

## Spin-fluctuation effects on superconductivity

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(Received 14 September 1990)

We have studied the effect of spin fluctuations on select properties of high- $T_c$  superconductors with the pairing mechanism left largely unspecified. The specific-heat jump at  $T_c$  and its slope are calculated for various characteristic spin-fluctuation spectra. The zero-temperature gap edge and second critical magnetic field are also considered. Results specific to a marginal Fermi-liquid model are presented. Finally we consider the effect of spin fluctuations on the isotope effect.

### I. INTRODUCTION

There is substantial evidence that magnetic interactions are important in the high- $T_c$  superconductors.<sup>1-11</sup> In both the La-Sr-Cu-O and the Y-Ba-Cu-O systems there is a transition from a nonsuperconducting insulating magnetically ordered phase to a metallic superconducting phase.<sup>3-5</sup> There is also evidence, at least in the La-Sr-Cu-O system, that superconductivity and antiferromagnetic order may coexist.<sup>12</sup> Additionally, there have been several theoretical proposals which incorporate the existence of antiferromagnetic order or spin fluctuations as the mechanism for pairing.<sup>10,11</sup> In this paper we take the opposite approach and study some of the properties of a superconductor in which the spin fluctuations (SF) are suppressing the superconductivity. We have cast the problem within the framework of Eliashberg theory<sup>13</sup> and therefore we assume that there is some boson exchange mechanism which is responsible for the superconductivity. It could, for example, be charge fluctuations as in some recent models.<sup>14-18</sup> We will not specify what that boson is. However, we do not believe that the superconductivity in these materials can be described by phonons alone. Thus, we take the approach that whatever the pairing exchange mechanism is, its character frequency will be higher than that of a phonon. As such, we will consider weak to moderately strong coupling as the realistic regime in which to discuss the oxides. For completeness, we have studied a much larger range of coupling strength.

The marginal Fermi-liquid model (MFL), developed to describe the copper oxides, has been reviewed by Varma.<sup>14</sup> It is closely related to our work although there are some differences. An essential feature of the MFL model is that there is coupling to both charge (pair-enhancing) and spin (pair-breaking) fluctuations. Both the charge- and spin-fluctuation kernels have the same frequency dependence, but differ in absolute strength. They also have some temperature dependence, but this is not very important near  $T_c$ . Thus, the MFL model corresponds to the special case when the characteristic energy associated with the charge and spin fluctuations is the same, and as such is a subcase of our calculations.

It should be stressed that, in reality, the superconduct-

ing transition itself could lead to modifications of the kernels that enter the equations for superconductivity and that self-consistent modifications may be required, at lower temperatures, due to the opening up of the superconducting gap. These modifications go beyond the scope of the present work and are not expected to be dominant.

In Sec. II we present the equations studied and describe the model spectra employed. In Sec. III we present numerical results for the specific-heat jump and the slope of the specific heat at  $T_c$ . Section IV deals with the gap ratio and the upper critical field. Section V contains a discussion of the isotope effect and conclusions are in Sec. VI.

### II. FORMALISM

The isotropic Eliashberg equations, written on the imaginary axis, including spin fluctuations are<sup>19-22</sup>

$$\begin{aligned} \Delta(i\omega_n)Z_s(i\omega_n) \\ = \pi T \sum_{m=-\infty}^{\infty} [\lambda^-(m-n) - \mu^*] \frac{\Delta(i\omega_m)}{[\Delta^2(i\omega_m) + \omega_m^2]^{1/2}} \end{aligned} \quad (2.1)$$

and

$$\begin{aligned} \omega_n Z_s(i\omega_n) \\ = \omega_n + \pi T \sum_{m=-\infty}^{\infty} \lambda^+(m-n) \frac{\omega_m}{[\Delta^2(i\omega_m) + \omega_m^2]^{1/2}}, \end{aligned} \quad (2.2)$$

where

$$\lambda^{\pm}(m-n) = 2 \int_0^{\infty} \frac{\omega [\alpha^2 F(\omega) \pm P(\omega)]}{\omega^2 + (\omega_m - \omega_n)^2} d\omega, \quad (2.3)$$

and  $\alpha^2 F(\omega)$  and  $P(\omega)$  are the electron-boson (phonon, charge fluctuation, etc.) and electron-spin-fluctuation spectral densities, respectively, and  $i\omega_n = i\pi T(2n-1)$ ,  $n \in I$  are the Matsubara frequencies. In all our work we have set the Coulomb pseudopotential  $\mu^*$  to zero for numerical simplicity.

For both the boson and spin fluctuations we have employed Einstein spectral densities of the form

$$\begin{aligned}\alpha^2 F(\omega) &= \frac{\omega_E \lambda^E}{2} \delta(\omega - \omega_E), \\ P(\omega) &= \frac{\omega_P \lambda^P}{2} \delta(\omega - \omega_P),\end{aligned}\quad (2.4)$$

with  $\lambda^E$  and  $\lambda^P$  the mass enhancement parameters for  $\alpha^2 F(\omega)$  and  $P(\omega)$ , respectively. In order to calculate thermodynamic quantities we utilize the Bardeen-Stephen expression for the free-energy difference between the normal and superconducting states<sup>23</sup>

$$\begin{aligned}F_n - F_s &= N(0)\pi T \\ &\times \sum_{m=-\infty}^{\infty} \{[\bar{\Delta}^2(i\omega_m) + \bar{\omega}^2(i\omega_m)]^{1/2} - |\bar{\omega}(i\omega_m)|\} \\ &\times \left[ 1 - \frac{|\bar{\omega}_m^0|}{[\bar{\Delta}^2(i\omega_m) + \bar{\omega}^2(i\omega_m)]^{1/2}} \right],\end{aligned}\quad (2.5)$$

$$\bar{\omega}^0(i\omega_n) \equiv \omega_n + \pi T \sum_{m=-\infty}^{\infty} \lambda^+(m-n) \text{sgn} \omega_m$$

with  $N(0)$  the single-spin electronic density of states at the Fermi energy.

The specific-heat jump is readily obtained from the free-energy difference through the standard thermodynamic relations and is given by

$$\frac{\Delta C}{\gamma T_c} = \frac{T}{\gamma T_c} \frac{d^2 \Delta F(T)}{dT^2}.\quad (2.6)$$

We also calculate the upper critical field. It is obtained from the following equations<sup>24</sup>

$$\begin{aligned}\Delta(i\omega_n) Z_s(i\omega_n) \\ = \pi T \sum_{m=-\infty}^{\infty} [\lambda^-(m-n) - \mu^*] \frac{\bar{\Delta}(i\omega_m)}{\chi^{-1}(\bar{\omega}(i\omega_m))},\end{aligned}\quad (2.7)$$

$$\chi(\bar{\omega}(i\omega_m)) = \frac{2}{\sqrt{\alpha}} \int_0^{\infty} dq e^{-q^2} \tan^{-1} \left[ \frac{q\sqrt{\alpha}}{|\bar{\omega}(i\omega_m)|} \right],\quad (2.8)$$

where  $\alpha \equiv \frac{1}{2} e H_{c2}(T) v_F^2$ .  $e$  is the electronic charge and  $v_F$  is the Fermi velocity. In order to avoid any  $v_F$  dependence, we present results for the reduced upper critical field defined by

$$h_{c2}(t) \equiv \frac{H_{c2}(T)}{\left[ T_c \left| \frac{dH_{c2}(T)}{dT} \right| T_c \right]}.\quad (2.9)$$

$t \equiv T/T_c$  is the reduced temperature.

### III. SPECIFIC-HEAT JUMP

We have solved Eqs. (2.1) and (2.2) numerically and used the results to calculate the specific heat given by Eq. (2.6). In our calculations, we chose a critical temperature ( $T_c^0$ ) for a pure system which we hold fixed. We then chose a value of  $\omega_E$  and calculate  $\lambda^E$  to give us our

chosen  $T_c^0$ . We then added spin fluctuations at some frequency  $\omega_P$ , and calculate a  $\lambda^P$  which will suppress the critical temperature to 100 K. Two values of  $T_c^0$ , 150 and 200 K were used. For both values of  $T_c^0$ , the results were qualitatively the same. We will only show results for  $T_c^0 = 200$  K. In our calculations, we have varied the frequencies of both the pairing and spin-fluctuation spectra. We use the parameters  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$  to discuss the results. It has been shown for materials that are well described by the electron-phonon interaction that the parameter  $T_c/\omega_{\text{in}}$  can be used to characterize the superconducting properties of a material.<sup>25</sup> Here  $\omega_{\text{in}}$  is the Allen-Dynes parameter.<sup>26</sup> For an Einstein spectra,  $\omega_{\text{in}} \equiv \omega_E$ . Our numerical studies have spanned the range of 0–2 for both  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$ . We point out that conventional phonon materials lie in the range  $0 \leq T_c/\omega_{\text{in}} \leq 0.25$  so that our range of parameters goes way beyond the probable physical region.

In Fig. 1 we display  $\lambda^P$ , the electron-spin-fluctuation mass-enhancement factor versus  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$ . We note that  $\lambda^P$  rises rapidly for small values of both parameters and then levels off. For  $T_c^0 = 200$  K, the maximum value of  $\lambda^P$  is 1.7 for

$$\frac{T_c^0}{\omega_E} = \frac{T_c^0}{\omega_P} = 2.0.$$

In Fig. 2 we show  $\lambda^E$  versus  $T_c^0/\omega_E$ . We note that, for  $T_c^0/\omega_E = 2.0$ ,  $\lambda^E \approx 120$ , which is way beyond the likely physical range but is nevertheless included for completeness. If we restrict ourselves to a  $\lambda^E \leq 5.0$ , we find that we only need  $\lambda^P \leq 1.0$  to suppress  $T_c$  from 200 to 100 K. For very weak coupling in both the pairing and spin fluctuations, a  $T_c$  suppression of 50% is achieved with  $\gamma^P \approx 0.05$ . Thus, even weakly coupled spin fluctuations can have a dramatic effect upon the critical temperature of a superconductor. Such weakly coupled excitations would be difficult to detect experimentally in the superconducting properties.

Figure 3 displays the normalized specific-heat jump ( $\Delta C/\gamma T_c$ ) with  $\gamma$  the Sommerfeld constant. For  $T_c^0/\omega_E$

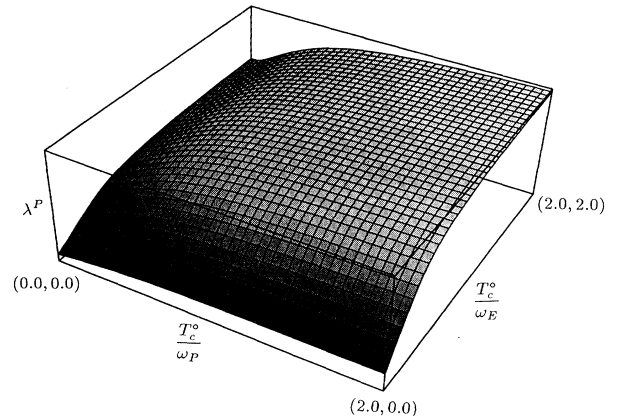


FIG. 1. Electron-spin-fluctuation mass-enhancement factor  $\lambda^P$  vs  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$  for  $T_c/T_c^0 = 0.5$ . The surface has a height of  $\approx 0.05$  at (0,0) and a maximum value of  $\approx 1.7$  at (2,2).

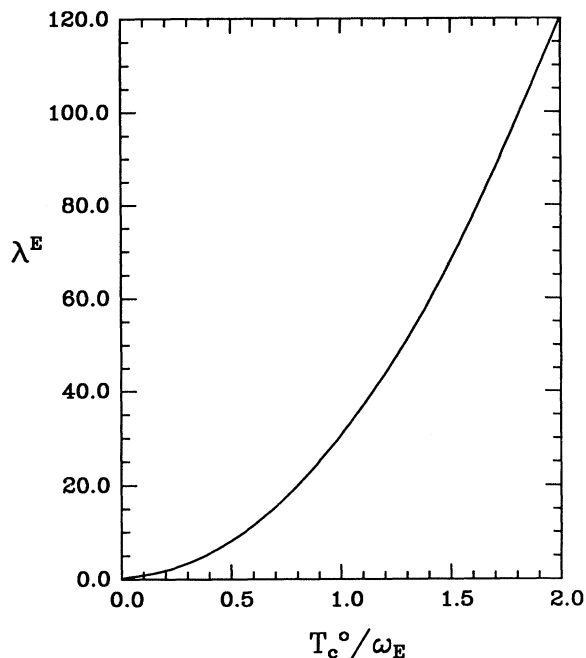


FIG. 2. Electron-boson mass-enhancement factor  $\lambda^E$  vs  $T_c^0/\omega_E$ .  $\lambda^E$  is determined by choosing an  $\omega_E$  and then calculating  $\lambda^E$  to give  $T_c^0=200$  K. For  $T_c^0/\omega_E \geq 0.5$ ,  $\lambda^E$  appears to be unphysically large.

and  $T_c^0/\omega_P$  equal to zero, we obtain the usual BCS value of 1.43. As  $T_c^0/\omega_E$  increases,  $(\Delta C/\gamma T_c)$  increases, reaches a maximum of  $\approx 4.1$  for  $T_c^0/\omega_E=0.4$ , and then decreases below the BCS value. As  $T_c^0/\omega_P$  increases, the specific-heat jump is enhanced and, for  $T_c^0/\omega_E=0.4$  and  $T_c^0/\omega_P=2.0$ , we find that  $(\Delta C/\gamma T_c)=9.6$ , which is much larger than the maximum value obtained without spin fluctuations.<sup>27</sup> It is interesting to note that, in the case of paramagnetic impurities, the specific-heat jump is always suppressed below its pure value.<sup>28</sup> Figure 4 shows the slope of the specific-heat difference at  $T_c$  normalized

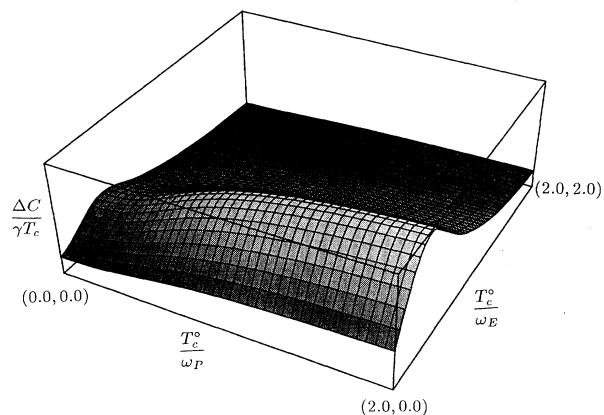


FIG. 3. Normalized specific-heat jump  $(\Delta C/\gamma T_c)$  vs  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$  for  $T_c/T_c^0=0.5$ . At  $(0,0)$  the height is 1.43, the BCS value. The maximum of 11.4 occurs at  $T_c^0/\omega_E=0.4$  and  $T_c^0/\omega_P=2.0$ . This is much larger than the maximum value that can be obtained in a purely attractive system.

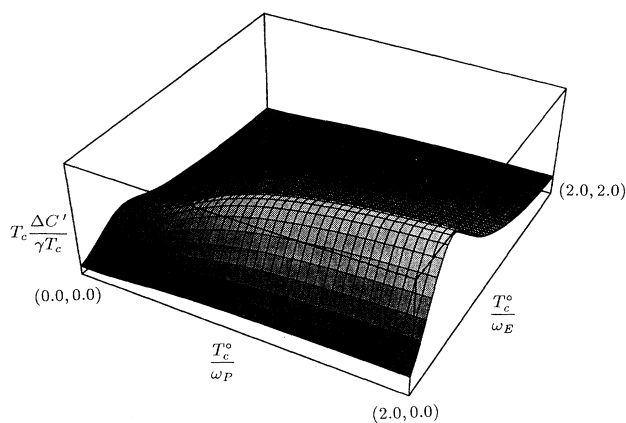


FIG. 4.  $(1/\gamma)(d\Delta C/dT)$  vs  $T_c^0/\omega_E$  and  $T_c^0/\omega_P$  with  $T_c/T_c^0=0.5$ . At  $(0,0)$ , we obtain the BCS value of 3.77. The maximum value of 23 occurs at  $T_c^0/\omega_E=0.4$  and  $T_c^0/\omega_P=2.0$ , the same place where the maximum of the specific-heat jump occurs.

by  $\gamma$ ,  $(1/\gamma)(d\Delta C/dT)$  ( $\gamma$  is the Sommerfeld value). For  $T_c^0/\omega_E=T_c^0/\omega_P=0$ , we obtain the BCS result of 3.77. As  $T_c^0/\omega_E$  increases, the normalized slope increases, reaches a maximum, and then decreases. For  $T_c^0/\omega_P=0$ , a maximum value of  $\approx 21$  is attained for  $T_c^0/\omega_E=0.4$ . The maximum value obtained was 67.3 for  $T_c^0/\omega_E=0.4$  and  $T_c^0/\omega_P=2.0$ . The slope of the specific heat behaves qualitatively like the specific-heat jump. This is not particularly surprising, as one would expect them to be correlated with one another in order to satisfy the entropy sum rule.

When we compare these results to those obtained for systems where no dynamic pair-breaking mechanism is included ( $\mu^*$ , a static, repulsive, Coulomb pseudopotential is included), we find that the results are qualitatively similar, but there are large quantitative differences. In the case of both the jump and the slope, other authors<sup>29</sup> find a maxima in these values at  $T_c/\omega_E=0.2$ . Note that the position of these maxima agrees with the values obtained here when we recall that  $T_c/T_c^0=0.5$ . However, the maxima obtained for the jump, with  $\mu^*=0.0$ , is  $\approx 3.4$ . Even in the weak-coupling limit for the spin fluctuations, we obtain a maximum of 4.1. Similarly, the maximum value for the slope in the purely attractive case is  $\approx 14.5$ , whereas we get a value, again in the weak-coupling SF regime, of  $\approx 21$ . Once again, as for the critical temperature, we see that even very weakly coupled spin fluctuations can have a dramatic effect upon the properties of a superconductor.

In order to measure the normalized jump or slope of the specific heat, it is necessary to know the value of the Sommerfeld constant  $\gamma$ . Due to the large critical temperatures and large value of the low-temperature critical fields,  $\gamma$  is not a well-known quantity for the high- $T_c$  superconductors. A quantity which contains information about both the jump and the slope in the specific heat is the ratio of the slope to the jump. In particular, we have calculated  $(T_c/\Delta C)(d\Delta C/dT)$ . This quantity is indepen-

dent of  $\gamma$ . In addition, if we restrict ourselves to values near  $T_c$ , one would hope that experimental results for this quantity would be reasonably insensitive to the details of the subtraction of the lattice contribution to the specific heat. Results of our calculations are shown in Fig. 5. Along the  $T_c^0/\omega_p=0.0$  line we see a sharp rise to the maximum of  $\approx 5.2$  of  $T_c^0/\omega_E=0.4$  and then a gradual fall as  $T_c^0/\omega_E$  increases further. In this case, the value does not fall below the BCS value of 2.64 which we obtain for

$$\frac{T_c^0}{\omega_E} = \frac{T_c^0}{\omega_p} = 0.0$$

As we move away from  $T_c^0/\omega_p=0.0$ , we see a further increase. For both  $T_c^0/\omega_E$  and  $T_c^0/\omega_p \gtrsim 0.5$ , a plateau is reached at  $\approx 7.25$ . As we move further out, a slow increase to 7.6 is observed at

$$\frac{T_c^0}{\omega_E} = \frac{T_c^0}{\omega_p} = 2.0.$$

Comparing these results to values obtained for pure systems, we find that they are larger. Akis and Carbotte<sup>29</sup> report values in the range of 2.64 (BCS) to 5.0. For  $\mu^*=0.0$ , they give a maximum value of 4.6.

We are able to compare these results with experiment. Akis and Carbotte<sup>29</sup> have analyzed specific-heat data of Junod *et al.*<sup>30</sup> for  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , and find a value for  $(T_c/\Delta C)(d\Delta C/dT)$  in the range of 8–14, depending upon the temperature interval that they use to calculate the slope. We note that there is evidence that the fluctuation regime in these materials is large,<sup>31</sup> which would tend to sharpen the specific-heat anomaly. As consequence, perhaps the lower bound of their estimate is the more relevant. Our results would seem to fit with the lower bound. However, we are only able to achieve these values in the strong-coupling regime for the pairing mechanism.

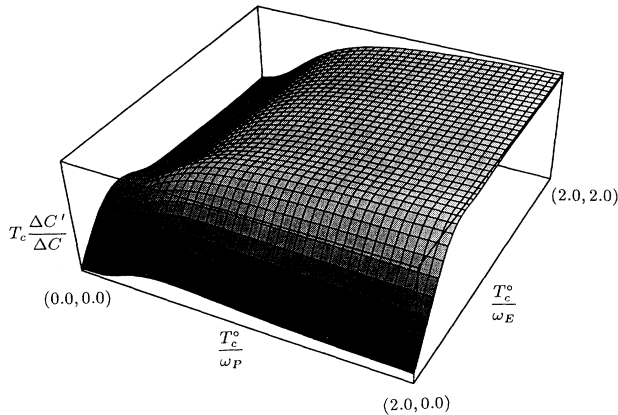


FIG. 5. Ratio of the temperature derivative of the specific heat to the specific heat at  $T_c$  vs  $T_c^0/\omega_E$  and  $T_c^0/\omega_p$  for  $T_c/T_c^0=0.5$ . This ratio is independent of  $\gamma$ , the coefficient of the linear term in the normal-state specific heat. We obtain the BCS result of 2.64 at (0,0) and a maximum of 7.6 at (2,2). At (0.5,0.5), we obtain 7.25.

We next consider the MFL model more explicitly. The coupling to the charge and spin fluctuations can be represented by a pair-creating spectral density

$$\alpha^2 F(\omega) = \lambda_\rho \left[ \frac{2}{\pi} \right] \tanh \left[ \frac{\omega}{2T} \right] \Theta(\omega_c - \omega) \quad (3.1)$$

and a pair-breaking spectral density

$$P(\omega) = \lambda_\sigma \left[ \frac{2}{\pi} \right] \tanh \left[ \frac{\omega}{2T} \right] \Theta(\omega_c - \omega). \quad (3.2)$$

The three parameters of the theory are the coupling strengths to the charge ( $\lambda_\rho$ ) and spin ( $\lambda_\sigma$ ) and the cutoff  $\omega_c$ . In presenting results, it is useful to introduce a parameter

$$g \equiv \frac{\lambda_\rho - \lambda_\sigma}{\lambda_\rho + \lambda_\sigma}, \quad (3.3)$$

which measures the relative amount of coupling to the spin and charge fluctuations. For  $g=1$ , there is no coupling to the spin fluctuations, and for  $g=0$  there is equal coupling to spin and charge fluctuations. For fixed values of  $g$  and  $\omega_c$ , the remaining parameter  $\lambda_\rho$  is fitted to give a  $T_c=100$  K, representative of the oxides. In Fig. 6 we show results for the jump and the slope of the specific heat at  $T_c$  as well as the ratio of the two quantities as a function of  $T_c^0/\omega_c$  for  $g=0.4, 0.5$ , and  $0.6$ . We note that

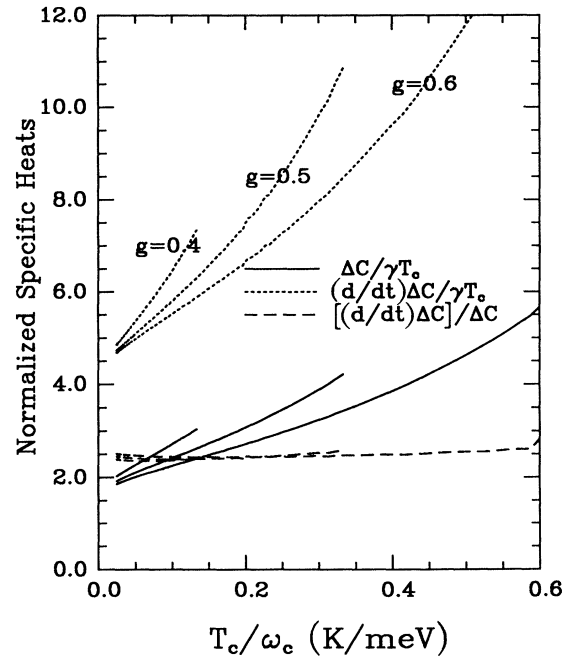


FIG. 6. The normalized specific-heat jump ( $\Delta C/\gamma T_c$ ) (solid curve), the slope of the normalized specific heat  $(1/\gamma)(d\Delta C/dT)$  (dotted curve), and the slope of the specific-heat difference normalized to the jump  $[T_c(d\Delta C/dT)/\Delta C]$  (dashed curve) vs  $T_c^0/\omega_c$  for the marginal Fermi-liquid model of Ref. 18. All quantities are evaluated at  $T_c$ . In all cases, the values obtained are greater than the BCS values, but less than the maximum values obtained with Einstein spectra.

both the normalized jump and slope rise quite rapidly with the value of  $T_c/\omega_c$ . Results terminate when convergence becomes difficult. In contrast, the ratio of slope to jump (dashed curve) is nearly constant and has a value around the BCS value of 2.64 in this model. The large slope-to-jump ratio observed in experiments cannot be explained in this way.

#### IV. $H_{c2}$ AND $[2\Delta(0)/k_B T_c]$

We now consider our results for the reduced upper critical field which were obtained by solving Eqs. (2.7) and (2.8). Figure 7 shows the reduced upper critical field versus reduced temperature  $t$ . For all curves  $T_c^0/\omega_E=0.05$  and  $T_c^0=200$  K. The curves for  $T_c^0/\omega_P=0.05$  and the curve for the system with no spin fluctuations lie on top of one another. Both of these curves seem to be tending smoothly to the BCS value of 0.73 at zero temperature. The spin fluctuations have no observable effect upon the reduced upper critical field in the weak-coupling regime. This is in marked contrast to both the critical temperature and the specific heat. As  $T_c^0/\omega_P$  is increased, the curves start deviating markedly from BCS. The last curve shown is nearly linear over a large temperature range and starts bending over only around the reduced temperature  $t \sim 0.1$ . In Fig. 8 we show  $h_{c2}(0)$  versus  $T_c^0/\omega_P$ . We observe that it starts off slightly below 0.73, dips, and then rises, reaching a value of  $\approx 0.88$  for  $T_c^0/\omega_P=2.0$ . This type of behavior is similar to the behavior seen by Schossmann *et al.*<sup>32</sup> as a function of  $T_c^0/\omega_E$ . They obtain a maximum value near 1.5 for  $T_c^0/\omega_E=1.5$ . Our maximum value is smaller than

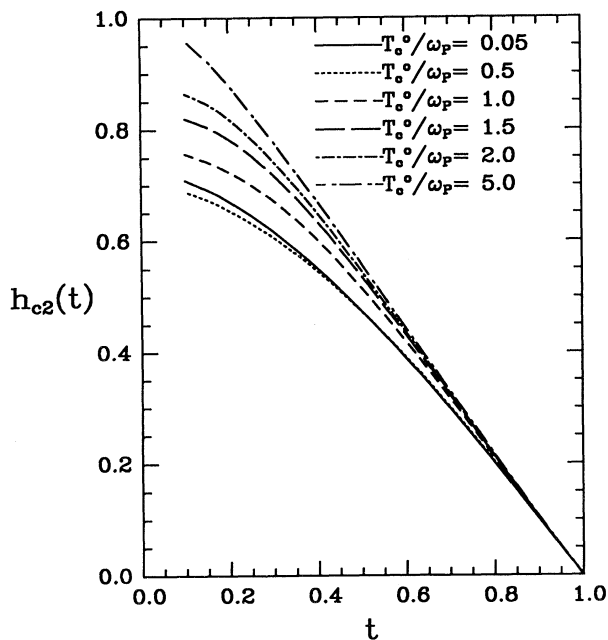


FIG. 7. Reduced upper critical field vs reduced temperature for  $T_c/T_c^0=0.66$ . For all curves  $T_c^0/\omega_E=0.05$ . The curve for  $T_c^0/\omega_P=0.05$  is almost indistinguishable from the curve one would obtain with no spin fluctuations which we do not show. The trend for increasing  $T_c^0/\omega_P$  is shown clearly in Fig. 8.

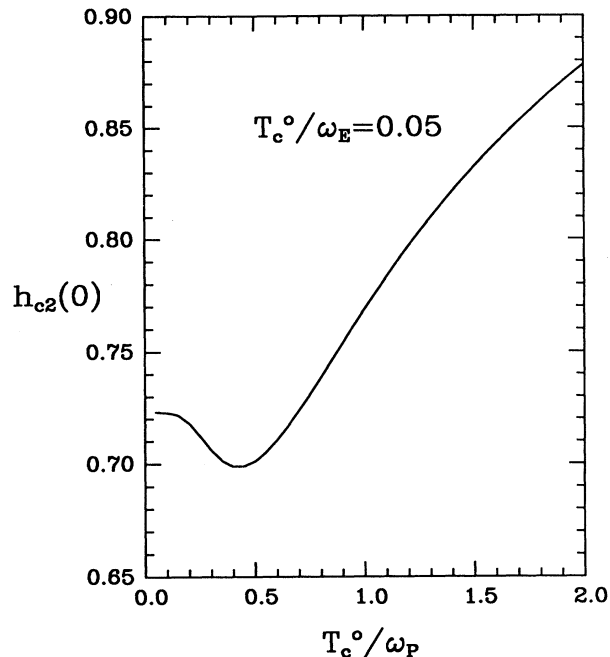


FIG. 8. The zero-temperature reduced critical field vs  $T_c^0/\omega_P$  for  $T_c/T_c^0=0.5$ . This type of behavior is qualitatively similar to that of a purely attractive system as a function of  $T_c^0/\omega_E$ . For  $T_c^0/\omega_P=0$ , we agree with the BCS result of 0.73.

this, although our curve is still increasing.

Figure 9 shows the ratio of  $[2\Delta(0)/k_B T_c]$  versus  $T_c^0/\omega_P$ . This quantity was also computed for  $T_c^0/\omega_E=0.05$ . The curve starts off slightly above the

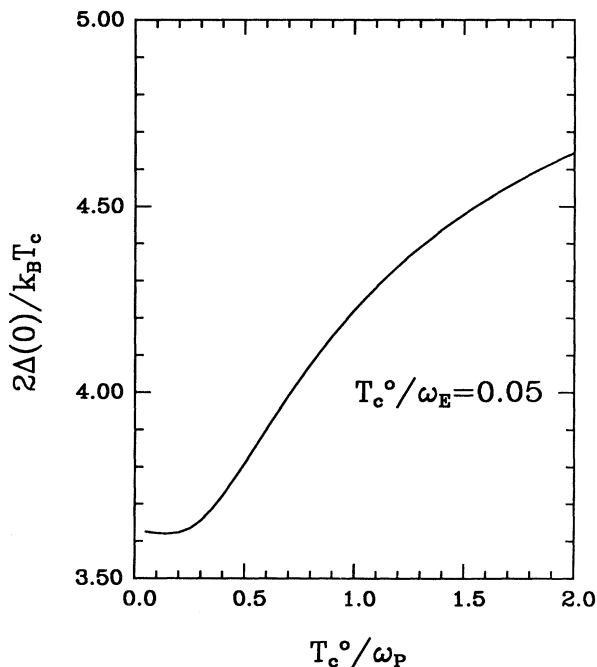


FIG. 9. The zero-temperature gap ratio vs  $T_c^0/\omega_P$  for  $T_c/T_c^0=0.5$  and  $T_c^0/\omega_E=0.05$ . The values obtained are all well below the maximum values that can be obtained in a purely attractive system.

BCS value of 3.53, exhibits a small dip, and then rises. The values obtained for these parameters are all well below the maximum possible value of approximately 13 that can be obtained in the extreme strong-coupling regime with no pair-breaking mechanism.<sup>33</sup> For comparison with conventional phonon superconductors, we remind the reader that Pb has an energy gap ratio of 4.5.

### V. ISOTOPE EFFECT

We now focus our attention upon the isotope effect that we would expect in such systems if we assume that the pairing interaction is due only to phonons. As we have already stated, we do not believe that phonons alone are responsible for the superconductivity in the high- $T_c$  superconductors. Indeed, our results for the isotope effect will demand that, if the scenario that we discussed is to be applicable, the pairing mechanism cannot be phonons alone. It could be mainly charge fluctuations, for example.

We have performed numerical as well as analytical calculations of the isotope effect  $\beta$ , which is given by

$$\beta \equiv \frac{d \ln(T_c)}{d \ln(M)}, \quad (5.1)$$

where  $M$  is the ionic mass. In all of the results below, we have assumed that the  $\alpha^2 F(\omega)$  kernel is due to phonons alone. Numerical results are shown in Fig. 10. This curve was calculated for  $T_c^0/\omega_E=0.05$ , and  $T_c^0=200$  K. We see that  $\beta$  is everywhere larger than  $\frac{1}{2}$ , the BCS result. The peak occurs at  $T_c^0/\omega_p=0.28$ . We can gain more insight into this result by considering the Rainer-Culetto formula for the isotope effect<sup>34</sup>

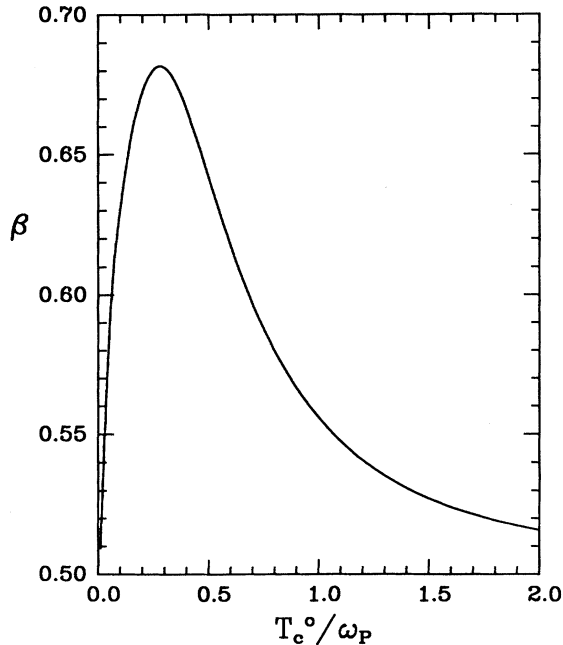


FIG. 10.  $\beta$ , the isotope effect coefficient, vs  $T_c^0/\omega_p$  for  $T_c^0/\omega_E=0.05$  and  $T_c/T_c^0=0.5$ . It is everywhere greater than or equal to  $\frac{1}{2}$ , the BCS value.

$$\beta_{\text{tot}} = \int_0^\infty d\omega R(\omega) \alpha^2 F(\omega). \quad (5.2)$$

$R(\omega)$  is defined as

$$R(\omega) = \frac{1}{2T_c} \left[ \frac{\delta T_c}{\delta \alpha^2 F(\omega)} + \omega \frac{d}{d\omega} \frac{\delta T_c}{\delta \alpha^2 F(\omega)} \right]. \quad (5.3)$$

For Einstein spectral densities  $\beta$  is simply equal to  $AR(\omega_E)$ , where  $A$  is the weighting factor of the electron-boson spectral density, i.e.,

$$\alpha^2 F(\omega) = A \delta(\omega_E - \omega).$$

We need to know the functional derivative of the critical temperature with respect to the electron-phonon spectral density in order to see why the isotope effect is larger than  $\frac{1}{2}$ . In Fig. 11 we show the functional derivative  $[\delta T_c / \delta \alpha^2 F(\omega)]$  for two cases: a 200-K superconductor with no spin-fluctuations, and the same system with its critical temperature suppressed to 100 K by spin fluctuations. In both cases  $T_c^0/\omega_E=0.05$ , and for the second case  $T_c^0/\omega_p=0.05$ . Both curves are everywhere positive definite, and the curve with spin fluctuations is everywhere larger than the curve for the pure system. In both cases, the electron-phonon spectral density is the same and it is sufficient to look simply at  $R(\omega_E)$  to see how  $\beta$  changes.

There are various factors contributing to the change in  $\beta$  when we add the spin fluctuations to the system. There

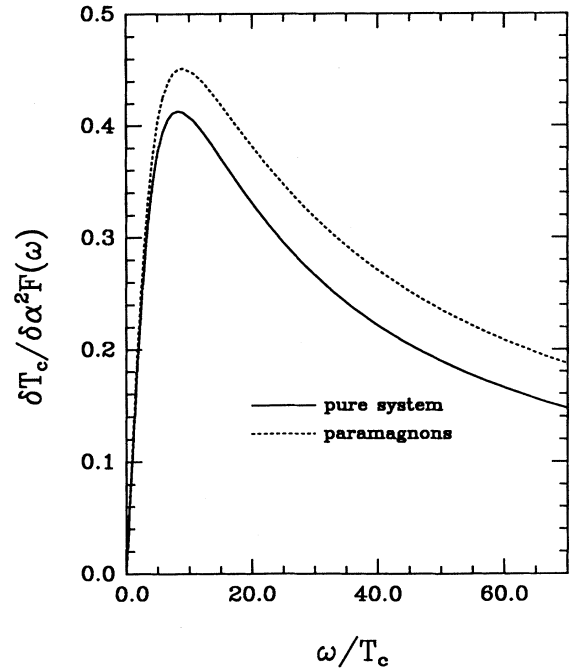


FIG. 11. Functional derivative of the critical temperature with respect to the electron-boson spectral density vs  $\omega/T_c$ . For both curves  $T_c^0/\omega_E=0.05$ , and for the system with spin fluctuations,  $T_c^0/\omega_p=0.05$  and  $T_c/T_c^0=0.5$ . The derivative for the purely attractive system is smaller and shifted to slightly lower  $\omega/T_c$  than the derivative for the system with the spin fluctuations.

is a suppression of  $T_c$  which tends to cause  $\beta$  to increase. In addition to this effect, there is a change in the functional derivative. One must remember that the functional derivative is plotted versus  $\omega/T_c$ , and hence the relevant data is at  $\omega/T_c=20.0$  for  $T_c=200$  K, and  $\omega/T_c=40.0$  for  $T_c=100$  K. One can see that both the functional derivative and its derivative with respect to frequency are smaller for the system with spin fluctuations. However, both of them have been reduced by less than  $\frac{1}{2}$  which, in combination with the factor of 2 coming from the  $T_c$  suppression, leads to an enhanced isotope

effect.

We can solve Eqs. (2.1) and (2.2) for the critical temperature using a square-well model<sup>35</sup> for both the pairing and spin-fluctuation spectra. In such a model we assume that  $\omega_{E,P} \gg T_c$  and approximate

$$\lambda^{E,P}(m) = \lambda^{E,P}(0) \Theta(\omega_{D,PM} - |\omega_m|). \quad (5.4)$$

We mean by  $\omega_{PM}$  the spin-fluctuation analogue of the Debye frequency. Solving for  $T_c$  in this approximation, one gets

$$T_c = \exp \left[ - \frac{(1 + \lambda^+(0) - \lambda^E(0) \ln(1.13\omega_E) + \lambda^P(0) \ln(1.13\omega_P))}{\lambda^-(0)} \right], \quad (5.5)$$

and using (5.1), one obtains for the isotope effect

$$\beta = \frac{1}{2} \frac{\lambda^{\text{ph}}(0)}{\lambda^-(0)}. \quad (5.6)$$

From Fig. 1 we see that, for small  $T_c^0/\omega_P$ ,  $\lambda^P$  is quite small, and hence  $\beta$  does not deviate significantly from  $\frac{1}{2}$ , as is shown in Fig. 10.

One can also solve for  $T_c$  in the limit of  $\lambda^{\text{ph}}$  going to infinity. In this limit, it has been found that  $T_c$  is given to a good approximation using a one-gap model<sup>26</sup>

$$\Delta(i\omega_n) = \begin{cases} \Delta_0, & \text{if } n = 1 \\ 0, & \text{otherwise} \end{cases}. \quad (5.7)$$

Using this model, Eqs. (2.1) and (2.2) give

$$\Delta_0 [1 + \lambda^+(0)] = \pi T [\lambda^-(0) + \lambda^-(1)] \Delta_0. \quad (5.8)$$

This can be solved for  $T_c$  in the limit of  $\omega_E \ll \omega_P \ll T_c$  to give

$$T_c = \frac{(\lambda^{\text{ph}})^{1/2} \omega_E}{\sqrt{2\pi}} \frac{1}{1 + 2\lambda^P}. \quad (5.9)$$

This gives  $\beta = \frac{1}{2}$ . Figure 10 shows  $\beta$  approaching  $\frac{1}{2}$  for large  $T_c^0/\omega_E$ .

## VI. CONCLUSIONS

Spin fluctuations can have a large effect on the value of the specific-heat jump at  $T_c$ , on its slope, and, consequently, the normalized slope-to-jump ratio which can be

as large as 7.68 for the parameter space surveyed. This value is larger than the maximum established by Akis and Carbotte for a pure boson-exchange mechanism which is 4.6 when the Coulomb pseudopotential  $\mu^* = 0$ . It is large enough to explain the lower bound presently established in specific-heat experiments. The value of 7.6, however, is only obtained when the average boson energy in the pairing channel is small. Other quantities considered were the ratio of the gap to critical temperature and the second critical magnetic field  $h_{c2}$ . Results for the specific heat were also obtained in the marginal Fermi-liquid model which, in some sense, is a subcase of the work presented here. In this case it was found, for the parameter space considered, that the jump and slope are always above the corresponding BCS value and rapidly increasing with the ratio of  $T_c$  to cutoff  $\omega_c$  in the fluctuation spectrum. The ratio of slope to jump was, however, found to be reasonably constant and nearly equal to the BCS value.

Finally, it was found that spin fluctuations can increase the value of the isotope coefficient  $\beta$ . In a phonon model for the pairing, spin fluctuations increase  $\beta$  above  $\frac{1}{2}$ .

## ACKNOWLEDGMENTS

This research was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC). J. P. Carbotte is also supported by the Ontario Center for Materials Research (OCMR) and by the Canadian Institute for Advanced Research (CIAR).

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