

Marginal-Fermi-liquid theory and the isotope effect

E. J. Nicol and J. P. Carbotte

Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1

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In the marginal-Fermi-liquid model, the coupling between two electrons is via charge (attractive) and spin (repulsive) fluctuations, and so it does not exhibit an isotope effect. To include this effect, an additional phonon contribution must be introduced. Using the case of $\text{YBa}_2\text{Cu}_3\text{O}_7$, for illustrative purposes, with a total isotope effect coefficient of $\beta_{\text{tot}} \cong 0.05$ at a T_c of 90 K, we find that the implied electron-phonon mass renormalization is very small for coupling to high-energy phonons but increases rapidly with decreasing phonon frequency or an increasing amount of spin fluctuations. Finally, we examine how β increases with decreasing T_c when charge fluctuations are reduced or spin fluctuations augmented.

I. INTRODUCTION

The oxygen isotope effect in $\text{YBa}_2\text{Cu}_3\text{O}_7$ has been measured by many authors.¹⁻⁸ In all cases, it is found to be small and of the order of 0.05, with some values as high as 0.1.⁸ Bourne *et al.*⁹ find that the Ba and Cu isotope effect coefficient is essentially zero as do several other groups.¹⁰⁻¹³ Thus, the total isotope effect coefficient β_{tot} is small, $\cong 0.05$. Small values for the isotope effect have also been found in the Tl and Bi copper oxides as reviewed by Katayama-Yoshida *et al.*¹⁴ These results favor a nonphonon, electronic mechanism for the pairing in the high- T_c oxides although other interpretations have been given by Phillips.¹⁵⁻¹⁷

More recently, new results by Crawford *et al.*¹⁸ in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ as a function of x and by Franck *et al.*¹⁹ in $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ have revealed that the oxygen isotope coefficient $\beta_{\text{ox}} \equiv -d \ln T_c / d \ln M_{\text{ox}}$, with M_{ox} the oxygen mass, can vary greatly with dopant x . By the time the critical temperature has been reduced to 30 K, β_{ox} is almost 0.5. This can be understood in terms of energy dependence in the electronic density of states near the Fermi energy on a scale of importance for superconductivity. Tsuei *et al.*²⁰ use a van Hove singularity while Schachinger, Greeson, and Carbotte²¹ employ a Lorentzian form. For the specific case of $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ an alternative explanation has been given by Carbotte, Greeson, and Perez-Gonzalez²² in terms of the pair breaking effect of the Pr dopant. While it is not yet well understood what changes occur in the electronic and spin structure of $\text{YBa}_2\text{Cu}_3\text{O}_7$ when the yttrium is replaced by praseodymium,²³ there is some evidence that the Pr ions act as ordinary paramagnetic impurities, strongly exchanged coupled to the holes in the CuO_2 planes. Other evidence suggests filling of mobile holes in the conducting plane by electrons donated by the substituted Pr. This would favor the energy-dependent density of states $N(\epsilon)$ model in which the chemical potential shifts away from the peak in $N(\epsilon)$ with a corresponding increase in β .

A model for the high- T_c oxides that has received considerable attention is the marginal-Fermi-liquid mod-

el.²⁴⁻²⁸ It appears to be able to explain many of the anomalous normal-state properties observed in the oxides.²⁴ Superconducting properties have also been worked out.²⁸⁻³³ In this model, charge (attractive) and spin (repulsive) fluctuations are involved in the pairing potential, and so $\beta=0$. It is interesting to investigate whether large values and rapid variation of the isotope coefficient β can be incorporated into this model without introducing a large phonon contribution. In this paper, we extend the model to include a phonon contribution and investigate what limits are put on the electron-phonon mass renormalization by the constraint $\beta=0.05$ in stoichiometric $\text{YBa}_2\text{Cu}_3\text{O}_7$. We also investigate how the isotope effect increases when the critical temperature is reduced through an increase in spin fluctuations or a decrease in the charge fluctuations keeping, in all cases, the electron-phonon interaction fixed.

In Sec. II, we present formalism and preliminary simple results while Sec. III contains our main results. A conclusion is found in Sec. IV.

II. FORMALISM AND SIMPLE RESULTS

All the work in this paper is based on the Eliashberg equations of the form

$$\Delta(i\omega_n)Z(i\omega_n) = \pi T_c \sum_m [\lambda^-(m-n) - \mu^*] \frac{\Delta(i\omega_m)}{|\omega_m|} \quad (1)$$

and

$$\omega_n Z(i\omega_n) = \omega_n + \pi T_c \sum_m \lambda^+(m-n) \text{sgn}(\omega_m), \quad (2)$$

where $\Delta(i\omega_n)$ and $Z(i\omega_n)$ are, respectively, the Matsubara gap and renormalization functions with $\omega_n = (2n-1)\pi T$. Here, T is the temperature and $n=0, \pm 1, \pm 2, \dots$. In Eqs. (1) and (2), μ^* is the usual Coulomb pseudopotential and $\lambda(n-m)$ is given in terms of the electron-exchange-boson spectral density $\alpha^2 F(\omega)$ for any boson exchange process of interest, i.e., phonons, plasmons, charge fluctuations, etc., by

$$\lambda^+ = \lambda^- = \lambda(n-m) = \int_0^\infty \frac{2\omega\alpha^2 F(\omega)}{\omega^2 + (\omega_n - \omega_n)^2} d\omega. \quad (3)$$

In the marginal-Fermi-liquid model,²⁴⁻³³ an essential feature is the coupling to both charge and spin fluctuations as described by Kuroda and Varma.²⁸ In this case the charge degrees of freedom, which are pair creating, couple to the superconducting electrons through a dimensionless coupling λ_ρ while coupling to spin is described by λ_σ . The modifications of Eqs. (1) and (2) are made by replacing $\lambda^-(m-n)$ by $(\lambda_\rho - \lambda_\sigma)F(m-n)$ and $\lambda^+(m-n)$ by $(\lambda_\rho + \lambda_\sigma)F(m-n)$ where in a simple approximation

$$F(m-n) = \frac{1}{\pi} \int_0^{\omega_c} \frac{2\omega \tanh\left[\frac{\omega}{2T}\right]}{\omega^2 + (\omega_m - \omega_n)^2} d\omega. \quad (4)$$

Here ω_c is an upper cutoff on the excitation spectrum. Note that the parameters of the theory are λ_ρ , λ_σ , and ω_c .

To add phonons to the marginal-Fermi-liquid model we need only to add to each of $\lambda^+ = (\lambda_\rho + \lambda_\sigma)F(n-m)$ and $\lambda^- = (\lambda_\rho - \lambda_\sigma)F(n-m)$ a phonon contribution of the form (3) with $\alpha^2 F(\omega)$ being the electron-phonon spectral density. A feature of this extended marginal-Fermi-liquid model which should be noted is that both spin and charge fluctuations are determined by the same kernel $F(m-n)$ while the phonons are different. For the purpose of this paper it will be sufficient to use a delta function model for the electron-phonon spectral density at a single Einstein energy ω_E , i.e.,

$$\alpha^2 F(\omega) = \frac{\omega_E \lambda_E}{2} \delta(\omega - \omega_E). \quad (5)$$

Here, λ_E is the electron-phonon mass enhancement factor. This parameter is often taken to be a measure of the strength of the electron-phonon interaction.

To start, let us consider a pure phonon model consisting of a number of different modes ω_{Ei} with associated mass enhancement factor λ_i where $\lambda_i = 2A_i/\omega_{Ei}$ for a spectral weight model $\alpha^2 F(\omega) = \sum_i A_i \delta(\omega - \omega_{Ei})$. If we use a square well model³⁴ in Eqs. (1) and (2) with a constant gap value (a very rough approximation) we can get an interesting result for T_c , namely,

$$T_c = 1.13 \left[\prod_i (\omega_{Ei})^{\lambda_i/\lambda_{\text{tot}}} \right] \left(e^{-(1+\lambda_{\text{tot}})/\lambda_{\text{tot}}} \right), \quad (6)$$

which is not expected to be accurate but which has a suggestive form. If all the ω_{Ei} 's are the same we recover the BCS result $T_c = 1.13\omega_E \exp[-(1+\lambda_{\text{tot}})/\lambda_{\text{tot}}]$ with $\lambda_{\text{tot}} \equiv \sum_i \lambda_i$. An interesting feature of Eq. (6), however, is that the partial isotope effect is

$$\beta_i \equiv -\frac{d \ln T_c}{d \ln M_i} = \frac{1}{2} \frac{\lambda_i}{\lambda_{\text{tot}}}, \quad (7)$$

where we have associated a different mass M_i with each ω_{Ei} . On summing Eq. (7), we recover the well-known re-

TABLE I. The isotope coefficient calculated from the exact solution of Eqs. (1) and (2) compared to the approximate form of Eq. (7).

i	ω_{Ei}	λ_i	β_i exact	β_i approx.
1	5	0.1	0.198	0.167
2	10	0.05	0.086	0.083
3	15	0.15	0.216	0.250
Total		0.3	0.5	0.5

sult that $\beta_{\text{tot}} \equiv \sum_i \beta_i = \frac{1}{2}$ for a pure phonon model. While we do not expect Eq. (7) to be very accurate, in Table I we show results for the β_i 's in a model with $T_c \cong 1$ K, $\lambda_1 = 0.1$ ($\omega_{E1} = 50$ meV), $\lambda_2 = 0.05$ ($\omega_{E2} = 10.0$ meV), and $\lambda_3 = 0.15$ ($\omega_{E3} = 15.0$ meV). On comparing results from complete numerical solutions of Eqs. (1) and (2) with results from Eq. (7) we see good but not exact agreement. We have found that as the λ_i 's are increased, the agreement becomes much worse. Nevertheless, we can use Eq. (7) to illustrate some important points in the discussion of the numerical results.

Suppose we now use an equation of the form of (6) for the extended marginal-Fermi-liquid model which includes a phonon contribution in addition to coupling in the pairing channel with charge (attractive) and spin (repulsive) fluctuations. It is

$$T_c = 1.13 \omega_E^{\lambda_E/(\lambda_E + \bar{\lambda}_-)} \bar{\omega}_c^{\bar{\lambda}_-/(\lambda_E + \bar{\lambda}_-)} \times e^{-(1+\lambda_E + \bar{\lambda}_+)/(\lambda_E + \bar{\lambda}_-)}, \quad (8)$$

from which it follows that

$$\beta = \frac{1}{2} \frac{\lambda_E}{\lambda_E + (\lambda_\rho - \lambda_\sigma)F(0)}. \quad (9)$$

In Eq. (8), $\bar{\lambda}_- \equiv \lambda^- F(0)$ and $\bar{\lambda}_+ \equiv \lambda^+ F(0)$, where $F(0)$ is the $m=n$ term of Eq. (4) with $T=T_c$. Because the spin fluctuation contribution, λ_σ , enters with a minus sign in the denominator of (9) it is clear that including spin fluctuations will lead to an enhancement of the isotope effect over its value when they are neglected. A similar result was first obtained by Williams and Carbotte³⁵ in a phonon-plus-paramagnon model, which corresponds closely to setting $\lambda_\rho = 0$ in (9). In this case $\beta > \frac{1}{2}$ is possible. As in the work of Carbotte, Greeson, and Perez-Gonzalez²² on paramagnetic impurities, the isotope effect is affected by the presence of magnetic fluctuations. This makes it very interesting to investigate the effects of a small phonon contribution added to a dominant charge and spin contribution in the marginal-Fermi-liquid model.

In our numerical work, we start by imposing two constraints on the parameters of the theory, which are now λ_ρ , λ_σ , ω_c , λ_E , and ω_E . We will insist that $T_c \cong 90$ K and $\beta \cong 0.05$. This is typical of the observed situation in stoichiometric $\text{YBa}_2\text{Cu}_3\text{O}_7$. This leaves three free parameters. Results do not depend much on ω_c and so we will fix this quantity at 200 meV. Further, we introduce a parameter $g \equiv (\lambda_\rho - \lambda_\sigma)/(\lambda_\rho + \lambda_\sigma)$ which is a measure of the admixture of charge to spin fluctuations in the marginal-

Fermi-liquid model. Results will then be presented as a function of g and ω_E .

III. RESULTS

While it is not our aim here to present fits to experimental data, the reader should keep in mind the experimental data for $Y_{1-x}Pr_xBa_2Cu_3O_7$. As the praseodymium concentration x is increased, the value of T_c is observed to drop steadily from 96 K in the stoichiometric compound. At the same time the oxygen isotope coefficient β_{ox} increases from 0.05 to a value around 0.45 at $T_c \approx 30$ K. The questions we ask are how much or how little electron-phonon interaction is necessary in the extended marginal-Fermi-liquid model to obtain the $\beta=0.05$ in the stoichiometric compound? And, can the variation of β with a change in T_c in $Y_{1-x}Pr_xBa_2Cu_3O_7$ be understood, at least qualitatively, within this model?

In Fig. 1, we show values of the phonon mass renormalization parameter λ_E as a function of the phonon energy ω_E for various values of g for the stoichiometric compound. In all cases, the values of λ_E required to achieve a $\beta=0.05$ and a $T_c=90$ K are small when ω_E is large but grows substantially with decreasing Einstein frequency. Also at fixed ω_E , λ_E values increase when g decreases, i.e., when more spin fluctuations are introduced in the system. This means that the introduction of spin fluctuations allows for an increase in phonon contribution at fixed T_c and β . Note that the difference between some ($g < 1$) and no spin fluctuations ($g = 1$) increases with a decrease in ω_E and can become very substantial. We can understand qualitatively this result from our Eq. (9), where increasing λ_σ at fixed λ_ρ must be compensated by an increase in λ_E to maintain β at 0.05.

While λ_E may get large as ω_E is reduced, this does not imply that phonons make an ever increasing contribution

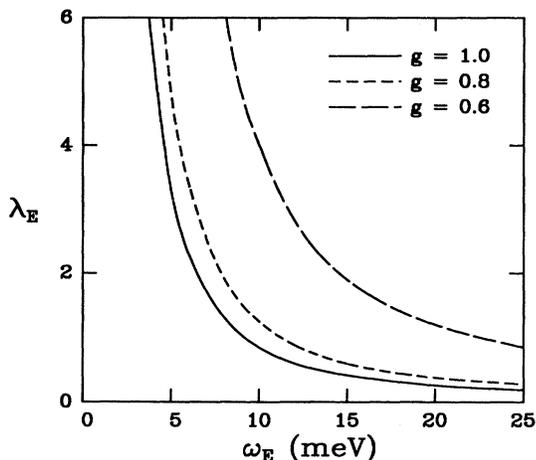


FIG. 1. The electron-phonon mass renormalization parameter λ_E as a function of ω_E for different values of g , the admixture of charge and spin fluctuations in the extended marginal-Fermi-liquid model. These curves were calculated for $\omega_c=200$ meV, $T_c=90$ K, and $\beta=0.05$. $g=1.0$ corresponds to no spin fluctuations.

to the value of T_c . In fact, in all cases shown in Fig. 1, introducing phonons increases T_c above its value for the marginal Fermi liquid, acting alone, by no more than 5 K. According to this measure the phonons are not very important. On the other hand, as we have just seen, the corresponding values of λ_E can get quite large and such values are consistent with a very small isotope effect. For modest values of the spin fluctuation parameter λ_σ this arises only when ω_E is very small and of the order of 5 meV. Coupling to mainly 5 meV phonons seems to us unlikely in oxide superconductors, for which the phonon

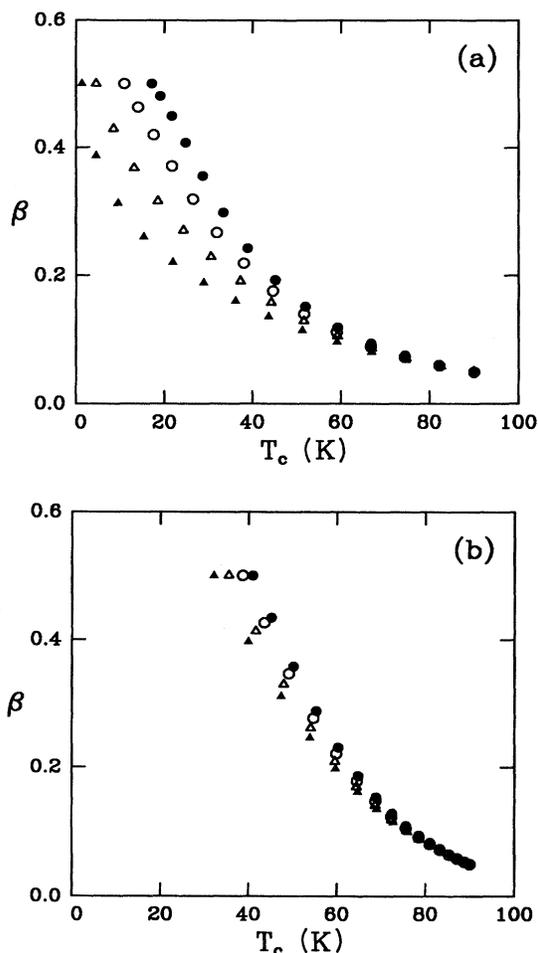


FIG. 2. (a) The isotope coefficient, β , as a function of T_c for various phonon frequencies: $\omega_E=5.0$ meV (solid circles), $\omega_E=10.0$ meV (open circles), $\omega_E=15.0$ meV (open triangles), and $\omega_E=20.0$ meV (solid triangles). In this graph, $g=1.0$ and the parameters in the extended marginal-Fermi-liquid model were chosen to give $\beta=0.05$ at a T_c of 90 K, corresponding to the stoichiometric compound. T_c was reduced by allowing the marginal-Fermi-liquid component to approach zero while keeping the phonon component fixed. β rises in this case to the BCS value of 0.5 where only the phonon component remains. (b) Similar to (a) but with $g=0.6$. Now the isotope coefficient β rises more sharply to $\beta=0.5$ due to a stronger phonon contribution.

spectrum can extend up to 100 meV.^{36,37} As the spin fluctuation contribution is increased, higher frequency phonons could be involved. We note, however, that large values of λ_E are inconsistent with resistivity data.³⁸

With respect to the experimental data for $Y_{1-x}Pr_xBa_2Cu_3O_7$, it is of some interest to change the parameters in our model so as to decrease T_c and see what effect this has on the corresponding β value. Of course, the marginal-Fermi-liquid model is phenomenological and does not have, at the moment, a foundation in microscopic theory. Thus, we do not know how the three parameters λ_ρ , λ_σ , and ω_c might be changing on praseodymium doping. In the absence of such guidance we will consider three very simple models for this change. In the first model we will keep λ_ρ fixed and decrease T_c by increasing the spin fluctuations. In a second, we simply reduce λ_ρ and λ_σ together by the same percentage amount. In the third, we will fix λ_σ and reduce λ_ρ . In all cases, the phonon contribution is in no way changed. Note that in the first and third models important charge and spin fluctuations, respectively, remain even when T_c become small and of the order of the value it would have with phonons alone, while in the second model the marginal-Fermi-liquid part of the interaction is gradually being phased out.

In Fig. 2(a), we show results for β as a function of T_c for an initial model in which $g = 1$ in the stoichiometric compound, i.e., there are no spin fluctuations. The value of the critical temperature is then reduced by switching off λ_ρ leaving the phonon contribution constant. As this is done β increases towards a value of 0.5 which occurs exactly when the only contribution to the T_c is from the

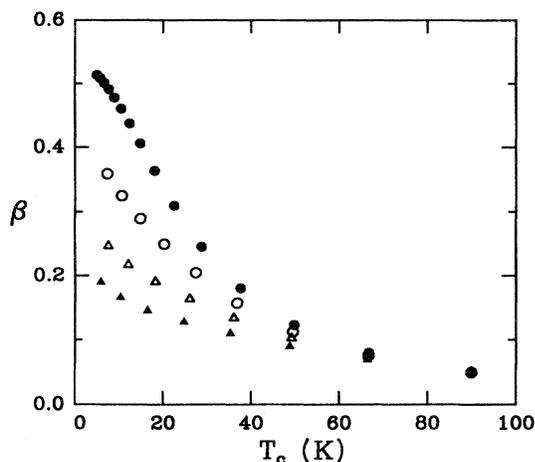


FIG. 3. β as a function of T_c for various phonon frequencies: $\omega_E = 5.0$ meV (solid circles), $\omega_E = 10.0$ meV (open circles), $\omega_E = 15.0$ meV (open triangles), and $\omega_E = 20.0$ meV (solid triangles). As in Fig. 2, marginal-Fermi-liquid parameters are chosen to give $\beta = 0.05$ at $T_c = 90$ K. Here $g = 1.0$ but curves for $g = 0.8$ and 0.6 were not very different. The model used for the reduction in T_c was to fix λ_ρ and increase the amount of spin fluctuations, λ_σ . This reduces T_c and also allows for the possibility of β exceeding the BCS value of 0.5, as exhibited by the $\omega_E = 5$ meV curve.

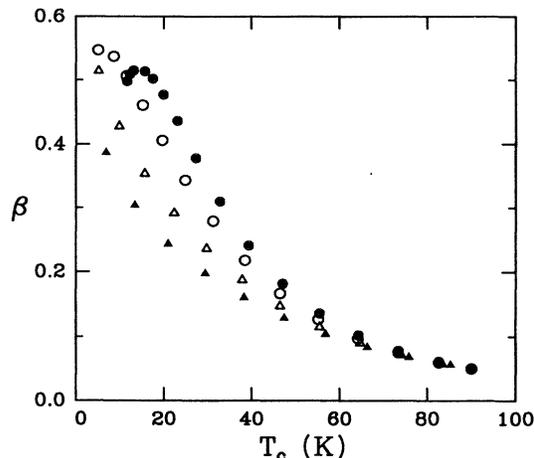


FIG. 4. β as a function of T_c for $g = 0.6$ and for various phonon frequencies: $\omega_E = 5.0$ meV (solid circles), $\omega_E = 10.0$ meV (open circles), $\omega_E = 15.0$ meV (open triangles), and $\omega_E = 20.0$ meV (solid triangles). As in Fig. 2, marginal-Fermi-liquid parameters are chosen to give $\beta = 0.05$ at $T_c = 90$ K. The model used for the reduction in T_c was to fix λ_σ and decrease the amount of charge fluctuations, λ_ρ . This reduces T_c and also allows for the possibility of β exceeding the BCS value of 0.5, as exhibited by the $\omega_E = 5, 10$, and 15 meV curves.

phonons acting alone. One can see this behavior on a qualitative manner from Eq. (9), where in the limit of $\lambda_\rho \rightarrow 0$ for $\lambda_\sigma = 0$, β increases to 0.5. However, we stress that the crude approximations leading to Eq. (9) do not make (9) quantitatively correct (especially for large T_c 's and large λ 's). It is important to be aware that as λ_ρ is decreased towards zero, the phonons with fixed ω_E and λ_E make an increasing contribution to T_c in absolute terms, i.e., the effect of the phonons is nonlinear and they are more effective in increasing T_c the smaller the marginal-Fermi-liquid component. In Fig. 2(b), we show a similar calculation for $g = 0.6$. Here, the rise to $\beta = 0.5$ is much sharper mainly because of a larger electron-phonon contribution. These curves reflect the trend in the experimental data in a more quantitative manner but require λ 's that would violate those derived experimentally from resistivity measurements.³⁸ Very similar trends for the variation of β with T_c value are found when λ_ρ is left fixed and the spin fluctuation λ_σ is increased so as to reduce T_c . Results are shown in Fig. 3. The rise in β is more gradual than for Fig. 2 but we note that at the lowest temperatures β can now be larger than 0.5, although not by much in the curves shown. This is not surprising since the value of T_c is depressed due to spin fluctuations and thus the T_c becomes small even though the charge fluctuations and the electron-phonon interaction remain large. Such a possibility is anticipated in the work of Carbotte, Greeson, and Perez-Gonzalez²² and Williams and Carbotte.³⁵ Again, referring to Eq. (9) for β , it is clear that an isotope coefficient $> \frac{1}{2}$ can be achieved when $\lambda_\sigma > \lambda_\rho$. Finally, Fig. 4 displays results for our third model, that of fixing λ_σ and decreasing λ_ρ . The

curves in this case fall in a region intermediate to the other two models and also exhibit an isotope coefficient that is greater than $\frac{1}{2}$ for the same reasons mentioned above.

In relation to the experimental results on $Y_{1-x}Pr_xBa_2Cu_3O_7$ it is interesting to note that a good part of the observed rise to $\beta=0.45$ at $T_c=30$ K can be understood simply on the basis of our simple model. In reality, of course, something more complicated is at work. Two possible suggestions are pair breaking and an energy dependence in the electronic density of states.

IV. CONCLUSIONS

We have calculated the isotope effect coefficient in the marginal-Fermi-liquid model with an additional phonon contribution. We have found that a large value of T_c with attendant small values of β (of order 0.05) is consistent with a small value of the electron-phonon mass renormalization parameter λ_E provided coupling is primarily to high-energy phonons. For coupling to low energies the corresponding λ_E values can be much larger al-

though the total contribution to the enhancement in overall T_c value is never greater than about 5 K. Also as the amount of spin fluctuations in the system is increased, the corresponding value for λ_E also increases. This effect is small for large ω_E but can be very substantial for low values. Finally, we find that, if T_c is reduced by either increasing the amount of spin fluctuations with all other parameters fixed, decreasing uniformly λ_ρ and λ_σ to zero, or decreasing λ_ρ only, the isotope coefficient increases sharply towards a value of $\frac{1}{2}$ or even above. The increase in β , however, is never large enough to explain presently available results for $Y_{1-x}Pr_xBa_2Cu_3O_7$ and remain consistent with the dc resistivity determination of λ .

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