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Isotopic mass and pressure dependent changes for extended s-wave superconductors

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Abstract. We consider a tight-binding model comprising a hopping and an attractive interaction term to obtain superconductivity. Exact expressions for the isotope-shift exponent (α) and the pressure coefficient of transition temperature (γ_P) are derived invoking the isotopic mass and pressure dependence of both the hopping and attractive interaction terms. The variations of α and γ_P are studied as a function of the chemical potential and the transition temperature. With proper choice of parameters we obtain large positive values of α for low-T_c samples and a minimum in α near optimum doping. It is found that γ_P is large and positive for low-T_c underdoped systems and small near optimum doping. These results qualitatively agree with the experimental results of hole-doped high-T_c oxides. The behaviour of γ_P for electron-doped oxide systems can also be explained from the model.

1. Introduction

Since the advent of superconductivity, isotopic substitution of atoms and application of pressure have been recognised as key factors affecting the transition temperatures (T_c). Following the discovery of high-temperature superconductors, several experiments for the isotopic mass [1–4] and the pressure dependence [5–8] on T_c have been performed. Since the majority of these systems become superconducting on doping with holes, the dopant dependent isotope-shift exponent ($\alpha = -\partial \ln T_c/\partial \ln M$) and pressure coefficient of the transition temperature ($\gamma_P = \partial \ln T_c/\partial P$) have been keenly studied over the years and certain general trends have emerged [9, 10].

α is large (exceeding the canonical value of 0.5, in some cases) in the underdoped region and attains a very small value at optimum doping where T_c is maximum. In many cases α is minimum at optimum doping and increases in the overdoped region. Anomalously, in Bi:2212 samples, small negative values of α in the overdoped region have been reported [4]. The pressure coefficient of T_c is positive for the hole-doped superconductors. It is large when T_c is small and is reduced significantly for high values of T_c. In the overdoped region negative values of the pressure coefficient at high pressures have been observed [10]. For electron-doped oxide systems the pressure coefficient is negative; its value is large for low-T_c samples and decreases with increasing T_c [8].

In this work our objective lies in obtaining the general trends of α and γ_P with doping from a minimal model, consisting of a hopping term and an effective attraction between the electrons, in the weak-correlation limit. In a previous work [11] we have calculated α within the polaronic theory of superconductors where the isotopic mass dependence occurs only in the hopping, to find $\alpha < 0$ for all doping. So, in order to understand all the salient

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features of α and γ_P with doping, we feel, a judicious choice is to invoke the mass and the pressure dependence of both the hopping and attractive interaction strengths and examine their relative roles in determining the behaviour of α and γ_P.

2. Model Hamiltonian and T_c

Following the discovery of high-T_c superconductors extensive studies have been made with local pairing interaction in narrow-band systems. Both weak- and strong-correlation models [12–17] have been considered in this context. In the weak-correlation limit, the minimal relevant model for studying superconductivity would comprise an attractive term for electrons in addition to a term describing band dispersion. Thus our model is

$$H = -t\sum_{i,j,\sigma} c_{i\sigma}^{+} c_{j\sigma} - V\sum_{i,j} n_i n_j - \mu\sum_{i,\sigma} n_{i\sigma} \tag{1}$$

where t and V are the hopping matrix element and effective attraction between electrons at nearest-neighbour sites, respectively. $c_{i\sigma}^{+}$ ($c_{i\sigma}$) is the usual electron creation (annihilation) operator and $n_{i\sigma} = (c_{i\sigma}^{+} c_{i\sigma})$ is the number operator corresponding to the ith site and spin state σ. μ is the chemical potential which is determined by the filling of the band (doping in the case of oxide systems).

For studying superconductivity, the second term on the r.h.s. of equation (1) is simplified in the mean-field spirit through the introduction of an order parameter

$$\Delta_0 = \tfrac{1}{2}\left(\langle c_{i\downarrow} c_{j\uparrow}\rangle + \langle c_{j\downarrow} c_{i\uparrow}\rangle\right). \tag{2}$$

Subsequent k-space transformation yields the Hamiltonian in the usual BCS form as

$$H = \sum_{k\sigma} \xi_k n_{k\sigma} + \sum_k \Delta_k \left(c_{k\uparrow}^{+} c_{-k\downarrow}^{+} + \text{HC}\right) \tag{3}$$

where $\xi_k = \epsilon_k - \mu$, $\epsilon_k = -tz\gamma_k$ and $\gamma_k = (1/z)\sum_j \exp(\mathrm{i}k \cdot R_{ij})$, R_{ij} being the nearest-neighbour lattice vector. For a square lattice $z = 4$ and $\gamma_k = \cos k_x + \cos k_y$. The superconducting gap parameter corresponding to an extended s-wave pairing is

$$\Delta_k = z\gamma_k V \Delta_0. \tag{4}$$

Using the Green function technique the superconducting correlation is obtained as

$$\left\langle c_{k\uparrow}^{+} c_{-k\downarrow}^{+}\right\rangle = -\frac{\Delta_k}{2E_k}\tanh\left(\beta E_k/2\right) \tag{5}$$

where $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ and $\beta = 1/k_B T$.

Combining (4) and (5) the self-consistent equation for the gap is obtained as

$$\Delta_k = z\gamma_k V \sum_q \gamma_q \left(\frac{\Delta_q}{2E_q}\tanh\left(\beta E_q/2\right)\right). \tag{6}$$

This leads to the equation for T_c given by

$$1 = zV\int_{-1}^{1} \mathrm{d}\epsilon_r\, N(\epsilon_r)\frac{\epsilon_r^2}{2(\epsilon_r - \mu_r)}\tanh\left(\beta_r^c \frac{\epsilon_r - \mu_r}{2}\right) \tag{7}$$

where the subscript r denotes a reduced variable expressed in units of the electronic half-bandwidth ($W = 4t$), i.e., $\epsilon_r = \epsilon/W$, $\mu_r = \mu/W$ and $\beta_r^c = W\beta^c$ ($\beta^c = 1/k_B T_c$). $N(\epsilon_r) = WN(\epsilon)$ where $N(\epsilon)$ represents the electron density of states (DOS).

3. Isotope-shift exponent and pressure coefficient of T_c

To derive expressions for the isotope-shift exponent ($\alpha = -\partial \ln T_c/\partial \ln M$) and the pressure coefficient of the transition temperature ($\gamma_P = \partial \ln T_c/\partial P$) one has to differentiate equation (7) with respect to M and P. The parameters which depend on the isotopic mass (M) are t, V and β_r^c. The relevant pressure dependent factors are t, V, β_r^c and μ_r, since the application of pressure is known to alter the carrier concentration in high-T_c oxide systems and hence μ_r.

The expressions for α and γ_P thus derived are

$$\alpha = -\frac{\partial \ln t}{\partial \ln M} + \left(\frac{\partial \ln t}{\partial \ln M} - \frac{\partial \ln V}{\partial \ln M}\right)\frac{1}{\beta_r^c z V_r I_1} \tag{8}$$

and

$$\gamma_P = \frac{\partial \ln t}{\partial P} + \left(\frac{\partial \ln V}{\partial P} - \frac{\partial \ln t}{\partial P}\right)\frac{1}{\beta_r^c z V_r I_1} + \left(\frac{I_2}{\beta_r^c} - \frac{I_3}{2}\right)\frac{1}{I_1}\frac{\partial \mu_r}{\partial P} \tag{9}$$

where

$$I_1 = \int_{-1}^{1} \mathrm{d}\epsilon_r\, N(\epsilon_r)\frac{\epsilon_r^2}{4}\,\mathrm{sech}^2\left(\beta_r^c\frac{\epsilon_r - \mu_r}{2}\right) \tag{10}$$

$$I_2 = \int_{-1}^{1} \mathrm{d}\epsilon_r\, N(\epsilon_r)\frac{1}{2}\left(\frac{\epsilon_r}{\epsilon_r - \mu_r}\right)^2 \tanh\left(\beta_r^c\frac{\epsilon_r - \mu_r}{2}\right) \tag{11}$$

and

$$I_3 = \int_{-1}^{1} \mathrm{d}\epsilon_r\, N(\epsilon_r)\frac{1}{2}\left(\frac{\epsilon_r^2}{\epsilon_r - \mu_r}\right)\mathrm{sech}^2\left(\beta_r^c\frac{\epsilon_r - \mu_r}{2}\right). \tag{12}$$

$\partial \mu_r/\partial P$ appearing in equation (9) may be expressed in terms of the change in the carrier concentration (n) as

$$\frac{\partial \mu_r}{\partial P} = \frac{1}{2N(\mu_r)}\,\frac{\partial n}{\partial P}. \tag{13}$$

The transition temperature (T_c) and the isotope-shift exponent (α) are calculated for a square (energy-independent) DOS

$$N(\epsilon_r) = \tfrac{1}{2} \qquad |\epsilon_r| \leqslant 1 \tag{14}$$

and a DOS with a van Hove singularity

$$N(\epsilon_r) = 0.209\,53 \ln\left|\frac{4}{\epsilon_r}\right| \qquad |\epsilon_r| \leqslant 1. \tag{15}$$

Plugging (14) and (15) into equation (13) we find that for a square DOS $\partial \mu_r/\partial P = \partial n/\partial P$ while for a DOS with a vHs $\partial \mu_r/\partial P = 0.209\,53 \ln |4/\epsilon_r| \partial n/\partial P$.

In view of the importance of the second-nearest-neighbour hopping in hole-doped high-T_c cuprates, as inferred from the Fermi surface obtained from photoemission experiments [18], we have examined its effect on α. The band dispersion including second-nearest-neighbour hopping is

$$\epsilon_k = -2t\left(\cos k_x a + \cos k_y a\right) - 4t_2 \cos k_x a \cos k_y a \tag{16}$$

where t_2 is the next-nearest-neighbour hopping integral. The isotope-shift exponent is calculated from equation (8) for the dispersion (equation (16)) using the integral I_1 (equation (10)) as

$$I_1 = \frac{1}{N}\sum_k \left(\frac{\epsilon_k}{2W}\right)^2 \mathrm{sech}^2\left(\beta^c\left(\frac{\epsilon_k - \mu}{2}\right)\right). \tag{17}$$

For $t_2 \neq 0$ we have calculated I_1 numerically exactly and consequently α.

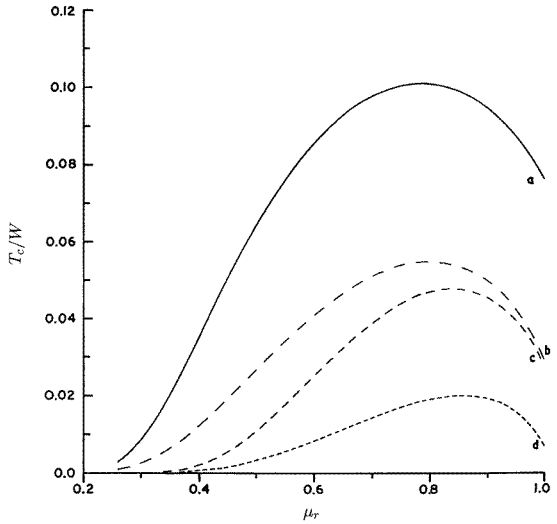

Figure 1. Variation of T_c/W with μ_r. Curves a and c are for $V_r = 0.625$ and 0.4 respectively and for a square DOS while b and d are for the same set of V_r values with a vHs in the DOS.

4. Results and discussions

Our interest lies in the study of T_c, α and γ_P as a function of doping (modelled through μ_r) and a qualitative comparison of their variations with the general trends emerging from experiments on various high-T_c cuprates. Naturally, a suitable choice of parameters such as V_r, the mass and pressure dependence of t and V and pressure dependence of carrier concentration (n) is essential.

We choose $V_r = 0.625$ and 0.4 respectively. Our choice of $(\partial \ln t)/\partial \ln M$ is guided by a recent experiment [19] on 1-2-3 compounds, where $(\partial \ln m^*)/\partial \ln M_0$ has been reported to be $\sim$0.6, m^* and M_0 being the effective mass of the charge carrier and average mass of the oxygen atom respectively. The effective mass of the charge carrier is inversely proportional to the effective hopping strength (leading to $\partial \ln t/\partial \ln m^* = -1$) and in accordance with the results of [19] we take $(\partial \ln t)/\partial \ln M = -0.6$. We treat $(\partial \ln V)/\partial \ln M$ as a free parameter.

For high-T_c oxide systems (hole doped) the carrier concentration (n) increases with pressure, and, by a general estimate [10] $(\partial \ln n)/\partial P \sim$ 7–10% GPa^{-1}, which corresponds to $\partial n/\partial P \sim$ 1–2 $\times 10^{-2}$ GPa^{-1}, for the concentration range $0.1 < n < 0.2$. For the La-214 system, however, the carrier concentration changes negligibly with pressure. As we have seen before, for a square DOS, $\partial n/\partial P = \partial \mu_r/\partial P$, so we choose $\partial \mu_r/\partial P$ in the range 0–1 $\times 10^{-2}$ GPa^{-1} for our study. The values of $(\partial \ln t)/\partial P$ and $(\partial \ln V)/\partial P$ are chosen as 1 and 2 respectively, in units of 10^{-2} GPa^{-1}, which may be reasonable for hole-doped superconductors.

In figure 1 we present the variation of T_c/W with μ_r for different values of V_r and for two different types of DOS (described in (14) and (15)). With decreasing attractive interaction strength, V_r, as expected, T_c values decrease for all carrier concentrations. However, for a given V_r, T_c values for a square DOS are higher than the corresponding values obtained with a vHs in the DOS.

In figures 2 and 3, α is plotted as a function of μ_r. From equation (8) it is evident

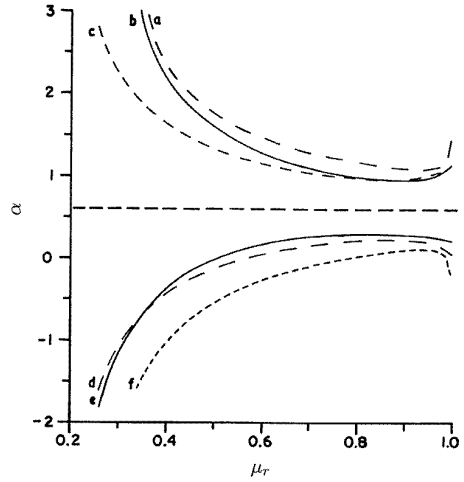

Figure 2. Variation of α against μ_r with $(\partial \ln t)/\partial \ln M = -0.6$. Curves a, b and c are for $(\partial \ln V)/\partial \ln M = -0.8$ while d, e and f are for $(\partial \ln V)/\partial \ln M = -0.4$. Other parameters for the curves are as follows: curves a and f, $V_r = 0.4$, vHs in DOS; curve b, $V_r = 0.4$, square DOS; curves c and e, $V_r = 0.625$, vHs in DOS; curve d, $V_r = 0.625$ and a square DOS.

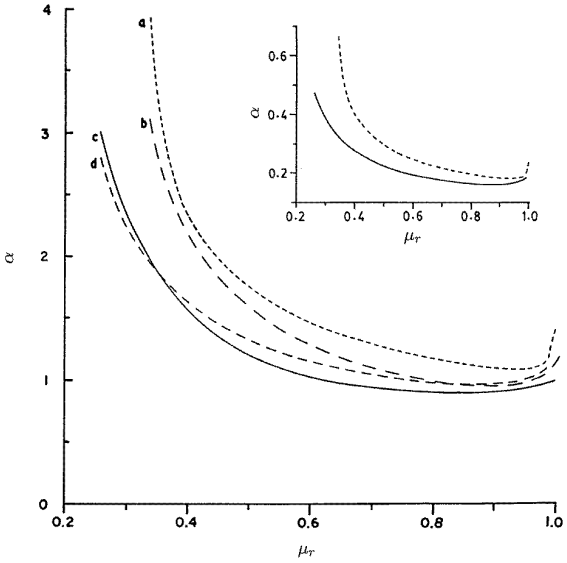

Figure 3. α against μ_r with $(\partial \ln t)/\partial \ln M = -0.6$ and $(\partial \ln V)/\partial \ln M = -0.8$. Curves b and c are for a square DOS and $V_r = 0.4$ and 0.625 respectively, while curves a and d are for a vHs in the DOS for the same set of V_r values. The solid and dotted inset curves are for $V_r = 0.625$ and 0.4 respectively and a vHs in the DOS; $(\partial \ln t)/\partial \ln M$ and $(\partial \ln V)/\partial \ln M$ are scaled down to values of -0.1 and -0.133 respectively to obtain realistic values of α.

that α depends on the choice of $(\partial \ln V)/\partial \ln M$, the nature of the DOS and V_r for a given value of $(\partial \ln t)/\partial \ln M$. In our earlier work [11], we have seen that if only the hopping strength depends on the isotopic mass, then $\alpha < 0$ for all μ_r, which corresponds to setting

$(\partial \ln V)/\partial \ln M = 0$ in the present model. However, in keeping with our tacit assumption in the present case that V too depends on M, we choose $(\partial \ln V)/\partial \ln M$ as -0.4 and -0.8. The former is larger while the latter is smaller than the value of $(\partial \ln t)/\partial \ln M$. Numerical exercises confirm that I_1 (equation (10)) is positive definite for all μ_r and three distinct features of α emerge, depending on the relative values of $(\partial \ln V)/\partial \ln M$ and $(\partial \ln t)/\partial \ln M$:

(i) For $(\partial \ln V)/\partial \ln M = (\partial \ln t)/\partial \ln M$, equation (8) yields $\alpha = -(\partial \ln t)/\partial \ln M$, which is a constant and independent of the nature of the DOS and μ_r.

(ii) For $(\partial \ln V)/\partial \ln M < (\partial \ln t)/\partial \ln M$, α decreases from large positive values when T_c is low to a near minimum at optimum doping and increases slightly on the overdoped side.

(iii) For $(\partial \ln V)/\partial \ln M > (\partial \ln t)/\partial \ln M$, α increases from large negative values for low values of μ_r to small positive values as μ_r increases.

In figure 2 the central dashed line corresponds to case (i) where α is constant and independent of doping, similar to the BCS case. The upper curves (a, b and c) correspond to case (ii) discussed above with $(\partial \ln V)/\partial \ln M = -0.8$, while the lower curves (d, e and f) correspond to case (iii), i.e. $(\partial \ln V)/\partial \ln M = -0.4$, holding $(\partial \ln t)/\partial \ln M = -0.6$ in all cases. Since all high-T_c oxides have positive values of α for all dopant concentrations, case (ii) discussed above is of more practical importance.

To understand the dependence of α on V_r and on the nature of the DOS, in figure 3 we plot α against μ_r for $V_r = 0.4$ and 0.625 and for both types of DOS (square and with a vHs), holding $(\partial \ln V)/\partial \ln M$ and $(\partial \ln t)/\partial \ln M$ fixed at -0.8 and -0.6 respectively. For DOSs of both types α is lower for the higher value of V_r over the entire range of μ_r. The minimum in α near optimum doping is more pronounced for the DOS with a vHs. The variation of α with μ_r is qualitatively consistent with the experimental trends of high-T_c oxide systems (i.e. α is large for underdoped materials and decreases to a minimum near optimum doping); however, the experimental values of α are much lower. It may be mentioned that, for a fixed ratio of $[(\partial \ln V)/\partial \ln M]/[(\partial \ln t)/\partial \ln M]$, the value of α at a particular filling and for a fixed V_r is just proportional to $(\partial \ln t)/\partial \ln M)$. Thus, the value of α can be lowered to any extent by decreasing the value of $(\partial \ln t)/\partial \ln M$. In the inset of figure 3 the variation of α with μ_r is shown for $(\partial \ln t)/\partial \ln M = -0.1$, keeping the ratio $[(\partial \ln V)/\partial \ln M]/[(\partial \ln t)/\partial \ln M]$ (=4/3) and other parameters the same as for the curves a and d of the main figure. As is expected, the values of α (in the inset) are six times lower than the corresponding values along the curves a and d of the main figure.

In figure 4 we have shown the effect of second-nearest-neighbour hopping (through the dimensionless parameter $r_2 = 2t_2/t$) on the behaviour of α along with the experimental data for La-214 and Co-substituted Y-123 systems for a comparison. Clearly, the inclusion of next-nearest-neighbour hopping enhances α considerably for small values of T_c and suppresses α slightly near $T_c \sim T_c^{max}$. We have taken $r_2 = 0.8$ and 0.9 as used by other workers [20]. There appears to be a reasonable agreement with experimental data for high values of r_2. It should be mentioned, however, that a quantitative comparison would be meaningful if accurate values of (isotopic) mass dependent parameters in cuprates could be determined. Only then can one conclude whether such a minimal model is sufficient to describe the isotopic behaviour of high-T_c cuprates. To bring down the minimum of α further as observed for the cuprates (e.g., for Bi-2212, $\alpha_{min} \sim 0.012$ [9]) additional terms such as pair tunnelling or a mass independent contribution to the attractive interaction may become necessary.

In figure 5 the variation of the pressure coefficient (γ_P) is shown with μ_r for

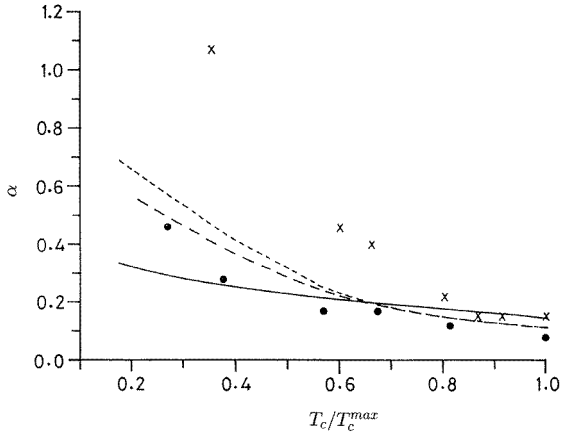

Figure 4. α against T_c/T_c^{max} with $(\partial \ln t)/\partial \ln M = -0.05$ and $(\partial \ln V)/\partial \ln M = -0.1$. The solid curve is for $r_2 = 0$ (only n.n. hopping) while the dashed curves are for $r_2 = 0.8$ (longer dash) and 0.9 (shorter dash). The crosses and full circles denote the data for La-214 and Co-substituted Y-123 systems, taken from [9].

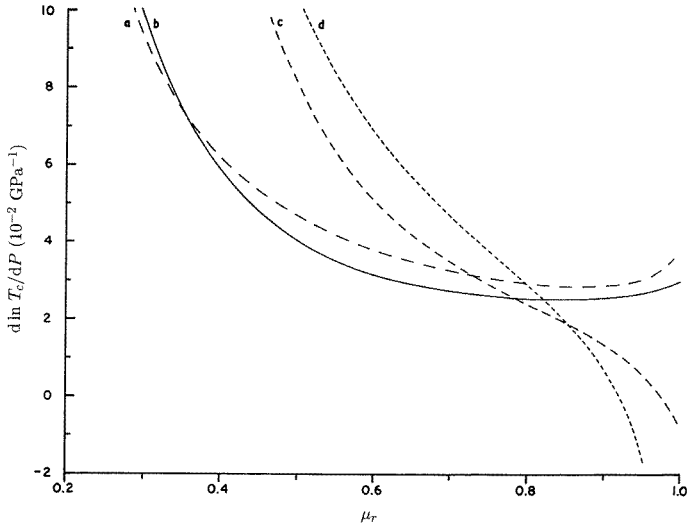

Figure 5. $(\partial \ln T_c)/\partial P$ against μ_r with $(\partial \ln t)/\partial P = 10^{-2}$ GPa^{-1}, $(\partial \ln V)/\partial P = 2 \times 10^{-2}$ GPa^{-1} and $V_r = 0.625$. Curves a and b are for $(\partial \mu_r)/\partial P = 0$ while c and d are for $(\partial \mu_r)/\partial P = 10^{-2}$ GPa^{-1}. Curves a and c are for a square DOS while b and d are for a vHs in the DOS.

different values of $\partial \mu_r/\partial P$ but fixed values of $(\partial \ln t)/\partial P$ and $(\partial \ln V)/\partial P$. We choose $\partial \ln V/\partial P > \partial \ln t/\partial P$ for which γ_P is positive in the entire range of μ_r provided $\partial \mu_r/\partial P$ is small. γ_P is large for low values of μ_r, where T_c is small, and decreases as μ_r (as well as T_c) increases. For $\partial \mu_r/\partial P = 0$ (curves a and b) γ_P reaches a minimum near optimum doping, while for $\partial \mu_r/\partial P = 1 \times 10^{-2}$ GPa^{-1} γ_P changes sign in the overdoped region and the slope of γ_P against μ_r is larger than that for the $\partial \mu_r/\partial P = 0$ case.

In figure 6 we show the variation of the pressure coefficient of T_c with T_c/T_c^{max} for two

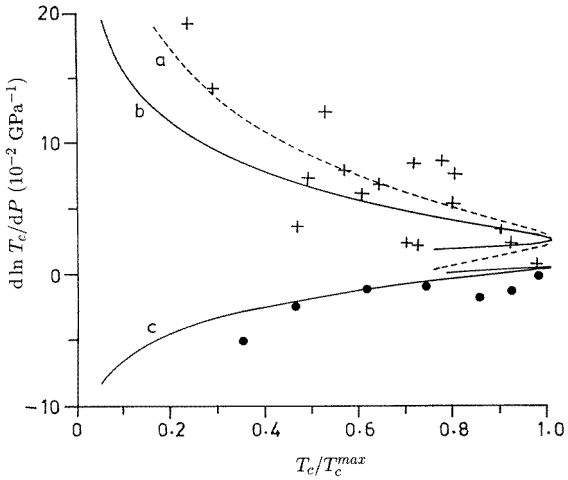

Figure 6. $(\partial \ln T_c)/\partial P$ against T_c/T_c^{max} for $V_r = 0.625$ and a square DOS. Values of $(\partial \ln t)/\partial P$ and $(\partial \ln V)/\partial P$ for curves a and b are the same as the ones used in figure 5. For curves a and b, $\partial \mu_r/\partial P = 0.3$ and 0.7 respectively in units of 10^{-2} GPa^{-1}. For curve c, $(\partial \ln t)/\partial P$, $(\partial \ln V)/\partial P$ and $\partial \mu_r/\partial P$ are chosen as 2, 1 and 0 in units of 10^{-2} GPa^{-1}. Superposed on the graph are the experimental data for both hole-doped (the Y-123 system, represented by the plus sign) and electron-doped (the $Nd_{2-x}Ce_xCuO_4$ system, represented by full circles) oxides taken from [10].

sets of values of $(\partial \ln V)/\partial P$ and $(\partial \ln t)/\partial P$, where T_c^{max} is the transition temperature at optimum doping. For $(\partial \ln V)/\partial P > (\partial \ln t)/\partial P$, the pressure coefficient is large and positive for underdoped systems having low T_c values, whereas for $(\partial \ln V)/\partial P < (\partial \ln t)/\partial P$ the pressure coefficient is negative for underdoped systems. In both cases the magnitude of the pressure coefficient decreases with increasing T_c values up to optimum doping. It may be mentioned that, for electron-doped oxide superconductors, γ_P is negative and its magnitude decreases with increasing T_c [8]. For a comparison with experimental results we have presented the data of hole-doped Y-123 and electron-doped Nd-214 systems in the same figure. The theoretical curves seem to corroborate the data fairly well. The effect of a next-nearest-neighbour hopping (relevant for hole-doped systems [21]) on the pressure coefficient is similar to that on α, namely, for low values of T_c, γ_P would increase substantially while it is expected to decrease slightly for $T_c \sim T_c^{max}$. For finite values of $\partial \mu_r/\partial P$ the increase of γ_P at low T_c would be sharper. Thus with a simple model considered here the variation of γ_P with T_c for both electron-doped and hole-doped oxide superconductors may be explained.

Finally, we should mention one of the limitations of our study. We have considered here only the case of extended s-wave pairing. However, substantial evidence in favour of d-wave pairing in high-T_c oxide systems has accumulated recently [22, 23]. Still the possibility of an anisotropic extended s-wave pairing has not been ruled out [24]. A study of α and γ_P for d-wave pairing has been recently made by Sil and Das [25] with a similar model. The qualitative behaviours of α and γ_P as a function of T_c, obtained by them, are similar to that for extended s-wave pairing obtained in the present study.

5. Summary

We derive exact analytical expressions for the isotope-shift exponent and the pressure coefficient of T_c considering the isotopic mass and pressure dependence of the hopping and attractive interaction strengths of a minimal model system, describing superconductivity. Theoretical predictions for α and γ_P with proper choice of parameters are qualitatively consistent with the experimental results of high-T_c oxide systems. A quantitative comparison for α is attempted taking into account next-nearest-neighbour hopping. The results are encouraging.

Acknowledgment

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