Isotope effect and resistivity in the Hubbard model for *d*-wave superconductivity

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For spin-fluctuation-induced *d*-wave superconductivity in a two-dimensional Hubbard model we calculate the suppression of T_c, the isotope exponent α, and the enhancement of the resistivity ρ due to additional phonon interaction. The smallest T_c suppression and the largest α values are obtained for interactions $\alpha^2F(\mathbf{q},\omega)$ which are enhanced at $\mathbf{q}=0$. For a reasonably large coupling constant λ_p the enhancement of ρ yields qualitative agreement with the data on $YBa_2Cu_3O_7$. However, the largest values of α (~ 0.2) lie at the lower limit of the measured values for reduced-T_c materials. [S0163-1829(96)02641-0]

There is growing experimental evidence that the Cooper pairs in the high-T_c cuprates have $d_{x^2-y^2}$-wave symmetry. This suggests a pairing mechanism due to exchange of antiferromagnetic spin fluctuations which can be described in the framework of the two-dimensional (2D) Hubbard model.[1] Many cuprates including $YBa_2Cu_3O_7$ exhibit a quite noticeable isotope effect at doping concentrations away from optimal doping.[2] The isotope effect can be estimated by including an electron-phonon interaction in the Hubbard model. This leads to a suppression of the superconducting transition temperature T_c for $d_{x^2-y^2}$-wave pairing and to a finite isotope exponent $\alpha=-d\ln(T_c)/d\ln(M)$. It has been claimed that coupling to *harmonic* phonon degrees of freedom gives values of α which are at least one order of magnitude smaller than the observed values of α.[3]

In this paper we reexamine this question by solving the following generalized Eliashberg equations for the quasiparticle self-energy components X_ν ($\nu=0,3,1$) where $X_0=\omega(1-Z)$ is the effective mass and damping, $X_3=\xi$ is the shift in the chemical potential, and $X_1=\phi$ the superconducting order parameter:[4,5]

$$X_\nu(\mathbf{k},\omega)=N^{-1}\sum_{\mathbf{k}'}\int_0^\infty d\Omega \times[P_s(\mathbf{k}-\mathbf{k}',\Omega)\pm\alpha^2F_j(\mathbf{k}-\mathbf{k}',\Omega)] \times\int_{-\infty}^{\infty}d\omega' I(\omega,\Omega,\omega')A_\nu(\mathbf{k}',\omega'). \quad (1)$$

Here the plus sign holds for X_0 and X_3 and the minus sign for X_1. The kernel I and the spectral functions A_ν of the normal ($\nu=0$, 3) and the anomalous ($\nu=1$) Green's function are given in Refs. 4 and 5. The spin fluctuation exchange interaction $P_s=(U^2/2\pi)\,\mathrm{Im}(3\chi_s-\chi_0)$ [where $\chi_s=\chi_{s0}(1-U\chi_{s0})^{-1}$ is the dynamical spin susceptibility] is calculated self-consistently from the spectral function A_ν of the dressed Green's functions. For simplicity we have left out here the charge-fluctuation exchange interaction P_c which has to be added to the electron-phonon interaction α^2F_i. For the latter we take a form for a single optical phonon branch where a coupling constant g_p multiplies a Lorentzian in frequency Ω of width Γ_0 around Ω_0, and a normalized form factor $F_i(\mathbf{q})$ as a function of momentum $\mathbf{q}$:

$$\alpha^2F_i(\mathbf{q},\Omega)=g_p\frac{1}{\pi}\frac{\Omega\Gamma_0^3}{[(\Omega-\Omega_0)^2+\Gamma_0^2]^2}F_i(\mathbf{q}) \quad (i=0,b,t) \quad (2)$$

with

$$F_0(\mathbf{q})\equiv 1, \quad F_b(\mathbf{q})=\sin^2(q_x/2)+\sin^2(q_y/2),$$
$$F_t=2-F_b. \quad (3)$$

The Eliashberg coupling constant λ_p becomes approximately

$$\lambda_p=\frac{2}{8t}\int_0^\infty d\Omega\,\Omega^{-1}\sum_{\mathbf{q}}\alpha^2F_i(\mathbf{q},\Omega) =\frac{g_p}{8t}\frac{1}{\pi}\left[\frac{\pi}{2}+\arctan\left(\frac{\Omega_0}{\Gamma_0}\right)+\frac{(\Omega_0/\Gamma_0)}{1+(\Omega_0/\Gamma_0)^2}\right]. \quad (4)$$

Here we used an average value $N(0)=1/8t$ for the density of states. Notice that in Ref. 5 we obtain $N(0)\approx 0.2/t$. Then g_p corresponds to the coupling strength U_p, and λ_p corresponds to the λ in Ref. 3. Indeed, in the limit $\Gamma_0/\Omega_0\to 0$ we obtain $\lambda_p=g_p/8t$. In most of our numerical calculations we take an optical phonon frequency $\Omega_0=0.3t\simeq 60$ meV and a half-width $\Gamma_0=0.1t$. Then $\Omega_0/\Gamma_0\gg 1$ which yields approximately $\lambda_p\simeq g_p/8$ (g_p in units of t).

We study here the effect of three quite different form factors where F_0 is constant, and form factors F_b and F_t are peaked at $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$ and $\mathbf{q}=(0,0)$. The latter form factors might apply to the breathing and tilting modes, respectively.[6] The form factor F_t can also describe the effect of electronic correlations which have been calculated for a Hubbard model plus an on-site electron-phonon interaction.[7] These correlations produce a forward scattering peak in the effective electron-phonon coupling which depends strongly on doping. With decreasing doping the momentum dependence becomes more and more pronounced at $\mathbf{q}=0$. For our doping value away from half filling, $\delta=1-n=0.15$, the enhancement function γ^2 due to vertex corrections[7] agrees roughly with our form factor $F_t(\mathbf{q})$ in Eq. (3).

We have solved Eq. (1) for a tight-binding band $\epsilon(\mathbf{k})$ including next-nearest-neighbor hopping $t'=-0.45t$ (t is

the nearest-neighbor hopping energy) which approximates the 2D Fermi line of $YBa_2Cu_3O_7$. For an effective coupling $J(\mathbf{q})$ with $J(\mathbf{Q})=U=3.7t$ and a chemical potential $\mu=-1.35$ yielding a renormalized band filling $n=0.85$ we obtain in the absence of the electron-phonon interaction ($g_p=0$) a $T_{c0}=0.0388t$ for $d_{x^2-y^2}$-wave pairing.[5] Below T_c the spectral density $\mathrm{Im}\chi_s(\mathbf{Q},\omega)$ exhibits a large peak in agreement with neutron scattering experiments. For finite g_p we solve the eigenvalue equation for the linearized equation (1) for $X_1\equiv\phi$. The transition temperature T_c is given by that temperature where the eigenvalue λ_d passes through unity. It turns out that T_c is suppressed in comparison to T_{c0} where the amount of suppression depends strongly on the form factor $F_i(\mathbf{q})$ of the electron-phonon interaction. For example, for form factor F_t we obtain for coupling strengths $g_p=2$ and 4 transition temperatures $T_c=0.0364t$ and $0.0337t$, or relative suppression $(T_c-T_{c0})/T_{c0}\equiv\Delta T_c/T_{c0}=-0.062$ and -0.131. For form factor F_0 and coupling strengths $g_p=2$ and 4 we obtain $T_c=0.0279t$ and $0.0195t$, or $\Delta T_c/T_{c0}=-0.282$ and -0.497. We find that the suppression of T_c is largest for form factor F_b ($\Delta T_c/T_{c0}=-0.466$ for $g_p=2$) which is plausible because the pairing interaction in the gap equation for $X_1\equiv\phi$ [see Eq. (1)] is $(P_s-\alpha^2F_i)$ where the repulsive spin fluctuation interaction P_s is peaked at $\mathbf{Q}$. Thus F_b is destructive for d-wave pairing. The suppression of T_c is relatively small for form factor F_t [see Eq. (3)] which is peaked at $\mathbf{q}=(0,0)$. This result is in line with previous results for combined spin fluctuation interaction P_s and electron-phonon interaction α^2F: If α^2F is sufficiently strongly peaked at $\mathbf{q}=(0,0)$, one obtains $d_{x^2-y^2}$-wave pairing even though α^2F is attractive.[8] For the constant form factor F_0 the suppression of T_c is intermediate between these two extrema for form factors F_b and F_t.

Assuming an isotopic mass dependence $\Omega_0\propto M^{-1/2}$ the isotope exponent α becomes

$$\alpha=\frac{1}{2}\frac{d\ln T_c}{d\ln(\Omega_0)}. \tag{5}$$

In calculating α one has to ensure that the electron-phonon coupling λ_p is kept fixed. This means according to Eq. (4) that for fixed g_p the ratio Ω_0/Γ_0 has to be kept constant when one evaluates Eq. (5) numerically from the difference ΔT_c as a function of $\Delta\Omega_0$. We quote here some results for α for the same parameter values given above for the calculations of ΔT_c. For form factor F_t we obtain for coupling constants $g_p=2$ and 4 the values $\alpha=0.069$ and 0.14. For form factor F_0 the results are $\alpha=-0.022$ and -0.065 for $g_p=2$ and 4, and for F_b we obtain $\alpha=-0.121$ for $g_p=2$. These examples show that the isotope exponent α for a given form factor varies almost linearly with coupling strength g_p, and for given g_p the values of α decrease in the sequence of form factors F_t to F_0 to F_b. On the other hand, we have seen above that the magnitude of the suppression, ΔT_c, of the transition temperature increases as one goes from F_t to F_0 and to F_b. These differences between the results for the three form factors can be seen more clearly in Fig. 1 where we have plotted α versus T_c (we set $t=200$ meV which yields $T_{c0}=90$ K). One sees that α increases almost linearly with decreasing T_c for form factor F_t while

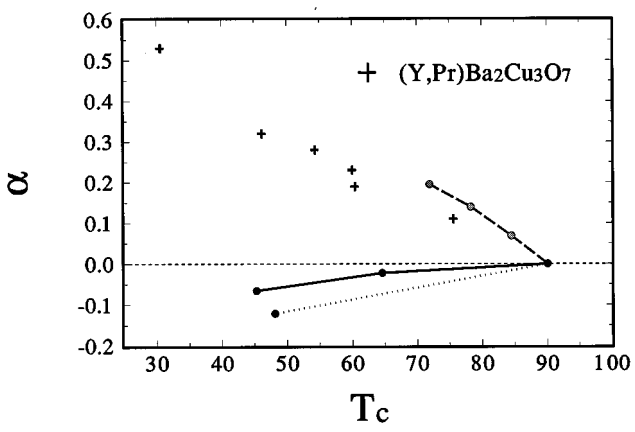

FIG. 1. Isotope exponent α vs T_c for $d_{x^2-y^2}$ pairing in a Hubbard model with on-site Coulomb repulsion $U=3.7t$, band filling $n=0.85$, and a Fermi surface approximating that of $YBa_2Cu_3O_7$. The circles refer to electron-phonon coupling constants $\lambda_p\simeq g_p/8=0.25$, 0.5, and 0.75, the solid line refers to constant form factor F_0 for the $\mathbf{q}$ dependence of the interaction $\alpha^2F(\mathbf{q},\Omega)$, the dashed line refers to $F_t(\mathbf{q})$ which is enhanced at $\mathbf{q}=0$, and the dotted line refers to $F_b(\mathbf{q})$ which has its maximum at $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$. The crosses are the experimental points for $(Y,Pr)Ba_2Cu_3O_7$ (Ref. 2).

α is negative and decreases almost linearly with decreasing T_c for form factors F_0 and F_b. For comparison we show also the data points (crosses) for $(Y,Pr)Ba_2Cu_3O_7$.[2] Here it should be pointed out that the theoretical curves refer to a fixed band filling $n=0.85$ while the experimental points refer to different values of α and T_c which have been obtained by varying the doping, that is, n. Thus our theoretical curves tell us merely that only the smaller experimental values of α ($\leqslant 0.2$) can be reached by going to coupling strengths $\lambda_p\simeq g_p/8$ up to 0.75, provided that the interaction is enhanced for small $\mathbf{q}$ like that for form factor F_t. Our curve for F_t in Fig. 1 lies substantially above the curve in Fig. 2 of Ref. 3 which has been obtained from the MMP (Ref. 9) model. Our curve for F_0 which shows small and negative α values and large T_c suppression agrees essentially with the curve in Fig. 2 of Ref. 3 which has been obtained for the Hubbard model with nearest-neighbor hopping at $n=0.86$ and $U/t=6$. The main difference between these two calculations is that we use a real frequency formulation and a finite width Γ_0 of α^2F around Ω_0 while in Ref. 3 the imaginary frequency formulation is used for an Einstein-phonon model.

The main constraints on our values of $\lambda_p\approx g_p/8$ are that the reduction of T_c and the enhancement of the resistivity ρ be not too large and in accordance with the experimental values. We calculate here the conductivity σ_1 with the help of the Kubo formula

$$\sigma_1=\frac{2\pi e^2}{\hbar^2 c}\int_{-\infty}^{\infty}d\omega(-\partial f/\partial\omega)\sum_{\mathbf{k}}\left[(\partial\epsilon/\partial k_x)^2+(\partial\epsilon/\partial k_y)^2\right]\times[A_0(\mathbf{k},\omega)+A_3(\mathbf{k},\omega)]^2. \tag{6}$$

Here, f is the Fermi function and c is the lattice constant perpendicular to the CuO_2 planes. The spectral functions A_0 and A_3 are calculated self-consistently from Eq. (1). It

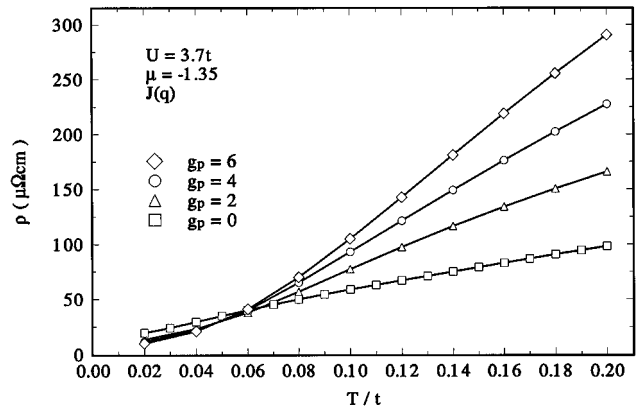

FIG. 2. Resistivity ρ vs T in the normal state for spin fluctuation alone (squares for $g_p=0$), and for additional electron-phonon interaction with form factor $F_t(\mathbf{q})$ and coupling constants $\lambda_p \simeq g_p/8=0.25$ (triangles), $\lambda_p \simeq g_p/8=0.5$ (circles), and $\lambda_p \simeq g_p/8=0.75$ (diamonds). (See notation in Fig. 1.) The curve for $\lambda_p=0.5$ agrees qualitatively with the resistivity ρ_a observed on $YBa_2Cu_3O_7$ (Ref. 9).

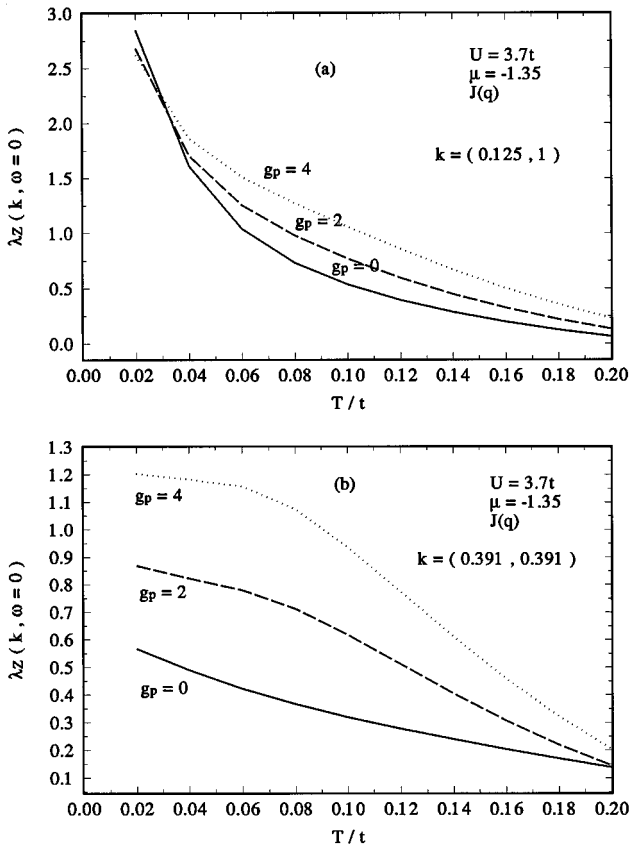

FIG. 3. Effective mass enhancement, $\lambda_Z \equiv \mathrm{Re}Z(\mathbf{k},\omega=0)-1$, vs T, for $g_p=0$, 2, and 4 (with F_0). (a) $\mathbf{k}=(0.125,1)$, (b) $\mathbf{k}=(0.391,0.391)$.

should be pointed out that no vertex corrections to the current correlation function have been taken into account. As an example we show in Fig. 2 the resistivity $\rho=(\sigma_1)^{-1}$ (in $\mu\Omega$ cm) versus T for a spin fluctuation plus phonon interaction with form factor F_t for coupling strengths $\lambda_p \simeq g_p/8=0.25$ (triangles), $\lambda_p \simeq g_p/8=0.5$ (circles), and $\lambda_p \simeq g_p/8=0.75$ (diamonds). For comparison we show also ρ for spin fluctuation interaction alone ($g_p=0$, squares). The first thing to note from Fig. 2 is that to a good approximation the curves are linear in T apart from the lowest temperatures where they tend quadratically toward zero. Second, the phonon contribution to ρ increases substantially with coupling constant λ_p and for increasing temperature T in comparison with the curve for $\lambda_p=0$. The reason for this behavior is the following: The magnitude of the resistivity is determined primarily by the interaction in a frequency range up to $\omega \sim T$. Since the spin fluctuations have most of their spectral weight at frequencies well below our phonon frequency, we can understand that the distance between the curves with and without phonons increases with temperature. The curve for $\lambda_p \simeq g_p/8=0.5$ shows that the resistivity does not become too large for these coupling constants. In fact, the agreement with the experimental ρ_a appears to be quite good.[10] For the constant form factor F_0 and coupling constants $g_p=2$ and 4 we obtain approximately the same values for the resistivity ρ as those for F_t shown in Fig. 2. We have also calculated the effective mass enhancement $\lambda_Z \equiv \mathrm{Re}Z(\mathbf{k},\omega=0)-1$ as a function of temperature T and momentum $\mathbf{k}$. In Fig. 3 we show our results with F_0 and coupling constant $g_p=0$, 2, and 4 at momentum $\mathbf{k}_a=(0.125,1)$ [see Fig. 3(a)] and $\mathbf{k}_n=0.391(1,1)$ [see Fig. 3(b)]. One sees that at the antinodal point $\mathbf{k}_a$ the spin fluctuation effect dominates (λ_Z increases rapidly for decreasing T as in a marginal Fermi liquid) while at the nodal point $\mathbf{k}_n$ the electron-phonon interaction dominates $[\lambda_Z(g_p)-\lambda_Z(g_p=0) \approx \lambda_p=g_p/8]$. These results show that the average mass enhancement is dominated by the spin fluctuation exchange. We have ascertained also that we indeed obtain $d_{x^2-y^2}$-wave pairing for the three form factors and for all coupling strengths considered by comparing the corresponding eigenvalue λ_d of the linearized gap equation for $X_1 \equiv \phi$ with the eigenvalue λ_s for a state ϕ having extended s-wave symmetry. For example, for form factor F_t, $g_p=6$, and $T=0.031t$ we find $\lambda_d=0.99$ and $\lambda_s=0.85$. For form factor F_0, $g_p=4$, and $T=0.020t$ we find $\lambda_d=0.99$ and $\lambda_s=0.46$.

We have varied the parameter values of our model in the following way. First, we have increased and decreased the phonon frequency Ω_0. Second, we have varied the width Γ_0 of the spectrum. Third, we have chosen form factors $F_i(\mathbf{q})$ which are more and more pronounced at $\mathbf{q}=0$ corresponding to the vertex corrections for smaller doping values δ away from half filling.[7] None of these modifications produced any sizable enhancement of the isotope exponent α. Finally we have increased the band filling n towards half filling $n=1$. For example, for $g_p=0$, $U=3.2t$, and $\mu=-1.1$ we obtain a renormalized band filling $n=0.93$ and a $T_{c0}=0.0278t$. For form factor F_t and $\lambda_p \simeq g_p/8=0.25$ we find a suppression $\Delta T_c/T_{c0}=-0.102$ and a value of $\alpha=0.072$. Again this value of α is nearly the same as that for $\mu=-1.35$ ($n=0.85$) quoted above.

In summary, we have studied the effect of different phonon interactions $\alpha^2F(\mathbf{q},\omega)$ on the spin-fluctuation-induced T_c for $d_{x^2-y^2}$-wave pairing in a 2D Hubbard model. For the Ω spectrum we take a Lorentzian of width Γ_0 around an optical phonon frequency $\Omega_0 \simeq 60$ meV, and for the $\mathbf{q}$ dependence we consider three different form factors $F_i(\mathbf{q})$ which

are constant ($i=0$), peaked at $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$ ($i=b$), or peaked at $\mathbf{q}=0$ ($i=t$). The latter form factor F_t is suggested by the effect of electronic correlations on the on-site phonon interaction in a Hubbard model.[7] Of course there may be other sources for form factor F_t of the interaction, for example, the phonon tilting modes.[6] We have calculated here the suppression of T_c, the isotope exponent α, and the enhancement of the normal-state resistivity ρ for different electron-phonon coupling constants λ_p and form factors $F_i(\mathbf{q})$. The suppression of T_c is found to be relatively small for F_t and largest for F_b. The values of α are positive for F_t while they are negative for F_0 and F_b. Our result, that form factor F_t yields small suppression of T_c and positive α, is plausible because, quite generally, the suppression of T_c decreases and even goes over to an enhancement of T_c for $d_{x^2-y^2}$-wave pairing as the peak in $\alpha^2F(\mathbf{q},\omega)$ at $\mathbf{q}=0$ becomes more and more pronounced.[8]

For a coupling value of $g_p=4$ ($\lambda_p\simeq 0.5$) the enhancement of the resistivity $\rho(T)$ for form factor F_t yields qualitative agreement with the data obtained on $YBa_2Cu_3O_7$ (see Fig.2) while the curve for $g_p=6$ ($\lambda_p\simeq 0.75$) yields somewhat too large values at higher T. The physically relevant effective mass enhancement $\lambda_Z\equiv \mathrm{Re}Z(\mathbf{k},\omega=0)-1$ turns out to be very anisotropic (see Fig. 3).

The corresponding values of the isotope exponent α for form factor F_t and $\lambda_p=0.75$, i.e., $\alpha\simeq 0.2$ (see Fig. 1) lie at the lower limit of the values which have been measured on $(Y,Pr)Ba_2Cu_3O_7$ (see crosses in Fig. 1).[2] It should be pointed out that the condition for global structural stability (Ref. 3), i.e., that $U_p<U$ is approximately satisfied up to $g_p=4$ since $U_p\cong g_p$ and since our effective U is larger than $J(\mathbf{Q})=U=3.7$ due to the $\mathbf{q}$ dependence of the coupling $J(\mathbf{q})$. The value $g_p=6$ (see Figs. 1 and 2) seems to lie at the limit of the requirement for global structural stability. The curves of α versus T_c for form factors F_0 and F_b lie far below the experimental values (see Fig. 1). All our attempts to increase α by varying the phonon frequency Ω_0, the width Γ_0 of our interaction $\alpha^2F(\mathbf{q},\Omega)$, the enhancement of this spectrum for small momentum transfer $\mathbf{q}$, or the band filling n have failed. Our negative values of α for constant form factor F_0 (see Fig. 1) are essentially in agreement with those found in Ref. 3. Our positive and larger values of α ($\leqslant 0.2$) for F_t cannot resolve the puzzle concerning the much larger values of α (up to about 0.5 in Fig. 1) which have been observed in nonoptimally doped, reduced-T_c cuprate materials.[2] We mention two attempts to resolve this puzzle. It has been shown that such large values of α can be obtained by exchange of *anharmonic* lattice tunneling excitations with reasonable coupling constants.[3] Another way to obtain substantially larger α and smaller T_c suppression is to assume *phonon-mediated d*-wave pairing with large enough $\lambda_{p,d}$.[11]

It should be pointed out that the *one-band* 2D Hubbard model for spin fluctuations and additional interaction for *harmonic* phonons is a minimum model for the cuprate superconductors. The FLEX approximation for this model yields a number of results which are consistent with experiments for larger doping concentrations. However, the failure to yield the observed decrease of T_c and the large increase of the isotope exponent α for decreasing doping concentration may indicate that the FLEX approximation or the model itself becomes invalid for low doping concentrations.

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