Experimental constraints on some mechanisms for high-temperature superconductivity

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Since its discovery, many mechanisms have been suggested to explain the phenomenon of high-temperature superconductivity in oxides. We propose that experimental data, along with theoretical models, can place constraints on or exclude many of these mechanisms. The isotope shift α, the transition temperature T_c, the ratio of the electronic-specific-heat jump to the normal-state specific heat $\Delta C/\gamma T_c$, and the superconducting gap ratio $2\Delta/k_B T_c$ are considered. We find limits on the applicability of solely phonon-based and combined phonon-electronic mechanisms.

I. INTRODUCTION

The advent of high-temperature superconductivity (HTS) in oxides[1,2] has led to an explosion of theoretical work aimed at explaining the properties of these materials. The many theories proposed range from minor variations on the phonon-based BCS-Eliashberg[3,4] theories to mechanisms completely independent of phonons, and both strong-coupling and weak-coupling theories have been suggested. Generally, these theories yield the high transition temperatures found in the oxide superconductors but differ in their predictions for other characteristic parameters of superconductivity such as the isotope effect parameter α, the gap ratio $2\Delta/k_B T_c$, the electronic-specific-heat discontinuity $\Delta C/\gamma T_c$, and some normal-state parameters. If it could be unequivocally determined whether the HTS oxides are weak- or strong-coupling superconductors, a large number of suggested mechanisms for HTS in the oxides could be eliminated. Although the experimental data do not yet clearly indicate strong or weak coupling, the aim of the present work is to show that the data can be used in conjunction with theory to constrain several of the suggested mechanisms. In Sec. II we summarize some relevant experiments and review predictions of the conventional theory in both the strong- and weak-coupling limits. In Sec. III, the theoretical basis for the calculations will be presented. Section IV contains the results, in which simple models are then used together with the experimental data to constrain and/or eliminate candidate theories. An exclusively phonon-based mechanism and a combined phonon-nonphonon mechanism are considered. The limitations of this method are discussed, and alternative explanations of the experimental results are examined.

II. SOME EXPERIMENTAL CONSTRAINTS

There are several experimental data which are crucial for determining the validity of a proposed theory for HTS in the oxides. Some of these are the energy gap ratio $2\Delta/k_B T_c$, the specific-heat jump $\Delta C/\gamma T_c$, and the isotope effect α. Both the energy gap ratio and the jump in specific heat can be used to distinguish between strong- and weak-coupling superconductors. If the HTS oxides are weak-coupling superconductors, a conventional phonon-mediated model would be excluded since phonons cannot give high T_c in the weak-coupling case. Historically, the isotope effect α has been used as an indicator of the importance of phonons for superconductivity in a given material.

Early determinations of the superconducting gap ratio $2\Delta/k_B T_c$ yielded a multitude of values ranging up to 20 in some of the HTS oxides, as compared to the theoretical values of 3.53 in the case of weak coupling and larger values in the case of strong coupling. More recent experiments using better materials have produced more reproducible results, but the values reported still vary widely, perhaps due to the anisotropy of the gap. Photoemission experiments[5] on Bi-Sr-Ca-Cu-O give a value for $2\Delta/k_B T_c$ of 8 ± 1.4, while tunneling experiments[6] yield 6.2 ± 0.3 for tunneling perpendicular to the c axis and 3.3 ± 0.3 for tunneling along the c axis. Reflectivity measurements on Bi-Sr-Ca-Cu-O,[7] however yield $2\Delta/k_B T_c=3.3$, with the temperature dependence of the gap substantially different from the BCS model prediction for temperatures near T_c. In Y-Ba-Cu-O, infrared conductivity[8] and reflectivity[9,10] experiments suggest that $2\Delta/k_B T_c\approx8$. In La-Sr-Cu-O, $2\Delta/k_B T_c$ varies[11] between 4 and 9, and for Ba-K-Bi-O, tunneling[12] yields 3.5 ± 0.5.

Another experiment which sheds light on the strong-versus-weak coupling question is the ratio of the specific-heat jump at T_c to the specific heat in the normal state at T_c, $\Delta C/\gamma T_c$. BCS theory predicts $\Delta C/\gamma T_c=1.43$, while strong-coupling effects increase this value. In La-Sr-Cu-O, $\Delta C/\gamma T_c=3.2$, while in Y-Ba-Cu-O, a value of 4.8 is found.[13,14] For Bi-Sr-Ca-Cu-O, $\Delta C/T_c$ has been found by two groups[15,16] to be 16 and 37 mJ/(mol K^2), respectively. Combining these results with a theoretical calculation,[17] $\gamma=5$ mJ/(mol K^2), yields values of $\Delta C/\gamma T_c$ of approximately 3 and 7. All of these values

are indicative of strong coupling.

In the case of the isotope effect, the simplest BCS model predicts that $\alpha=0.5$, while inclusion of the repulsive Coulomb interaction between the electrons reduces α. For weak-coupling superconductors, values of α between 0 and 0.5 are found, while in the strong-coupling limit, α is generally close to 0.5 except when the repulsive Coulomb interaction is very strong.[18,19] Therefore, absence of the isotope effect ($\alpha\approx 0$) does not exclude a phonon-based explanation of superconductivity for a given material.

In Ba-K-Bi-O, the reported values of α for oxygen substitution[20–22] vary between 0.22 and 0.4. In La-Sr-Cu-O at the maximum T_c composition, several groups[23–25] have reported $\alpha=0.14$, indicating that phonons play a significant role. In Y-Ba-Cu-O, the isotope effect is nearly absent[26–28] ($\alpha\approx 0.02$) although other groups[29,30] have observed larger shifts in T_c in experiments performed by different methods. A measurement[31] of α in Bi-Sr-Ca-Cu-O yielded $\alpha=0.034-0.048$.

III. THEORY AND CALCULATIONAL METHOD

Although the isotope effect is not a clear indicator of weak-versus-strong coupling, it can be used in conjunction with theoretical models to obtain information on superconducting mechanisms. In this section the theory for calculating the isotope shift parameter α and the superconducting gap $\Delta(T=0)$ is briefly reviewed. A more complete derivation is given in Ref. 32. The calculations are based on the nonlinear Eliashberg equations. The electron-phonon interaction spectrum $\alpha^2F(\omega)$ is used to define

$$\lambda(n-m)=2\int_0^\infty d\Omega\frac{\Omega\alpha^2F(\Omega)}{\Omega^2+(\omega_n-\omega_m)^2}\ , \tag{1}$$

where the Matsubara frequencies $\omega_n=(2n+1)\pi T$, n is an integer, and T the temperature. Near the transition temperature T_c, the Eliashberg equations may be linearized and simplified to yield

$$0=\sum_{m=0}^{N} S(n,m)\Delta'(i\omega_m) \tag{2}$$

with

$$S(n,m)=\lambda(n-m)+\lambda(n+m+1)-2\mu^*(\omega_c) -\delta_{nm}\left[2n+1+\lambda(0)+2\sum_{j=1}^{n}\lambda(j)\right], \tag{3}$$

where $N=\omega_c/(2\pi T)$, ω_c is the cutoff energy for the sums over the Matsubara frequencies, $\Delta'(i\omega_m)=\Delta(i\omega_m)/(2m+1)$, and $\Delta(i\omega_n)$ is the gap function at the Matsubara frequency ω_n. Also, μ^* is the Coulomb pseudopotential for the cutoff ω_c. Equations (2) and (3) define an eigenvalue problem and the transition temperature T_c is the temperature at which the largest eigenvalue equals zero.

In our calculations, the electron-phonon interaction spectrum $\alpha^2F(\omega)$ is modeled by a sum of Lorentzian peaks chosen to mimic the major features in $F(\omega)$, the experimental phonon density of states. In the following discussion, values of μ^* from these calculations will be reported as $\mu^*(\omega_{\rm rms})$, where $\omega_{\rm rms}$ is the rms phonon frequency. This is done so that the values of μ^* may be compared with those used in calculations within the two-square-well model, which uses $\mu^*(\omega_D)$. The relation between $\mu^*(\omega_c)$ which appears in the Eliashberg equations to $\mu^*(\omega_{\rm rms})$ is given by

$$\mu^*(\omega_{\rm rms})=\frac{\mu^*(\omega_c)}{1+\mu^*(\omega_c)\ln(\omega_c/\omega_{\rm rms})}\ . \tag{4}$$

The isotope effect α is calculated by shifting peaks in the electron-phonon interaction spectrum $\alpha^2F(\omega)$ to simulate isotopic substitution. The central frequency and the width of the Lorentzian peak in $\alpha^2(\omega)$ are scaled as $M^{-1/2}$ for a small change in M. Since the repulsive Coulomb interaction between the electrons is assumed to be constant, the values of μ^* and ω_c are not changed. The transition temperature is then calculated using the modified $\alpha^2F(\omega)$, and the isotope effect parameter is calculated from $\alpha=-(d\ln T_c)/(d\ln M)$.

To calculate $2\Delta/k_BT_c$, we need the gap at zero temperature $\Delta(0)$. Since $\Delta(T)$ is essentially constant for $T\ll T_c$, we approximate $\Delta(0)$ by $\Delta(0.1T_c)$. The linearization procedure applied above in the determination of T_c cannot be used here since $T\ll T_c$, so the nonlinear Eliashberg equations must be solved self-consistently. An initial guess for the gap function $\Delta(i\omega_n)$ is used, and the equations are then iterated to convergence. This procedure yields the gap function $\Delta(i\omega_n)$ at the Matsubara frequencies. A Padé approximant method[33] is used to analytically continue Δ onto the real axis, yielding $\Delta(\omega)$. The energy gap Δ_0 is given by the solution of $\Delta_0=\Delta(\Delta_0)$.

IV. RESULTS AND DISCUSSION

We focus here on mechanisms including phonons that have been proposed by several authors[34] to explain HTS in the oxides. Some of these suggestions rely solely on phonons as a mechanism for the superconductivity. Another class of theories has been in the area of combined phonon and electronic mechanisms. In this case an additional pairing boson is postulated, usually with a much higher and mass-independent characteristic energy. Such mechanisms can suppress the isotope effect while raising T_c due to the high value of the characteristic energy and the mass independence of the additional boson. A third possibility raised is that the phonons are unimportant and that HTS in oxides arises from a completely new mechanism, such as a magnetic mechanism. We will not consider such mechanisms in this paper. Our aim is to consider a few experimental data and use these as constraints to reduce the large number of candidates for mechanisms of HTS which involve some phonon coupling.

For the solely phonon-based mechanisms, the characteristic parameters of the interaction are an average phonon frequency $\langle\omega_{\rm ph}\rangle$ and the strength of the electron-phonon interaction $\lambda_{\rm ph}$. For electronic mechanisms, the relevant energy scale is that of the exchange boson (exci-

ton) and is given by ω_{el}. The strength of its coupling to the electrons is given by λ_{el}. Phonon-based mechanisms fall into the strong-coupling regime, due to the large value of $T_c/\langle\omega_{ph}\rangle$, while electronic mechanisms usually have weak coupling because of their higher characteristic frequency ω_{el}. Thus, in the phonon-based mechanisms, one expects the isotope effect to agree with the BCS model prediction of $\alpha=0.5$. The inclusion of the Coulomb pseudopotential results in $\alpha<0.5$. In a purely electronic mechanism, $\alpha=0$ since ω_{el} is independent of the ionic mass, while in a combined phonon-electronic mechanism, intermediate values of α are expected. The near vanishing of α in some of the high-T_c oxides has led to the claim that phonons cannot explain their superconductivity; we will examine this claim later in Sec. IV A.

For the weak-coupling case, the ratio of the superconducting gap to the transition temperature $2\Delta/k_BT_c=3.53$, while it may substantially exceed this value in the strong-coupling case. Physically, in the case of strong coupling, at T_c the thermally excited phonons reduce T_c via pair-breaking effects,[35] while the effect on Δ is much smaller since Δ is measured at $T\ll T_c$. In the extreme strong-coupling limit, $2\Delta/k_BT_c$ is predicted[36] to saturate at about 13.

Excluding the HTS oxides, the largest calculated value for $\Delta C/\gamma T_c$ in a real material is $\Delta C/\gamma T_c\sim 3$ in a Pb-Bi alloy.[37] Calculations[37] within Eliashberg theory indicate that an approximate upper limit of $\Delta C/\gamma T_c\leq 4$ exists. This limit is weakly dependent on the strength of the Coulomb pseudopotential μ^*, varying from 3.4 at $\mu^*=0$ to 3.9 at $\mu^*=0.3$. It has been shown[38] that the temperature dependence of the energy gap affects the value of $\Delta C/\gamma T_c$, and deviations from the BCS prediction for $\Delta(T)/\Delta(0)$ can lead to enhanced $\Delta C/\gamma T_c$ even if the gap ratio $2\Delta/k_BT_c$ lies in the weak-coupling regime.

A. Phonon-only mechanisms

It has been noted[39] that a model using purely phonon-mediated pairing can yield HTS, and an early attempt[40] to explain HTS in La-Sr-Cu-O showed that transition temperatures $T_c\sim 40$ K could be obtained in realistic calculations for La-Sr-Cu-O. These phonon-based mechanisms are strong-coupling mechanisms, implying that the energy gap $2\Delta/k_BT_c$ and the electronic-specific-heat jump $\Delta C/\gamma T_c$ will substantially exceed their weak-coupling limits of 3.53 and 1.43, respectively. The key obstacle to a phonon-based theory of HTS in the oxides is the extremely small isotope effect α found in the highest-T_c superconductors. An attempt by two of us[18] to reconcile a purely phonon-based mechanism with the high-T_c and small α found in the oxides failed in the case of Y-Ba-Cu-O but did not exclude such a mechanism in the case of La-Sr-Cu-O. For Y-Ba-Cu-O, it was shown that within a three-dimensional isotropic Eliashberg model using harmonic phonons, unphysically large values for the parameters λ and μ^* ($\lambda\sim 30$, $\mu^*\sim 0.45$) were required to reproduce the high T_c and small α seen experimentally. These calculations were performed using a phonon spectrum based on neutron-scattering experiments on Y-Ba-Cu-O. A more recent study[19] using a less constrained model of the phonon spectrum also found that both high T_c and small α may be obtained for nonphysical values of λ and the Coulomb pseudopotential μ^*.

The values of λ obtained in Ref. 19 are smaller than those found in Ref. 18 because Akis and Carbotte considered only a high-frequency Einstein phonon spectrum as opposed to the phonon spectrum modeled on experiment with a smaller $\langle\omega_{ph}\rangle$. In either case the necessary values of λ and μ^* are substantially greater than those found in conventional superconductors. For La-Sr-Cu-O, we found it unlikely that phonons could account for high T_c. The necessary values of λ and μ^* are $\lambda=3$ and $\mu^*\sim 0.3$. These values are outside the known ranges but not drastically so, leaving phonon-based superconductivity as a possibility for La-Sr-Cu-O. In the case of Ba-K-Bi-O, a spectrum of two Einstein peaks was used to reproduce the major features in the measured phonon density of states $F(\omega)$. Using this spectrum as a model $\alpha^2F(\omega)$, curves of constant $T_c\sim 30$ K and $\alpha=0.40$ were obtained in the (λ,μ^*) parameter space. Figure 1 shows the calculated curves of constant T_c and α, as well as a continuation of the constant α curve to smaller λ. The continuation of α was calculated from the two-square-well model with renormalization within which

$$\alpha=\frac{1}{2}\left[1-\left[\frac{\mu^*}{\lambda^*-\mu^*}\right]^2\right], \tag{5}$$

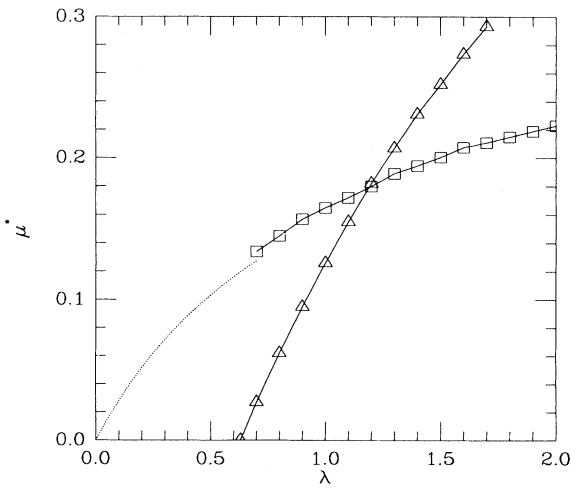

FIG. 1. Values of λ and μ^* for which $T_c=30$ K (triangles) or $\alpha=0.40$ (squares) calculated from the Eliashberg equations. These values are representative for Ba-K-Bi-O. The solid lines are guides to the eye. The dotted line represents the values of λ and μ^* for which $\alpha=0.4$ from the renormalized two-square-well model. The intersection of the solid lines at $(\lambda,\mu^*)=(1.2,0.18)$ indicates that these values of the parameters are consistent with a phonon-mediated coupling model. In contrast, a similar study for Y-Ba-Cu-O led[18] to unphysical values of λ.

where $\lambda^*=\lambda/(1+\lambda)$. The two different methods of calculating α agree well in the moderate-coupling range ($\lambda\sim0.6$). The intersection of the constant-T_c and constant-α curves yields values for the parameters (λ,μ^*) consistent with a model of solely phonon-mediated coupling. From Fig. 1, the intersection occurs at $\lambda=1.2$ and $\mu^*(\omega_{\rm rms})\approx0.18$, where $\omega_{\rm rms}=50$ meV. The calculated gap ratio is $2\Delta/k_BT_c=4.0$, which agrees with the experimental value of 3.5 ± 0.5 cited above. These values for λ and μ^* are well within the range of those for known BCS superconductors, suggesting that phonons may be responsible for superconductivity in Ba-K-Bi-O.

Although phonons are capable of yielding high T_c for reasonable coupling strengths, conventional BCS/Eliashberg theory predicts that the combination of high T_c and small α excludes the purely phonon mechanism for the highest-T_c oxides. Many authors have therefore been led to introduce additional features to the phonon mechanism in order to suppress the isotope effect, including anharmonic phonons, interactions with defects, and lower dimensionality. Generally, these models yield a reduced isotope effect and high T_c, but they lack clear predictions of T_c and α. In the 1970s Hui and Allen[41] showed that an anharmonic potential had only a small effect on the strength of the electron-phonon interaction. More recently, it has been proposed[42] that a double-well potential could lead to enhanced coupling strengths, but its effect on the transition temperature and the isotope effect are unclear.

B. Combined phonon-electron mechanisms

To account for the high T_c of the oxides, electronic or combined phonon and electronic mechanisms have been proposed by many authors. In general, higher-energy cutoffs characteristic of electronic mechanisms lead to larger prefactors in the T_c equation and higher T_c; however, this may not always be the case.[43] By considering the experimental values of α and T_c, constraints may be placed on the range of energies of the electronic mechanisms added to the phonons.

The electron-phonon interaction spectrum $\alpha^2F(\omega)$ is modeled by a few δ-function peaks designed to represent the major peaks in the phonon density of states $F(\omega)$ as measured by neutron scattering. In the calculation of the isotope effect α, these peaks are shifted as described in Sec. III above. An additional mass-independent peak of arbitrary frequency is added to simulate the nonphonon mechanism, instead of using a negative μ^* which is an attractive Coulomb pseudopotential as has been done by other authors.[44] Physically, a single peak in $\alpha^2F(\omega)$ corresponds to a pairing boson of a specific energy, while a negative μ^* implies a constant attractive interaction acting over all energies up to the cutoff ω_c.

The frequencies and relative weights of the phonon peaks are fixed, while an overall scaling factor is used to yield the desired coupling strength $\lambda_{\rm ph}$. The strength $\lambda_{\rm el}$ and frequency $\omega_{\rm el}$ of the nonphonon interaction are allowed to vary freely. By imposing two constraints on these three free parameters $(\lambda_{\rm ph},\lambda_{\rm el},\omega_{\rm el})$, any two of the parameters may be obtained as functions of the third. The constraints chosen are that the calculated transition temperature T_c and isotope effect α must match the experimental results for the material under consideration. The energy scale of the nonphonon interaction, $\omega_{\rm el}$, is chosen as the one free parameter, yielding $\lambda_{\rm ph}$ and $\lambda_{\rm el}$ as functions of $\omega_{\rm el}$. For a given $\omega_{\rm el}$, $\lambda_{\rm ph}$ and $\lambda_{\rm el}$ are varied until the calculated α and T_c agree with the experimental values. The $\lambda_{\rm ph}$ resulting from this calculation is then compared with experimental and theoretical estimates to constrain the range of $\omega_{\rm el}$. The gap ratio $2\Delta/k_BT_c$ is also obtained as a function of $\omega_{\rm el}$. Within the constrained range of $\omega_{\rm el}$ as determined by comparison of $\lambda_{\rm ph}$ with estimates from experiment and theory, the calculated $2\Delta/k_BT_c$ gives some indication of whether such a combined mechanism would be strong or weak coupling.

The results obtained earlier[45] were somewhat surprising in that a combined phonon-electronic mechanism was found to be inconsistent with the estimates of $\lambda_{\rm ph}$ for Y-Ba-Cu-O, but not for the lower-T_c oxides. Figure 2 shows the calculated values of $\lambda_{\rm ph}$, λ, and $\lambda_{\rm ph}/\lambda$ taken from Ref. 45 and a calculation of $2\Delta/k_BT_c$ for Y-Ba-Cu-O ($T_c=93$ K, $\alpha=0.02$). For a high-energy electronic mechanism with $\omega_{\rm el}>100$ meV, the constraints on α and T_c limit $\lambda_{\rm ph}$ to lie between 0.05 and 0.10, well below (by a

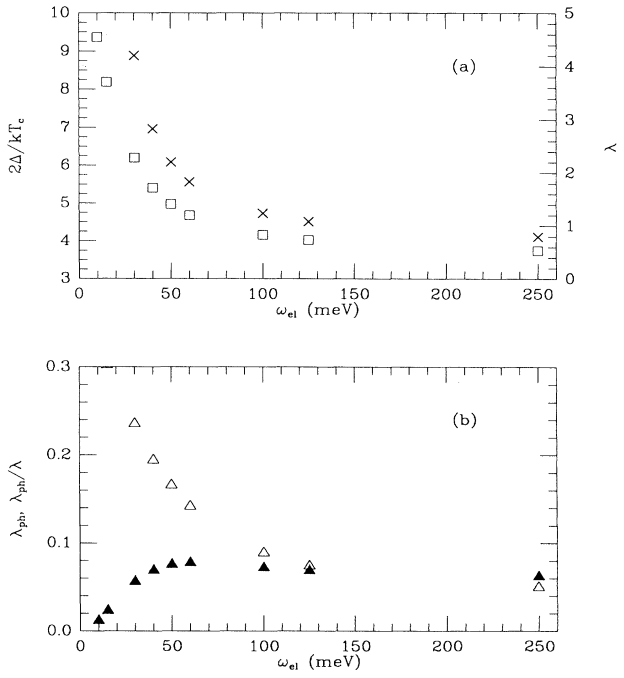

FIG. 2. Calculated parameters plotted against the characteristic energy $\omega_{\rm el}$ of the nonphonon interaction giving measured values of α and T_c appropriate for Y-Ba-Cu-O. (a) Total coupling $\lambda=\lambda_{\rm ph}+\lambda_{\rm el}$ (crosses, right-hand scale), and the gap ratio $2\Delta/k_BT_c$ (squares, left-hand scale). (b) Phonon-mediated coupling $\lambda_{\rm ph}$ (open triangles) and the fraction of phonon-mediated coupling $\lambda_{\rm ph}/\lambda$ (filled triangles).

factor of 3–10) the estimates of λ_{ph}. A recent experimental estimate[46] based on pump-probe experiments yielded $\lambda_{ph} \sim 0.9$ for Y-Ba-Cu-O, far above the calculated λ_{ph} for the combined mechanism considered here. Even for ω_{el} between 10 and 100 meV, our calculations give $\lambda_{ph} < 0.3$ and thus a low-energy phonon-nonphonon mechanism can also be excluded in Y-Ba-Cu-O. For $\omega_{el} < 10$ meV, λ becomes extremely large ($\lambda \geq 13$). Such values of λ are unphysical due to the onset of electron localization and/or lattice instabilities at extremely strong coupling. However, as is clear from Fig. 2, for small values of ω_{el} the theory is consistent with values of λ_{ph} and λ that are physically acceptable. The large values of $2\Delta/k_B T_c$ measured in Y-Ba-Cu-O indicate that a strong-coupling mechanism is most likely to be responsible for superconductivity in Y-Ba-Cu-O. In one experiment,[8] however, no structure was found in the conductivity above the energy gap, suggesting that the conventional model may be inapplicable to Y-Ba-Cu-O. If the conventional model of pair-breaking via thermal quasiparticle effects applies, then these large values of $2\Delta/k_B T_c$ also exclude a high-energy electronic mechanism, since the calculated $2\Delta/k_B T_c$ is large only for $\omega_{el} < 100$ meV.

The general behavior of λ_{ph}, λ, and λ_{ph}/λ can be understood as follows. As ω_{el} is decreased, λ must increase to keep T_c constant. Similarly, λ_{ph}/λ must be roughly constant to keep α at its fixed value. Consequently λ_{ph} increases as ω_{el} decreases.

In the present calculations the failure of the combined electronic-phonon mechanism to yield superconductivity in Y-Ba-Cu-O may be related to the use of an isotropic three-dimensional model that assumes a Fermi-liquid ground state. An alternative is that the Eliashberg theory is incorrect for an attractive interaction represented by a δ-function potential.

Figure 3 shows the results for La-Sr-Cu-O ($T_c \sim 40$ K, $\alpha = 0.14$). We concluded that an electronic mechanism can be excluded for $\omega_{el} > 70$ meV, since the estimates[40,47] of λ_{ph} exceed the calculated values by a factor of 2 to an order of magnitude. The calculated values of $2\Delta/k_B T_c$ and λ fall into the strong-coupling regime for the admissible range of ω_{el}. Strong coupling in La-Sr-Cu-O is also suggested by the experimental result $\Delta C/\gamma T_c = 3.2$, well above the weak-coupling limit of 1.43.

A similar analysis has been performed for Ba-K-Bi-O ($T_c \sim 27$ K, $\alpha = 0.40$) and the calculated λ_{ph}, λ, and $2\Delta/k_B T_c$ are shown in Fig. 4. No experimental estimates of λ_{ph} are available, but the value found for $2\Delta/k_B T_c$ is consistent with the experimental value for all ω_{el}. There-

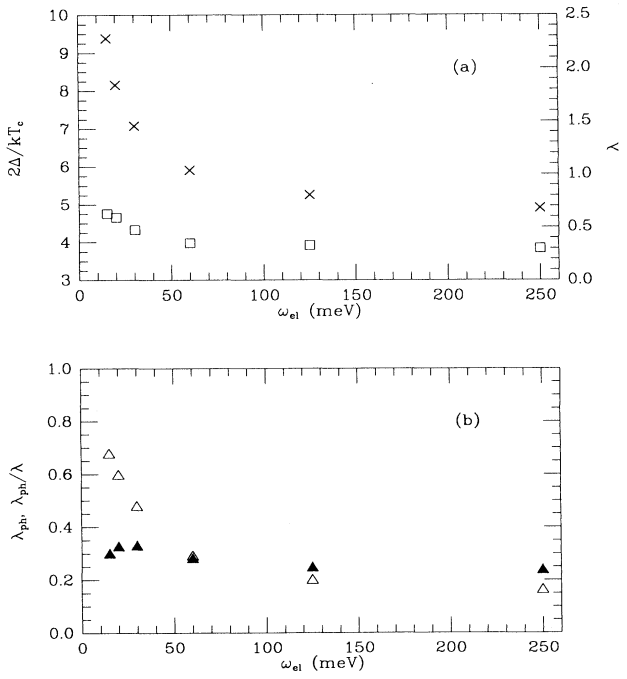

FIG. 3. Calculated parameters plotted against the characteristic energy ω_{el} of the nonphonon interaction giving measured values of α and T_c appropriate for La-Sr-Cu-O. (a) Total coupling $\lambda = \lambda_{ph} + \lambda_{el}$ (crosses, right-hand scale), and the gap ratio $2\Delta/k_B T_c$ (squares, left-hand scale). (b) Phonon-mediated coupling λ_{ph} (open triangles) and the fraction of phonon-mediated coupling λ_{ph}/λ (filled triangles).

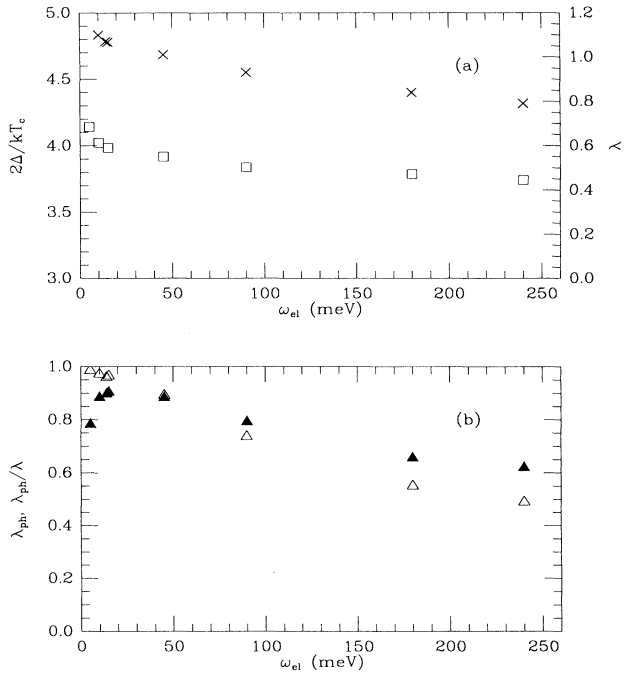

FIG. 4. Calculated parameters plotted against the characteristic energy ω_{el} of the nonphonon interaction giving measured values of α and T_c appropriate for Ba-K-Bi-O. (a) Total coupling $\lambda = \lambda_{ph} + \lambda_{el}$ (crosses, right-hand scale), and the gap ratio $2\Delta/k_B T_c$ (squares, left-hand scale). (b) Phonon-mediated coupling λ_{ph} (open triangles) and the fraction of phonon-mediated coupling λ_{ph}/λ (filled triangles). Hence $\lambda_{ph} < 0.9$ for Ba-K-Bi-O.

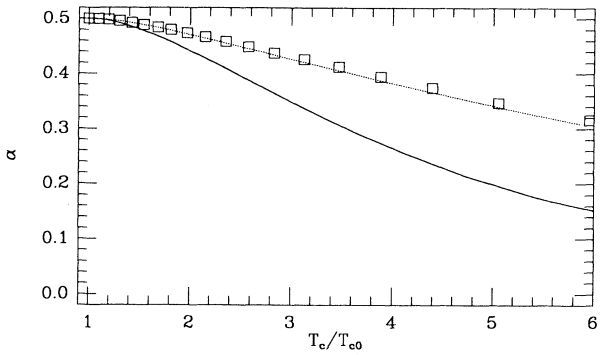

FIG. 5. The isotope effect α is plotted vs the normalized transition temperature T_c/T_{c0} for different models with a phonon coupling of $\lambda=0.5$ and an attractive Coulomb pseudopotential of varying strength. The solid line represents the results from Ref. 48, the dotted line the results from the McMillan (Ref. 50) equation, and the squares exact numerical calculations using the Eliashberg theory. The results from Ref. 48 do not agree with those from the McMillan equation or the exact numerical results. To allow comparison of the different models, the transition temperatures have been normalized by dividing by T_{c0}, the transition temperature calculated by including only the phonon interaction.

fore, a combined phonon-nonphonon mechanism cannot be excluded for Ba-K-Bi-O.

For the Bi-based HTS oxides, the measured values of the isotope effect are small and close to that observed for Y-Ba-Cu-O. We therefore expect that, given a reasonably similar phonon spectrum for Y-Ba-Cu-O and Bi-Sr-Ca-Cu-O, similar limits on λ_{ph} will be obtained. If the phonon contribution is similar to that in Y-Ba-Cu-O, as was found in a recent experiment,[46] then a high-energy electronic mechanism could also be excluded in Bi-Sr-Ca-Cu-O.

Other authors[19,44,48] have also done calculations of the isotope effect within a combined phonon-nonphonon model. A calculation using the Eliashberg theory and a similar model for the phonon spectrum (but with only one peak for the phonons) showed[19] that the isotope effect was strongly reduced by the addition of nonphonon coupling.

A more recent proposal[48] examines the combined mechanism within a model similar to the two-square-well model,[49] but with a second interaction that may be attractive as well as repulsive. In the case of an attractive Coulomb (or nonphonon) interaction, modeled via a negative μ^*, they also obtain a decrease in isotope effect with increasing nonphonon coupling (at constant λ_{ph}). In Fig. 5, the results from the modified two-square-well model presented in Ref. 48 are compared with those from our calculations using the McMillan[50] equation and the strong-coupling (Eliashberg) theory. The Eliashberg theory calculations were performed with a single Einstein (δ-function) peak for $\alpha^2F(\omega)$ and a negative μ^* to simulate the added attractive interaction. Figure 5 shows the calculated value of α as a function of T_c, normalized to the value of T_c calculated with $\lambda=0.5$ and no additional interaction. The exact Eliashberg calculation agrees well with the results from the McMillan equation, while the two-square-well model of Ref. 48 clearly exaggerates the deviation of the isotope effect from the BCS value of 0.5 at large T_c due to the neglect of strong-coupling effects.

V. CONCLUSIONS

Based on measurements of the isotope effect and T_c, a solely phonon-mediated mechanism can be excluded in the cases of Y-Ba-Cu-O and Bi-Sr-Ca-Cu-O within the assumptions of our models. In La-Sr-Cu-O, it seems unlikely that phonons alone can account for HTS, while phonons remain a good candidate in Ba-K-Bi-O. The isotope effect and T_c data can also be used to constrain combined phonon-nonphonon mechanisms within Eliashberg theory for La-Sr-Cu-O and Y-Ba-Cu-O.

The experimental evidence cannot yet conclusively determine whether the Cu-O–based HTS oxides fall into the category of strong or weak coupling, while for Ba-K-Bi-O, the available experimental data are consistent with either a purely phonon or mixed phonon-electronic mechanism with moderately strong coupling. In the three Cu-based HTS oxides considered here, the specific-heat discontinuity $\Delta C/\gamma T_c$ is indicative of strong coupling, while the isotope effect α tends to argue for weaker coupling. The results for $2\Delta/k_BT_c$ are mixed, since different techniques give widely varying values for $2\Delta/k_BT_c$. It is possible that these contradictory results could be reconciled by the addition of other effects, such as lower dimensionality, anharmonicity, or a non-BCS temperature dependence of the gap, but there are few quantitative predictions from such theories.

We have shown how a few experimental data can be used to constrain the range of possible models for HTS in the oxides. Hopefully, future experiments will determine whether the HTS oxides are strong- or weak-coupling superconductors and will help determine the appropriate theory for HTS.

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