involving the buckling mode of oxygen in the cuprate exist, as shown below. We further argue that the effective hole-hole interaction produced by this model favors d-wave SC at low carrier concentration once the AF induced hole dispersion is used.

The modified Holstein model proposed here is

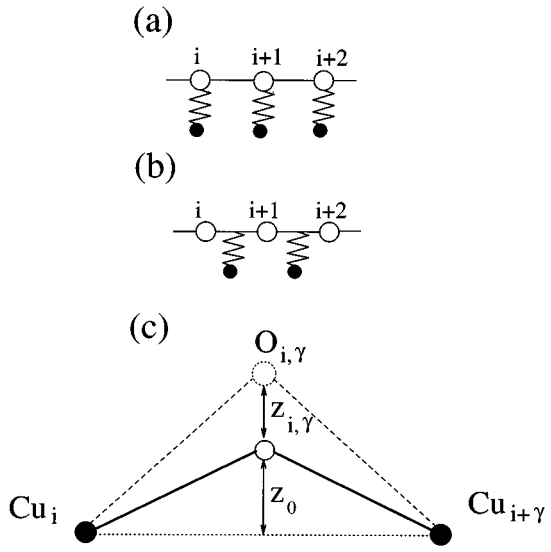

FIG. 1. (a) Graphical representation of the standard Holstein model with an oscillator attached to each lattice site **i**. (b) In the new model Eq. (1) the oscillators are attached to the oxygen positions, i.e., at half-distance between coppers. (c) O buckling mode studied in this paper. z_0 is the O equilibrium position, and $z_{\mathbf{i},\gamma}$ is the displacement from equilibrium in the z direction.

$$H=\sum_{\mathbf{k}\sigma}[\epsilon_{\mathrm{AF}}(\mathbf{k})-\mu]\bar{c}^{\dagger}_{\mathbf{k}\sigma}\bar{c}_{\mathbf{k}\sigma}+\sum_{\mathbf{i},\gamma=\hat{\mathbf{x}}\hat{\mathbf{y}}}\left(\frac{p^2_{\mathbf{i}\gamma}}{2M}+\frac{M}{2}\omega^2 z^2_{\mathbf{i},\gamma}\right)$$
$$+g\sum_{\mathbf{i},\gamma=\hat{\mathbf{x}}\hat{\mathbf{y}}}(z_{\mathbf{i},\gamma}+z_{\mathbf{i},-\gamma})(\hat{n}_{\mathbf{i}\uparrow}+\hat{n}_{\mathbf{i}\downarrow}), \quad (1)$$

where $\epsilon_{\mathrm{AF}}(\mathbf{k})$ is the hole dispersion obtained *after* the influence of AF correlations has been taken into account (this is important since the resulting q.p.'s are *weakly* interacting and thus the peak in the DOS is not removed by correlations or disorder[10]). $\bar{c}$ ($\bar{c}^{\dagger}$) is a fermion destruction (creation) operator located at Cu with standard fermionic anticommutation relations (these fermions represent ''holes'' in the cuprates), $\hat{n}_{\mathbf{i}\sigma}=\bar{c}^{\dagger}_{\mathbf{i}\sigma}\bar{c}_{\mathbf{i}\sigma}$ is the number operator, **i** labels sites of a 2D square lattice, $\gamma=\hat{\mathbf{x}},\hat{\mathbf{y}}$ are unit vectors along the axis directions, and $z_{\mathbf{i},\gamma}$ and $p_{\mathbf{i},\gamma}$ are the coordinate and momentum of the oscillators of mass M and frequency ω at half-distance between adjacent sites to mimic oxygens. As hole dispersion we use $\epsilon_{\mathrm{AF}}(\mathbf{k})/eV=0.165\cos k_x\cos k_y+0.0435(\cos 2k_x+\cos 2k_y)$, which corresponds to the hole dispersion in an AF background at half-filling,[8] but it should be approximately valid also at finite x as long as ξ_{AF} is not negligible. Holes move within the same sublattice. The spin index in Eq. (1) does not play an important role and working with spinless fermions leads to similar results. Using Eq. (1) we will study small fermionic (hole) densities to mimic the physics of the cuprates.

What cuprate phonons can lead to Eq. (1)? The in-plane breathing mode where O oscillates along the Cu-Cu link is not useful since it produces an effective hole nearest-neighbor (NN) *repulsion*. In principle O phonons transverse to the Cu-Cu link have a coupling quadratic in the displacement that is negligible. However, several authors[13,14] noticed that the *buckling* of the Cu-O-Cu link leads to a linear electron-phonon coupling in $YBa_2Cu_3O_{7-\delta}$. In this tilting mode [Fig. 1(c)] the O atom oscillates in the $\hat{\mathbf{z}}$ direction about an equilibrium position z_0 with a buckling angle $\beta=5°$ and a frequency that here we take as $\hbar\omega_{\mathrm{buck}}=12$ meV.[15,13] While buckling effects are not present in all cuprates, nevertheless it serves our purpose of identifying at least one phononic mode that in combination with strong correlations can lead to d-wave SC. Note that in this exploratory study we are also neglecting the coupling to other phonon modes of similar energy that may lead to repulsive interactions.

Let us discuss recent work related to the ideas described here. Song and Annett[13] studied d-wave phononic SC using the in-plane O breathing mode. However, further analysis showed that this mode does not lead to d-wave SC.[13] They also studied the O buckling mode with a tight-binding dispersion finding d-wave SC, but concluded that it would not produce a large enough T_c.[16] The key difference with our approach is that we here use an AF-induced DOS with a large peak which boots T_c to high values. In other related work, Yonemitsu *et al.*.[17] coupled the apical phonon modes to the t-J model forming a SC polaron pair condensate. AF correlations affect the hole propagation as in our approach, but they found ''nodeless'' d-wave or p-wave pairing, contrary to our $d_{x^2-y^2}$ result. Finally, using a mean-field approximation for the t-J model with phonons, Normand *et al.*[14] studied anomalies at T_c associated to the Y-Ba-Cu-O buckling mode. α_{O} was reported in agreement with experiment but the calculation was done only at x_{opt}.

Returning to the main idea, let us derive the buckling-mode induced hole-phonon coupling. Consider the Coulomb energy of carriers at the Cu ions in the presence of the NN O ions,[18]

$$H_{\mathrm{Coulomb}}=\frac{ee^*}{\epsilon}\sum_{\mathbf{i},\sigma,\gamma}\bar{c}^{\dagger}_{\mathbf{i}\sigma}\bar{c}_{\mathbf{i}\sigma}\left(\frac{1}{|\mathbf{R}_{\mathbf{i}}-\mathbf{r}_{\mathbf{i},\gamma}|}+\frac{1}{|\mathbf{R}_{\mathbf{i}}-\mathbf{r}_{\mathbf{i},-\gamma}|}\right), \quad (2)$$

where e is the electron charge, $e^*=-2e$ is the O-ion charge, ϵ is the dielectric constant, $\mathbf{R}_{\mathbf{i}}$ denotes the Cu positions which are assumed nonfluctuating, and $\mathbf{r}_{\mathbf{i},\gamma}$ denotes the vibrating O positions (interactions at distances larger than a are assumed negligible due to screening effects). In Eq. (2) we define $\mathbf{r}_{\mathbf{i},-\gamma}=\mathbf{r}_{\mathbf{i}-\gamma,\gamma}$. The Cu-O distance can be expanded in the z direction small O-ion displacement, $z_{\mathbf{i},\gamma}$, as $|\mathbf{R}_{\mathbf{i}}-\mathbf{r}_{\mathbf{i},\gamma}|=(a/2)(1+2z_0^2/a^2)+(2z_0/a)z_{\mathbf{i},\gamma}+\cdots$, $a\gg z_0\gg z_{\mathbf{i},\gamma}$ is assumed. The hole-phonon interaction becomes

$$H_{h\text{-ph}}=-\frac{8ee^*z_0}{\epsilon a^3}\sum_{\mathbf{i},\sigma,\gamma}\bar{c}^{\dagger}_{\mathbf{i}\sigma}\bar{c}_{\mathbf{i}\sigma}(z_{\mathbf{i},\gamma}+z_{\mathbf{i},-\gamma}). \quad (3)$$

In **k** space we arrive to the fermion-boson Hamiltonian,

$$H_{h\text{-ph}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}\mathbf{q}\gamma\sigma}g_{\mathbf{q},\gamma}\bar{c}^{\dagger}_{\mathbf{k}\sigma}\bar{c}_{\mathbf{k}-\mathbf{q}\sigma}(b_{\mathbf{q},\gamma}+b^{\dagger}_{-\mathbf{q},\gamma}), \quad (4)$$

where N is the number of Cu sites, $b_{\mathbf{q},\gamma}$ ($b^{\dagger}_{\mathbf{q},\gamma}$) is the destruction (creation) phonon operator with momentum **q**, and the electron-phonon coupling has the form

$$g_{\mathbf{q},\gamma}=-\left(\frac{16ee^*}{\epsilon a^2}\right)\left(\frac{z_0}{a}\right)\sqrt{\hbar/2M\omega_{\mathrm{buck}}}\cos\left(\frac{q_\gamma}{2}\right), \quad (5)$$

where M is the the O mass.[19] The coupling strength is estimated as $g_{\mathbf{q}=\mathbf{0},\gamma}\approx(1-2)\times10^{-2}$ eV where we used

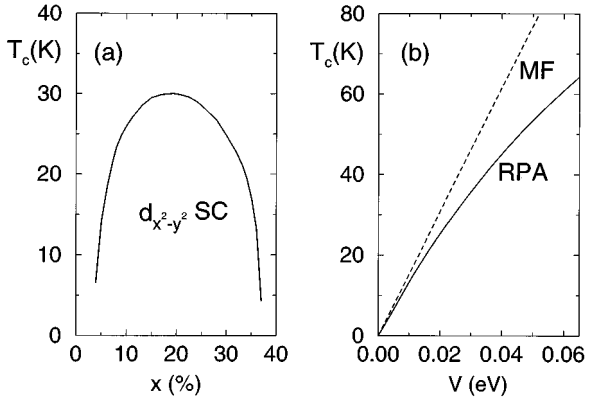

FIG. 2. (a) T_c vs x using $\epsilon_{\rm AF}(\mathbf{k})$ as dispersion, and Eq. (6). The coupling $g_{\mathbf{q}=\mathbf{0},\gamma}$ is set to 0.018 eV. The SC state is d-wave. (b) T_c vs coupling $V=g^2_{\mathbf{0},\gamma}/\omega_{\rm buck}$ at optimal density in the mean-field approximation (dashed line) to model Eq. (8). The solid line represents the results after RPA corrections are included. $V\sim 0.02$ eV is the coupling necessary to recover the T_c obtained in (a).

$\epsilon\approx 10-20$,[20] $a\approx 3.8$ Å, $z_0\approx 0.17$ Å,[15] and $M=16$ a.u. This is in agreement with Ref. 13, and it is at least one order of magnitude *less* than typical electron-phonon couplings in normal metals, which is natural due to the reduction caused by the geometric factor z_0/a.

Let us analyze the effective hole-hole interaction caused by phonons in nonretarded form. This simplification should not change the symmetry of the SC condensate, and other qualitative features discussed below. Standard manipulations lead to the interaction (natural units)

$$H^{h\text{-}h}_{\rm int}=\frac{1}{2N}\sum_{\mathbf{kpq}\sigma\sigma'} V^{\rm eff}_{\mathbf{k},\mathbf{p}}\bar{c}^{\dagger}_{\mathbf{p}\sigma}\bar{c}^{\dagger}_{-\mathbf{p}+\mathbf{q}\sigma'}\bar{c}_{-\mathbf{k}+\mathbf{q}\sigma'}\bar{c}_{\mathbf{k}\sigma}, \qquad (6)$$

where $V^{\rm eff}_{\mathbf{k},\mathbf{p}}$ is given by

$$V^{\rm eff}_{\mathbf{k},\mathbf{p}}=-2\sum_{\gamma}\frac{g^2_{\mathbf{p}-\mathbf{k},\gamma}\omega_{\rm buck}}{\omega^2_{\rm buck}-[\epsilon_{\rm AF}(\mathbf{p})-\epsilon_{\rm AF}(\mathbf{k})]^2}. \qquad (7)$$

Since we are considering a dilute gas of holes and a short-range potential Eq. (7), this problem can be studied with the gap equation: $\Delta_{\mathbf{p}}=-\Sigma_{\mathbf{k}}(V^{\rm eff}_{\mathbf{k},\mathbf{p}}\Delta_{\mathbf{k}}/2E_{\mathbf{k}})\tanh(E_{\mathbf{k}}/2T)$, where $E_{\mathbf{k}}=\sqrt{[\epsilon_{\rm AF}(\mathbf{k})-\mu]^2+\Delta^2_{\mathbf{k}}}$, and $\Delta_{\mathbf{k}}$ is the SC gap. The numerical solution of this equation produces SC in the $d_{x^2-y^2}$ channel. To obtain T_c vs x the linearized gap equation was solved.[21] Naively, the small hole-phonon coupling induced by the buckling mode should produce a small T_c. However, the large peak in the hole DOS caused by flat bands can boost T_c.[10,11] The results are shown in Fig. 2(a). T_c is maximized when μ reaches the maximum in the DOS producing an "optimal doping."[10,11] For the couplings and the approximations described in this paper, which are standard, T_c reaches 30 K, which can be made higher by tuning the q.p. dispersion to increase the boosting DOS. Thus, the experimental d-wave character of the SC phase, and the x dependence of T_c can be qualitatively reproduced by the small fermion-phonon coupling induced by the buckling mode of Y-Ba-Cu-O, if $\epsilon_{\rm AF}(\mathbf{k})$ is used as dispersion.

Finding d-wave SC from Eqs. (6) and (7) is natural. To visualize this effect, assume interacting on-shell holes. Then, transforming Eq. (6) into real space we get

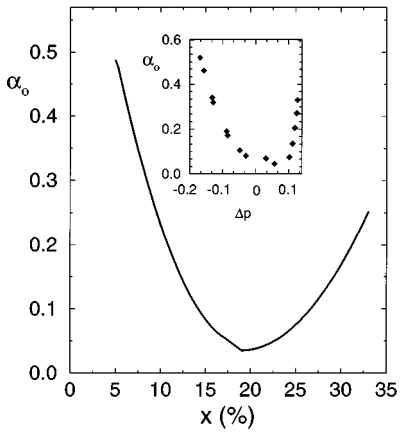

FIG. 3. $\alpha_{\rm O}$ vs x using $\epsilon_{\rm AF}(\mathbf{k})$, and $g_{\mathbf{q}=\mathbf{0},\gamma}=0.018$ eV. The inset shows experimental results for $\alpha_{\rm O}$ vs Δp, which is the concentration of mobile holes per CuO plane relative to the optimal value corresponding to $YBa_2Cu_3O_7$, when T_c is reduced by doping with Pr, Ca, Zn and/or Co [from J. P. Franck *et al.*, Phys. Rev. B **44**, 5318 (1991); J. P. Franck *et al.*, in *Lattice Effects in High-T_c Superconductors* (World Scientific, Singapore, 1992), p. 148; and references therein].

$$H^{h\text{-}h}_{\rm int}=-\sum_{\mathbf{i}}\frac{g^2_{\mathbf{0},\gamma}}{\omega_{\rm buck}}\hat{n}^2_{\mathbf{i}}-\frac{1}{2}\sum_{\langle\mathbf{ij}\rangle}\frac{g^2_{\mathbf{0},\gamma}}{\omega_{\rm buck}}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{j}}, \qquad (8)$$

where $\langle\mathbf{ij}\rangle$ denote NN sites. The first term in Eq. (8) is an on-site attraction which is suppressed trivially by the hard-core properties of the holes in the t-J model from which the dispersion is derived.[8] The second term provides the NN attraction that leads to an interaction of the form corresponding to the well-known "t-U-V" ($U>0, V<0$) model that has the tendency to form d-wave condensates.[22] However, there are several crucial differences between our model and the t-U-V model. More remarkable is the fact that the AF dispersion used here allows the formation of a d-wave condensate at *low* particle density, while the t-U-V model (where a $\cos k_x+\cos k_y$ dispersion is used) has s-wave SC in this regime.[22] Optical conductivity measurements in underdoped cuprates clearly show that the number of carriers grows as the number of holes, and thus we should study a dilute gas of quasiparticles as carried out in this paper. Our ideas go beyond previous studies of d-wave SC that have used the t-U-V model in spite of its shortcomings such as having a T_c maximum at half-filling and a strong competition with phase separation.[22] Combining the potential Eq. (7) with the AF dispersion[8] is the proper way to mimic the phenomenology of the cuprates. In addition, the phonons in Eq. (1) produce an isotope effect which of course does not exist in the electronic t-U-V model. Note also that the instantaneous Coulombic repulsion at distance a would tend to suppress an effective attraction of AF origin, since both spin waves and holes in AF backgrounds have velocities dominated by the exchange J, and thus there are no obvious sources of retardation in the system. On the other hand, the retardation intrinsic to phononic mechanisms avoids such a problem in the present approach.

In Fig. 2(b), we show that corrections to the mean-field approach change T_c only by a small amount. We solved numerically the self-consistent equation $G=G_0+G_0VGG$,

where G_0 (G) is the noninteracting (full) Green's function, and V is the random phase approximation (RPA) effective potential. With the normal state G, we found the anomalous self-energy in the SC state following a standard procedure. Details will be given in a future publication.[23] We only remark that the effective model described here is in the weak-coupling regime since the heavy dressing of the holes by AF fluctuations was already considered in the dispersion, and the electron-phonon coupling is intrinsically small. Then, it is not surprising that corrections beyond mean field are not important [Fig. 2(b)]. The sharp features in the hole DOS are not washed out by disorder or quasiparticle interactions as shown in Ref. 10.

We also remark that $\alpha_O \approx -(\Delta T_c/T_c)(M/\Delta M)$ vs x has the proper shape compared to experiments (Fig. 3). The isotope coefficient can be as low as 0.05 at $x_{\rm opt}$. The minimum in α_O is caused by the van Hove singularity in the dispersion, as remarked in previous papers.[11] Away from $x_{\rm opt}$, α_O recovers the value close to 0.5 as in standard phononic systems. The behavior of α_O is regulated equally by ΔT_c and T_c, i.e., ΔT_c vs x is not constant in our calculation, but minimized at $x_{\rm opt}$.

Summarizing, here we have proposed a model where phononic pairing occurs between holes that are strongly dressed by AF fluctuations. The model may be applicable to the cuprates if the normal-state correlation $\xi_{\rm AF}$ at $x_{\rm opt}$ is proven not strong enough to produce pairing (currently under much discussion). Within the gap equation formalism, we found $T_c \sim 30$ K when the buckling mode of Y-Ba-Cu-O is considered. Although the hole-phonon coupling is much smaller than in normal metals, the large hole DOS boots T_c to realistic values. The same effect leads to an O-isotope coefficient that is small at $x_{\rm opt}$ but becomes close to 0.5 in the underdoped and overdoped regimes. The symmetry of the condensate produced by the buckling mode in *combination* with the AF induced hole dispersion is $d_{x^2-y^2}$ even in the low density of carriers regime. These ideas may provide a tentative unified explanation for several puzzling experimental features observed in the cuprates, especially the presence of an abnormal Fermi liquid at $T > T_c$, a nonzero isotope effect, and a d-wave SC condensate.

We thank J. F. Annett, J. P. Franck, and M. Norman for useful correspondence. Support by ONR Grant No. (N00014-93-0495) and the NHMFL are acknowledged.

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