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Research Article

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Variation of Isotope Coefficient with Number of CuO_2 Layers in High TC Superconductors

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Abstract

In this paper, an effort has been made to study the isotope coefficient in high T_C Superconductors by using the variation of isotopic coefficient with the number of CuO_2 layers and the variation of isotope coefficients on transition temperature T_C. The Hamiltonian for CuO_2 layers using BCS type model and extra term of interlayer interaction between CuO_2 layers has been considered. Expressions for isotope effect (α) and transition temperature (T_C) are obtained and numerically calculated for experimental values by using Green's function technique.

Keywords: Isotope effect; CuO_2 layers; Isotope coefficient; High T_C superconductors

Introduction

After the discovery of high T_C cuprate superconductors in 1986 [1] at 35 K, the field is buzzing with research activities. Efforts to increase the transition temperature are currently going on. Till now the highest reached T_C under pressure is 164 K in $HgBa_2Ca_2Cu_3O_{8+8}$ [2]. These cuprates have unconventional properties both in normal and superconducting state [3,4]. Till date there is no consensus on the origin of pairing mechanism. It is now widely suggested that spin fluctuation driven pairing mechanism provides a good agreement between theory and experiments [5]. However, there are several experimental observations which clearly indicate that this purely electronic picture is incomplete and lattice effects have to be taken into account [6-8]. Isotope shift of T_C is regarded as the defining signature of superconducting pairing resulting from phonons. In high T_C superconductors, a small isotope effect is found [9-11]. Suppression of this effect is not explained within conventional BCS theory which predicts that the critical temperature T_C and isotope mass M are related by $T_C \propto M^{-\alpha}$ where α=0.5 for all elements. To explain the small isotope effect in high T_C compounds, many mechanisms including resonance valence bond [12], excitons [13], Plasmon's [14] and antiferromagnetic spin fluctuation mediated pairing are proposed [15]. Daemen and Overhauser [16] 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. Here we present the variation of isotope coefficients with number of CuO_2 layers and the variation of isotope coefficients on transition temperature T_C [17-22]. As the trilayer material has highest (T_C) in these cuprates but it has very small isotope coefficient (α). Clearly the argument that a mechanism other than an electron phonon interaction dominates the superconductivity based only on a small (α) in a cuprate with relatively high (T_C) is inappropriate. The observed CuO_2 layer dependence of the isotope effect indicates that the interlayer coupling between the adjacent CuO_2 planes is necessary for superconductivity in layered cuprates [23-26]. For monolayer materials having lower (T_C) the interlayer coupling plays a less important role and (T_C) can be mainly controlled by the phonon coupling yielding a larger size of isotope coefficient with increasing the number of CuO_2 layers in a unit cell, the interlayer coupling begins to play an important role in enhancing (T_C) and the isotope effect is expected to be small.

Formulation

The model Hamiltonian for our system can be described as

$$H = H_{intra} + H_{inter}$$

$$H_{intra} = \sum_{km\sigma} E_k a^{+}_{mk\sigma} a_{mk\sigma} - V \sum_{mkk'} a^{+}_{mk\uparrow} a^{+}_{m-k\downarrow} a_{m-k'\downarrow} a_{mk'\uparrow}$$

$$H_{inter} = -W \sum_{mnkk'} a^{+}_{mk\uparrow} a_{n-k'\downarrow} a_{mk'\uparrow}$$

$$H = \sum_{km\sigma} E_k a^{+}_{mk\sigma} a_{mk\sigma} - V \sum_{mkk'} a^{+}_{mk\uparrow} a^{+}_{m-k\downarrow} a_{m-k'\downarrow} a_{mk'\uparrow} - W \sum_{mnkk'} a^{+}_{mk\uparrow} a^{+}_{n-k\downarrow} a_{n-k'\downarrow} a_{mk'\uparrow} \quad (1)$$

Where $a^{+}_{mk\sigma}, a_{mk\sigma}$ denote the fermions creation and annihilation operator respectively, k is the wave vector and σ is spin index for fermions.

In our present analysis we use a Green's function, defining as

$$G^{\uparrow\uparrow}_{mnkk'} = \langle\langle a_{mk\uparrow}, a^{+}_{nk'\uparrow} \rangle\rangle \quad (2)$$

Equation of motion is written as

$$\omega G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi} + \langle\langle [a_{mk\uparrow}, H], a^{+}_{nk'\uparrow} \rangle\rangle$$

Evaluating the commutator $[a^{+}_{m-k\downarrow}, H]$ using the Hamiltonian (1) we get

$$[a_{mk\uparrow}, H] = E_K a_{mk\uparrow} - \sum_{k'} (V) a^{+}_{m-k\downarrow} a_{m-k'\downarrow} a_{mk'\uparrow} - \sum_{nk'} (W) a^{+}_{n-k\downarrow} a_{n-k'\downarrow} a_{mk'\uparrow}$$

And writing the equation of motion as

$$\omega G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi} + \langle\langle [a_{mk\uparrow}, H], a^{+}_{nk'\uparrow} \rangle\rangle \quad (3)$$

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Putting the value of commutator $\left[a_{mk\uparrow}, H\right]$ in equation (3) we get

$$\omega G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi} + \left\langle\left\langle E_k a_{mk\uparrow}, a^+_{nk'}\right\rangle\right\rangle - \sum_{k'} V \left\langle\left\langle a^+_{m-k\downarrow} a_{m-k'\downarrow} a_{mk'\uparrow}, a^+_{nk'\uparrow}\right\rangle\right\rangle - \sum_{k'} W \left\langle\left\langle a^+_{n-k\downarrow} a_{n-k'\downarrow} a_{mk'\uparrow}, a^+_{nk'\uparrow}\right\rangle\right\rangle$$

$$\text{Or } (\omega - E_k) G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi} - \left[\Delta v + \sum_n \Delta W\right] G^{\downarrow\uparrow}_{mn-kk'} \quad (4)$$

Now we introduce the order parameter Δ such as

$$\Delta_{rr} = \sum_k V_{rr}(kq)\left\langle C^+_{rk\uparrow} C^+_{r-k\downarrow}\right\rangle, \qquad \Delta_{rj} = \sum_k V_{rj}(kq)\left\langle C^+_{jk\uparrow} C^+_{j-k\downarrow}\right\rangle$$

Where $G^{\downarrow\uparrow}_{mn-kk'}$ is another Green's function which may be written as

$$G^{\downarrow\uparrow}_{mn-kk'} = \left\langle\left\langle a^+_{m-k\downarrow}, a^+_{nk'\uparrow}\right\rangle\right\rangle \quad (5)$$

This Green's function may also be written in terms of equation of motion as

$$\omega G^{\downarrow\uparrow}_{mn-kk'} = \left\langle\left\langle \left[a^+_{m-k\downarrow}, H\right]; a^+_{nk'\uparrow}\right\rangle\right\rangle \quad (6)$$

Evaluating the commutator $[a^+_{m-k\downarrow}, H]$ using the Hamiltonian

$$a^+_{m-k\downarrow}, H = \left[a^+_{m-k\downarrow}, \sum_{km\sigma} E_k a^+_{mk\sigma} a_{mk\sigma} - V \sum_{mkk'} a^+_{mk\uparrow} a^+_{m-k\downarrow} a_{m-k'\downarrow} a_{mk'\uparrow} - W \sum_{mnkk'} a^+_{mk\uparrow} a^+_{n-k\downarrow} a_{n-k'\downarrow} a_{mk'\uparrow}\right]$$

Putting the commutator $E_{(-k)} = E_k$ from (7) in equation (6) we get

$$\omega G^{\downarrow\uparrow}_{mn-kk'} = -E_k \left\langle\left\langle a^+_{mk\downarrow}, a^+_{nk'\uparrow}\right\rangle\right\rangle - V \sum_{k'} \left\langle\left\langle a^+_{mk'\uparrow}, a^+_{m-k'\downarrow}\right\rangle\right\rangle \left\langle\left\langle a_{mk\uparrow}, a^+_{nk'\uparrow}\right\rangle\right\rangle - W \sum_{nk'} \left\langle\left\langle a^+_{mk'\uparrow}, a^+_{n-k'\downarrow}\right\rangle\right\rangle \left\langle\left\langle a_{mk'\uparrow}, a^+_{nk\uparrow}\right\rangle\right\rangle$$

But from the law of conservation of energy

$$E_{(-k)} = E_k$$

$$(\omega + E_k) G^{\downarrow\uparrow}_{mn-kk'} = -\left(\Delta V + \sum_{\substack{n \\ m\neq n}} \Delta W\right) G^{\uparrow\uparrow}_{mnkk'} \quad (8)$$

In equation (4) we finally obtained the equation

$$(\omega - E_k) G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi} - \left(\Delta V + \sum_{\substack{n \\ m\neq n}} \Delta_n W\right) G^{\downarrow\uparrow}_{mn-kk'} \quad (9)$$

Multiply $(\omega+E_k)$ in equation (9) and putting the value of $(\omega - E_k) G^{\uparrow\uparrow}_{mnkk'}$ from equation (8) then we get the Green's function $G^{\uparrow\uparrow}_{mnkk'}$ as

$$\left(\omega^2 - E_k^2\right) G^{\uparrow\uparrow}_{mnkk'} = \frac{1}{2\pi}(\omega + E_k) - \left(\Delta V + \sum_n \Delta W\right)(\omega + E_k) G^{\downarrow\uparrow}_{mn-kk'} \quad (10)$$

Multiplying by $(\omega+E_k)$ in the equation (8) and putting the value of $(\omega - E_k) G^{\uparrow\uparrow}_{mnkk'}$ from equation (9) we get the Green's function as

$$G^{\uparrow\uparrow}_{mnkk'} = \frac{\omega + E_k}{2\pi\left[\left(\omega^2 - E_k^2\right) + \left(\Delta V + \sum_n \Delta_n W\right)\left(\Delta V + \sum_n \Delta_n W\right)\right]}$$

$$\left(\omega^2 - E_k^2\right) G^{\downarrow\uparrow}_{mnkk'} = -\left(\Delta V + \sum_{\substack{n \\ m\neq n}} \Delta_n W\right)(\omega - E_k) G^{\uparrow\uparrow}_{mnkk'}$$

We know from equation (9)

$$G^{\downarrow\uparrow}_{mn-kk'} = -\frac{\left(\Delta V + \sum_n \Delta W\right)}{2\pi\left(\omega^2 - E_k^2 - \left(\Delta V + \sum_n \Delta_n W\right)^2\right)} \quad (11)$$

Using the Green's function, we can obtain the expression for order parameter Δ_{mn} and correlation parameter γ the order parameter Δ_{mn} may be written as

$$\Delta_{mn} = \sum_{k'} V \left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle \quad (12)$$

Correlation function $\left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle$ is related to Green's function $G^{\downarrow\uparrow}_{mn-kk'}$ as

$$\left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty} \frac{G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon) - G^{\uparrow\uparrow}_{mn-kk'}}{e^{\omega/KT} - \eta} d\omega \quad (13)$$

Where η=-1 for fermions, K=Boltzmann constant and T= Temperature

Green's function $G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon)$ and $G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon)$ may be expressed as

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon) = \frac{-\left(\Delta V + \sum_n \Delta_n W\right)}{2\pi\left[(\omega + i\varepsilon)^2 - E_k^2 - \left(\Delta V + \sum_n \Delta_n W\right)^2\right]} \quad (14)$$

$$\therefore \xi_q^2 = E_k^2 + \left(\Delta V + \sum_n \Delta_n W\right)^2$$

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon) = -\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{4\pi\xi_q}\left\{\frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 - \varepsilon^2} - i\pi\delta(\omega - \xi_q) - \frac{(\omega + \xi_q)}{(\omega - \xi_q)^2 - \varepsilon^2} + i\pi\delta(\omega + \xi_q)\right\} \quad (15)$$

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon) = \frac{-\left(\Delta V + \sum_n \Delta_n W\right)}{2\pi\left[(\omega - i\varepsilon)^2 - E_k^2 - \left(\Delta V + \sum_n \Delta_n W\right)^2\right]} \quad (16)$$

$$\therefore \xi_q^2 = E_k^2 + \left(\Delta V + \sum_n \Delta_n W\right)^2$$

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon) = \frac{-\left(\Delta V + \sum_n \Delta_n W\right)}{2\pi\left[(\omega - i\varepsilon)^2 - \xi_q^2\right]}$$

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon) = -\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{4\pi\xi_q}\left\{\frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 + \varepsilon^2} + i\pi\delta(\omega - \xi_q) - \frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 + \varepsilon^2} + i\pi\delta(\omega - \xi_q)\right\} \quad (17)$$

Substitute both the Green's function $G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon)$ and $G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon)$ from equation (13) and then after solving we get correlation function.

$$G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon) - G^{\downarrow\uparrow}_{mn-kk'}(\omega - i\varepsilon) = -\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{4\pi\xi_q}\left(2i\pi\delta(\omega - \xi_q) - 2i\pi\delta(\omega + \xi_q)\right) \quad (18)$$

$$\therefore \left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty} \frac{G^{\downarrow\uparrow}_{mn-kk'}(\omega + i\varepsilon) - G^{\downarrow\uparrow}_{mn-kk'}}{e^{\omega/KT} - \eta} d\omega$$

Where η=-1

$$\left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty} -\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{4\pi\xi_q}\left(\frac{2i\pi\delta(\omega - \xi_q) - 2i\pi\delta(\omega + \xi_q)}{e^{\omega/KT} - \eta}\right) d\omega$$

$$\left\langle a^+_{mk'\uparrow} a^+_{m-k'\downarrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty} -\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{4\pi\xi_q}\left(\frac{2i\pi\delta(\omega - \xi_q) - 2i\pi\delta(\omega + \xi_q)}{e^{\omega/KT} - \eta}\right) d\omega = \frac{\left(\Delta V + \sum_n \Delta_n W\right)}{\xi_q}\left[\frac{1}{e^{\frac{\xi_q}{KT}} + 1} - \frac{1}{e^{\frac{-\xi_q}{KT}} + 1}\right]$$

Put $x = \dfrac{\xi_q}{kT}$

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$$\left\langle a^{+}_{mk'\uparrow} a^{+}_{m-k'\downarrow} \right\rangle = \frac{\left(\Delta V + \sum_n \Delta_n W\right)}{2\xi_q}\left[\frac{1}{e^{x}+1} - \frac{1}{e^{-x}+1}\right] \quad (19)$$

$$\therefore \frac{1}{e^{x}+1} - \frac{1}{e^{-x}+1} = \frac{e^{-x/2}+e^{x/2}}{e^{-x/2}+e^{x/2}} = \tanh\frac{x}{2} = \tanh\frac{\xi_q}{2kT}$$ Using in (19) we get

$$\left\langle a^{+}_{mk'\uparrow} a^{+}_{m-k'\downarrow} \right\rangle = \frac{\left(\Delta V + \sum_n \Delta_n W\right)}{\xi_q}\left(\tanh\frac{\xi_q}{2kT}\right) = \frac{\Delta V + \sum_n \Delta_n W}{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}} \tanh\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2} \quad (20)$$

Then we can obtained the expression of or dr parameter Δ_{ir} by substituting correlation function in equation (12)

$$\Delta_{ir} = \sum_{k'} V_{ir}\left(k'_q\right)\left\langle c^{+}_{ik'\uparrow} c^{+}_{i-k'\downarrow}\right\rangle = \sum_{k'} V_{ir}\left(k'_q\right)\left\langle a^{+}_{mk'\uparrow} a^{+}_{m-k'\downarrow}\right\rangle$$

$$\Delta_{mn} = \sum_{k'} V_{ir}\left(k'_q\right)\frac{\Delta V + \sum_n \Delta_n W}{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}} \tanh\frac{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}}{2kT}$$

Converting summation over K into integration with cut-off energy $\hbar\omega_D$ from the Fermi level we get

$$\Delta_{mn} = N_0 \int_0^{\hbar\omega D} V_{ir}\left(k'_q\right)\frac{\left(\Delta V + \sum_n \Delta_n W\right)}{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}} \tanh\frac{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}}{2kT} dE_q \quad (21)$$

$$\therefore \frac{1}{N_0 V} = \int_0^{\hbar\omega D} \frac{1}{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}} \tanh\frac{\sqrt{E_q^{\,2} + \left(\Delta V + \sum_n \Delta_n W\right)^2}}{2k_B T} dE_q \quad (22)$$

At $T = T_C, \Delta = 0$

$$\frac{1}{N_0 V} = \frac{1}{2K_B T_C}\int_0^{\hbar\omega_D} \frac{1}{\left(\frac{E_q}{2K_B T_C}\right)} \tanh\frac{E_q}{2k_B T_C} dE_q \quad (23)$$

$$\therefore \frac{1}{N_0 V} = \frac{1}{2K_B T_C}\int_0^{\frac{\hbar\omega_D}{2K_B T_C}} \frac{1}{x}\tanh x\left(2k_B T_C\right)dx$$

Or $\dfrac{\hbar\omega_D}{2K_B T_C} e^{0.8185} = \exp^{\frac{1}{N_0 V}}$

$$\therefore T_C = (1.13072)\frac{\hbar\omega_D}{2K_B}\exp^{-\frac{1}{N_0 V}} \quad (24)$$

The Isotope effect coefficient is

$$\alpha = -\frac{d\ln T_C}{d\ln M} \quad (25)$$

Using equation (29) and (30) we get

$$\alpha = \frac{d}{d\ln M}\left[\log(1.13072)\frac{\hbar\omega_D}{K_B} + \log e^{-\frac{1}{N_0 V}}\right] \quad (26)$$

Put $T_C \propto M^{-\frac{1}{2}}, or T_C = KM^{-\frac{1}{2}}$

$$\therefore \alpha = -\frac{d}{4d\log V}\left[2\log V\right] - \frac{d}{4d(\log V)}\left(\frac{1}{N_0 V}\right) \quad (27)$$

Differentiating we get

$$\frac{1}{N_0 V} = \left(2(1+2\alpha)\right) \quad (28)$$

Now from equation (24) we get

$$T_C = 1.13072\frac{\hbar\omega_D}{K_B}\exp\left(-2(2\alpha+1)\right) \quad (29)$$

By solving equation (33), we get α as

$$\alpha = \frac{1}{4N_0 V\left(1+\frac{D}{N_0}\right)} - \frac{1}{2} \quad (30)$$

The values of α and T_C are calculated from equation (29) and (30) respectively for various values of different CuO_2 layers (Table 1).

Results and Discussion

The numerical analysis of equation (29) and (30) have been calculated for different CuO_2 layers taking $\frac{D}{N_0} = 0.2(for n=1)$ and $\frac{D}{N_0} = 0.6(for n=3)$. Figure 1a is plotted between isotope coefficient (α) and number of CuO_2 layers (n) per unit cell. Figure shows that as increasing number of CuO_2 layers per unit cell, isotope coefficient (α) linearly decreases. For n=1, the value of (α) is 0.34 and it decreases continuously with number of CuO_2 layers. At n=3, isotope coefficient (α) is 0.1317 which is very low. This systematic reduction of isotope coefficient with increasing CuO_2 layers indicates that isotope effect can be negligible for multi-layer cuprates. This result is good agreement with experimental result made by Chen et al. Figure 1b is plotted between transition temperature (T_C) and isotope coefficient. The curve shows that as increasing (α), the transition temperature exponentially decreases so for lower isotope coefficient T_C will be maximum and T_C decreases for higher values of (α). So we can say that as increasing number of CuO_2 layers, (α) decreases and the transition temperature increases. This result also supported by Chakravarty et al.

Conclusion

First of all Hamiltonian for CuO_2 layers using BCS type model

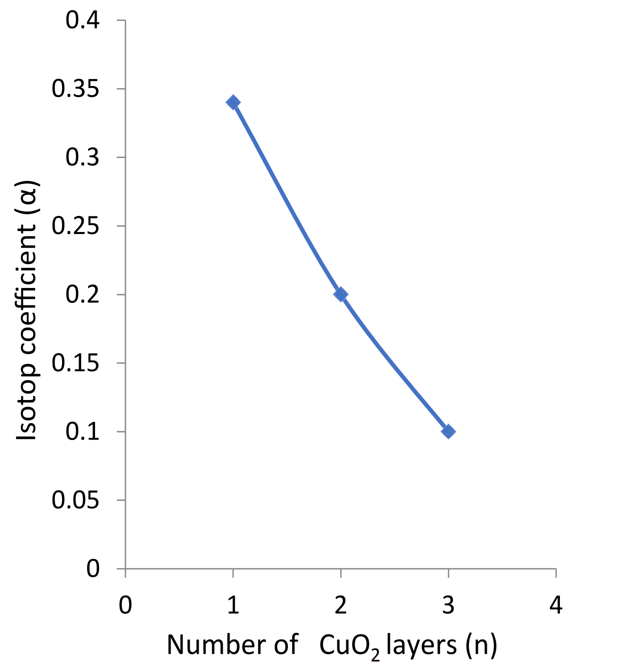

Figure 1a: Isotope coefficient (α) VS number of CuO_2 layers (n).

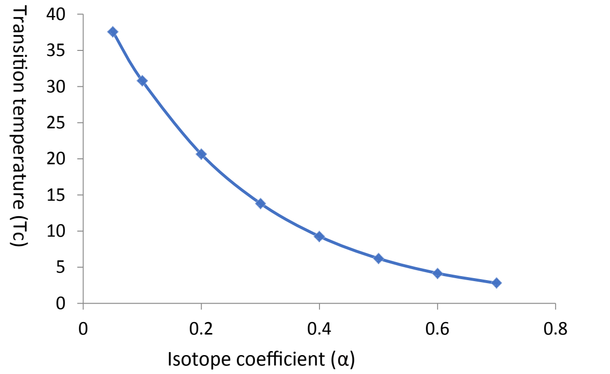

Figure 1b: Transition temperature (T_C) VS Isotope coefficient (α).

S No	α	T_c
1	0.05	37.586
2	0.1	30.772
3	0.2	20.627
4	0.3	13.827
5	0.4	9.268
6	0.5	6.212
7	0.6	4.164
8	0.7	2.791

Table 1: Table for values of (α) and (T_C).

and extra term of interlayer interaction between CuO_2 layers has been considered, using this equation expression for isotope effect (α) and transition temperature (T_C). Expression obtained is numerically solved using Green's function technique and then the value of isotope effect (α) and transition temperature (T_C) is calculated. The graph is plotted between isotopic coefficient and number of CuO_2 layers. The second graph is plotted between isotope effect (α) and transition temperature (T_C). Then conclusion is drawn comparing with available experimental result. The tri layer material has highest (T_C) in these cuprates but it has very small isotope coefficient (α). Clearly the argument that a mechanism other than an electron-phonon interaction dominates the superconductivity based only on a small (α) in a cuprate with relatively high (T_C) is inappropriate. The observed CuO_2 layer dependence of the isotope effect indicates that the interlayer coupling between the adjacent CuO_2 planes is necessary for superconductivity in layered cuprates. For monolayer materials having lower (T_C) the interlayer coupling plays a less important role and (T_C) can be mainly controlled by the phonon coupling yielding a larger size of isotope coefficient with increasing the number of CuO_2 layers in a unit cell, the interlayer coupling begins to play an important role in enhancing (T_C) and the isotope effect is expected to be small.

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