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# A STUDY OF ISOTOPE EFFECT AND EVALUATION OF CRITICAL EXPONENT 'α' OF HIGH $T_c$ SUPERCONDUCTOR

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## ABSTRACT

Using the theoretical model of S. Yoksan, we have studied the isotope effect in high $T_c$ superconductors. This model takes into account the nearest neighbor interlayer hopping. Our theoretical results indicate that the value of isotope exponent α of high $T_c$ superconductor is very small.

**Key words**: Isotope effect, Critical exponent, Nearest neighbor interlayer hopping, High $T_c$-Superconductor.

## INTRODUCTION

One of the most interesting experimental properties of high $T_c$ superconductors is the small isotope effect. The suppression of this effect is not explained with the conventional BCS theory predicts that the critical temperature $T_c$ and the isotope mass M are related by $T_c M^{-\alpha}$, where $\alpha = 0.5$ for all elements[1-3].

To explain the almost absence of the isotope effect in high $T_c$ compounds, many authors have proposed various mechanisms including resonating valence bond[4], excitons[5], plasmons[6] and ant ferromagnetic spin fluctuation mediated pairing[7]. Fund and Kwok[8] suggested a local volume change due to oxygen deficiency as a cause of this effect. Su et al.[9] interpreted experimental data as evidence for the free carrier negative U-centre interaction, Seki and Tanabe[10] investigated the influence of the singularity enhanced density of states in a bond asymmetric high $T_c$ material. Daemen and Overhauser[11] surprisingly found that the existence of a short range attraction in addition to the conventional phonon pairing interaction suppresses the isotope effect significantly at high temperatures.

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In these calculations the authors assumed the constant electronic density of states at the Fermi level. As is well known, high temperature superconductors have a two dimensional structure. Various calculations[12-17] shows that there is a logarithmic singularity in density of states, one therefore expects that this singularity plays a dominant role in causing the anomalous behavior of the isotope effect.

## Theoretical formulation

Using the theoretical model given by Daemen and Overhauser[11] one assumes that the pairing interaction written as –

$$V_{kk}' = \begin{cases} -V_1 - V_2, \text{ for } 0 < E \hbar\omega_D \\ -V_2 \text{ for } \hbar\omega_D < E < 4t \end{cases} \quad \ldots(1)$$

is independent of the phonon frequency. Here $V_1$ is the phonon mediated interaction and $V_2$ is the extra interaction which may be of non electron phonon origin. E is the electron energy measured from the Fermi energy, $\omega_D$ is the Debye cut-off energy and 4t is the energy cut-off for $V_2$.

As it has been shown by experiments that in the oxide superconductors the carriers is still the Copper pair, one thereby assumes that a solution of the BCS integral equation.

$$\Delta(k) = \frac{1}{2}\sum_a \frac{V(k-q)\,\Delta(q)}{\sqrt{E^2+\Delta^2(a)}} \tanh \frac{\sqrt{E^2+\Delta(q)}}{2\,_\beta T} \quad \ldots(2)$$

Based on equation (1) has the following form –

$$\Delta\,(k,T) = \begin{cases} \Delta_o(T)\,\Delta_1, & \text{if } E < \hbar\omega_D \\ \Delta_o(T)\,\Delta_2, & \text{if } E > \hbar\omega_D \end{cases} \quad \ldots(3)$$

Here $\Delta_1$ and $\Delta_2$ are temperature independent constants. Upon substituting equation (3) into (2), one obtains the following equations.

$$\Delta_o \left[1 - (V_1 + V_2)\sum_1 (T)\right] = \Delta_2 V_2 E_2\,(T)$$

$$\Delta_1 V_2 E_1\,(T) = \Delta_2\,[1 - V_2 E_2\,(T)] \quad \ldots(4)$$

When

$$E_1\,(T) = \int_o^{\hbar\omega_D} \frac{dEN\,(E)}{\sqrt{E^2 + \Delta_0^2\,\Delta_1^2}} \tanh \frac{\sqrt{E^2 + \Delta_0^2\,\Delta_1^2}}{2k_\beta T}$$

$$E_1(T) = \int_{\hbar\omega_D}^{4t} \frac{dEN(E)}{\sqrt{E^2 + \Delta_0^2\,\Delta_2^2}} \tanh \frac{\sqrt{E^2 + \Delta_0^2\,\Delta_2^2}}{2k_\beta T} \quad \ldots(5)$$

One obtains equation (5) by replacing the summation over q by the energy integrals. Now in the Hubbard model on a two-dimensional square lattice, the Hamiltonian is –

$$H = \sum_{ij\sigma} tC_{i\sigma}^{+} + C_{1\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \quad \ldots(6)$$

here *t* denotes the transfer integral, and U the renormalized on site Coulomb interaction, the number operation $n_{i\sigma} - C_{i\sigma}^{+} C_{1\sigma}$. In case of the nearest neighbor hopping, the band energy is E (k)= -2t ($\cos k_x + \cos k_y$).This gives rise to the density of states in the form –

$$N(E) = \begin{cases} 2\pi^{\frac{1}{2t}}\, k = \left[1 - \left(\frac{E}{4t}\right)^2\right] & |E| < 4t \\ 0 & |E| > 4t \end{cases} \quad \ldots(7)$$

When K is the complete elliptic integral of the first kind, and N (E) is non-zero only when 0 < E < 4t, for E ~ 0, N (E) takes the form –

$$N(E) = \frac{1}{2\pi^2 t} \ln \left| \frac{E}{16t} \right| \quad \ldots(8)$$

AT $T = T_c$, $\Delta_0 (T) = 0$, with the aid of the expression for N(E) one can be see that the integrals in equation (5) are dominate around E=0, so one approximate equation (5) as –

$$\sum_{1}(T_c) = \frac{1}{2\pi^2 t} F\left(\frac{\hbar\omega_D}{2k_\beta T_c}\right)$$

$$\sum_{2}(T_c) = -\frac{1}{2\pi^2 t}\left\{F\left(\frac{4t}{2\pi^2 t}\right) - F\left(\frac{\hbar\omega_D}{2k_\beta T_c}\right)\right\} \quad \ldots(9)$$

With the function F defined by –

$$F\left(\frac{4t}{2\pi^2 t}\right) = \int_{6}^{\hbar\omega_D} \frac{dx \ln x}{x} \tanh \frac{8tx}{k_\beta T_c} \quad \ldots(10)$$

When equation (4) are compatible one arrives at the following condition.

$$\left(\frac{\hbar\omega_D}{2k_\beta T_c}\right)+\sigma F\left(\frac{4t}{2k_\beta T}\right)+\lambda\sigma F\left(\frac{\hbar\omega_D}{2k_\beta T_c}\right)\times\left[F\left(\frac{4t}{2k_\beta T_c}\right)-F\left(\frac{\hbar\omega_D}{2k_\beta T_c}\right)\right]=0 \qquad \ldots(11)$$

Here one has introduced the variable $\lambda=\frac{V_2}{2\pi^2 t}$ and $\sigma=\frac{V_1}{2\pi^2 t}$.

## $T_c$ Calculation

To calculate[13] the critical temperature $T_c$, one evaluates F and finds that –

$$F\left(\frac{Y}{2k_\beta T_c}\right)=-\frac{1}{2}\ln^2\left(\frac{k_\beta T_c}{4t}\right)+0.819\ln\left(\frac{k_\beta T_c}{2t}\right)+\frac{1}{2}\ln^2\left(\frac{Y}{16t}\right)-1 \qquad \ldots(12)$$

Putting F in equation (11) and rearranging, one arrives at the equation for $T_c$.

$$k_\beta T_c = 1.13\ \hbar\omega_D \exp\left\{\frac{\frac{1}{\lambda+\sigma^*}-0.6646}{\ln\left(\frac{\hbar\omega_D}{16t}\right)}\right\} \qquad \ldots(13)$$

Where

$$\sigma^* = \frac{\sigma}{1-\frac{\sigma}{2}\ln\left(\frac{4t}{\hbar\omega_D}\right)\ln\left(\frac{64t}{\hbar\omega_D}\right)} \qquad \ldots(14)$$

In the pure electron-phonon mechanism, i.e. when $V_1 \neq 0$ and $V_2 = 0$ and $\sigma = 0$ and and equation (13) gives.

$$k_\beta T_c = 1.13\ \hbar\omega_D \exp\left\{\frac{1}{\frac{V_1}{2\pi^2 t}\ln\left(\frac{2\pi^2 t}{16t}\right)}\right\} \qquad \ldots(15a)$$

In the dominate non electron-phonon process, i.e. when $V_2 >> V_1$, we have $\lambda\rightarrow 0$ and $\sigma \neq 0$ equation (13) gives.

$$k_\beta T_c = 8t \exp\left(\sqrt{\frac{4\pi^2 t}{V_2}}\right) \qquad \ldots(15b)$$

Here the quantity of $\frac{1^2}{2\pi} t \left| \ln\left(\frac{\hbar\omega_D}{16t}\right) \right|$ is analogous to the density of states at the Fermi level of the BCS theory. If this quantity is large, $T_c \sim \omega_D$. Thus the logarithmic singularity yields a function $\left| \frac{1}{\left(\frac{\hbar\omega_D}{16t}\right)} \right|$ giving an important enhancement of $T_c$.

For $V_2 \neq 0$, one calculates T, as a function of $\frac{\sigma}{\lambda}$ for different ratios $\frac{\hbar\omega_D}{16t}$.

## α Calculation

The isotope effect exponent can be derived from equation (13) as

$$\alpha = \frac{d \ln T_c}{d \ln M} \qquad \ldots(16)$$

In the phonon-mediated paIrIng scheme $\omega_D$ is proportional to $M^{-\frac{1}{2}}$, when M is the average mass of the atom constituting the specimen under consideration, using equation (13) in equation (16), one finds-

$$\alpha = \frac{1}{2}\left\{1 - \left[\left[1 - \lambda\left(0.6646 + \ln\frac{\hbar\omega D}{16t} \ln\frac{\hbar\omega_D}{1.134\hbar\omega_D}\right)\right]^2 - \frac{\ln(k\beta Tc/1.134\hbar\omega_D)}{\ln\left(\frac{\hbar\omega_D}{16t}\right)}\right\}\right. \qquad \ldots(17)$$

in the limit of low $T_c$, it is straight forward to show that equation (17) can be estimated as –

$$\alpha = \frac{1}{2}\left\{1 - \left[\left[1 - \lambda \ln\left(\frac{\hbar\omega_D}{16t} \times \ln\frac{k_\beta\omega_D}{1.134\hbar\omega_D}\right)\right]^2\right\}\right. \qquad \ldots(18)$$

Here the quantity

$$\left| \frac{V_1}{2\pi^2 t} \ln\left(\frac{\hbar\omega_D}{16t}\right) \right|$$

in this model is equivalent to $N_0V_1$ in equation (12).

In a refined version of α, one calculates it directly by differentianting equation (11) with respect to M and get

$$\frac{\hbar\omega_D}{16t}$$

Were

$$H\left(\frac{Y}{2k_\beta T_c}\right) = \int_0^{\frac{y}{16t}} \frac{dx}{x} \tanh\left(\frac{8tx}{k_\beta T_c}\right) \qquad \ldots(19)$$

## RESULTS AND DISCUSSION

In this paper, we have studied the isotope effect in high $T_c$ superconductor within the conventional BCS theory. By passing that there exist the usual attractive interaction, Originating from the phonon exchange and an attractive interaction from the unknown origin. One calculates the transition temperature $T_c$ and the isotope effect exponent $\alpha$. The possible singular behaviour in the density of states and the relative importance of the attractive interaction $T_c$ and $\alpha$ are investigated. It is found that the singularity contributes to the enhancement of $T_c$. For high critical temperature, the second attractive interactions must be the stronger of the two. One also observes that the behaviour of the exponent $\alpha$ depends sensitively on the relative magnitude of the two interactions. The results are shown in Table 1.

**Table 1**

| **High $T_c$ superconductor** | **$T_c$ (K)** | **$\Theta_D$ (K)** | **T (K)** | **$\lambda$** | **$\alpha^{theo}$** | **$\alpha^{expt}$** |
|---|---|---|---|---|---|---|
| $La_{2-x}Sr_xCuO_4$ | 37 | 240 | 5000 | 0.02 | 0.19 | 0.16 |
| $YBa_2Cu_3O_7$ | 92 | 450 | 6000 | 0.01 | 0.09 | 0.018 ± 0.004 |
| $Bi_2Sr_2Ca_2Cu_3O_{10}$ | 107 | 535 | 6925 | 0.025 | 0.048 | 0.026 ± 0.02 |
| $Ba_0.6K_0.4BO_3$ | 32 | 186 | 4783 | 0.022 | 0.40 | 0.042 ± 0.05 |
| $(T1_0.5Pb_0.5)\ Sr_2Cu_2Cu_3O_9$ | 122 | 639 | 7447 | 0.039 | 0.037 | 0.027 ± 0.003 |

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