



## Influence of Interlayer coupling and pseudogap on Isotope effect in layered high $T_c$ cuprate superconductors

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**ABSTRACT:** In the present investigations, we have studied the influence of interlayer coupling and pseudogap on the isotope effect on the basis of the BCS- Hamiltonian that includes the coupling between the planes and an attractive interaction containing both the electronic and phononic contribution to pairing for the high- $T_c$  cuprate like  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  having two  $\text{CuO}_2$  planes per unit cell. Employing Green's function equations of motion technique, we obtain the expressions for the superconducting order parameter, transition temperature and hence the isotope effect coefficient ( $\alpha$ ). On the basis of numerical computation of isotope effect, we have pointed out that it increases with the coupling between the planes and decreases with the transition temperature. The presence of the pseudogap in the quasiparticle spectrum enhances the isotope effect coefficient. These results are viewed in terms of recent experimental study on isotope effect in layered cuprate superconductors.

### I. INTRODUCTION

The isotope effect which provided a proof of electron-phonon based mechanism (BCS theory) of conventional superconductor now became one of the poorly understood properties in high  $T_c$  layered cuprates superconductors. The isotope effect is quite anomalous in high- $T_c$  cuprates superconductors [1] and its value is found to be small compared to BCS value ( $\alpha = 0.5$ ). Further, the oxygen isotope effect ( $\alpha$ ) pointed out to depend on doping level and decreases with increase in  $T_c$ . These features of  $\alpha$  can not be understood within the frame work of BCS theory. In order to understand the anomalous behavior of  $\alpha$ , several theoretical attempts [2,3] have been made.

Recently, the existence of the pseudogap in the doped normal state of cuprates has been verified by several experimental probes like ARPES and NMR measurements [4,5,6]. The magnitude of the pseudogap has the same momentum dependence as that of d-wave superconducting gap in cuprates. Due to pseudogap features, the electronic density of states around the Fermi level is found to be energy dependent which may also affect  $T_c$  and hence isotope effect in doped cuprates. So far, the microscopic origin of pseudogap and its influence on isotope effect in doped cuprates is not clearly understood from theoretical point of view. Further due to layered structure of  $\text{CuO}_2$  planes the recent ARPES measurements predicted that coupling

between the  $\text{CuO}_2$  planes is important as electronic spectra of these systems show different features for single plane and multi-  $\text{CuO}_2$  plane per unit cell cuprates [7]. Since isotope effect ( $\alpha$ ) in high-  $T_c$  cuprates depend on  $T_c$  and  $T_c$  is a function of number of  $\text{CuO}_2$  planes in a unit cell. This implies that isotope effect may also be influenced by coupling between the planes. Therefore, in the present work we have planned to include interlayer coupling and pseudogap in the study of isotope effect in layered cuprate superconductors.

### II. THEORETICAL FORMULATION

We consider BCS-type Hamiltonian containing the terms coupling between the  $\text{CuO}_2$  plane and an attractive interaction arising due to both, phononic and electronic mechanism. Such a model Hamiltonian be applicable for bilayer systems. The model Hamiltonian for our bilayer system in superconducting state can be given as

$$H = \sum_{\mathbf{k}\sigma} (\tilde{\epsilon}_{\mathbf{k}} - \mu) a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \sum_{\substack{\mathbf{r}\mathbf{s}\mathbf{k}\sigma \\ \mathbf{r} \neq \mathbf{s}}} t_{\mathbf{r}\mathbf{s}}^{-} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma}^{-}$$

$$- \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V(\bar{\mathbf{k}}, \bar{\mathbf{k}}') a_{\mathbf{k}\sigma}^{\dagger} a_{-\mathbf{k}-\sigma}^{-} a_{-\mathbf{k}'-\sigma}^{+} a_{\mathbf{k}'\sigma}^{-}$$

.... (1)

Where  $r, s=1, 2$  are layer indices within the unit cell. In equation(1), first term represents the kinetic energy of free charge carriers (holes) within the planes and second term represents the momentum dependent interlayer coupling between the  $\text{CuO}_2$  layers within the unit cell and  $\mu$  is the chemical potential. The interlayer coupling is found to have the momentum dependence of the form  $t_{k_\perp} = -\frac{t_\perp}{2} (\cos k_x a - \cos k_y a)^2$ . The planar

quasiparticle energy is expressed as  $\tilde{\epsilon}_{\bar{k}} = \sqrt{\epsilon_{\bar{k}}^2 + E_g^2(\bar{k})}$ , where we have introduced the pseudogap  $E_g(\mathbf{k})$  in phenomenological manner having momentum dependence of the form of d-wave superconducting order parameter as  $E_g(\mathbf{k})=E_g(\cos k_x - \cos k_y)$ . The last term in the model is attractive interaction where we have assumed anisotropic attractive Interaction  $V(\bar{k}, \bar{k}')$  containing contributions from electronic as well as phonon based mechanism. i.e.

$$V(\bar{k}, \bar{k}') = V_e(\bar{k}, \bar{k}') + V_p(\bar{k}, \bar{k}') \quad \dots(2)$$

Applying BCS mean field decoupling followed by canonical transformation we linearized the Hamiltonian and applying the Green function equations of motion approach, and following standard procedure [5], we obtain the expression of the superconducting order parameter containing electronic and phononic contributions as.

$$\Delta_p = \frac{V_p}{4N} \sum_{|\epsilon_{\bar{k}'}| \leq \omega_e} |\chi(\bar{k}')|^2 \frac{\tanh\left(\frac{\beta \epsilon_{\bar{k}'}}{2}\right)}{E_{\bar{k}'}} \Delta_{ep} + \frac{V_p}{4N} \sum_{\omega_e < |\epsilon_{\bar{k}'}| \leq \omega_p} |\chi(\bar{k}')|^2 \frac{\tanh\left(\frac{\beta \epsilon_{\bar{k}'}}{2}\right)}{E_{\bar{k}'}} \Delta_p \quad \dots(2)$$

where,

$$E_{\bar{k}} = \sqrt{(\tilde{\epsilon}_{\bar{k}} - \mu)^2 + |\Delta_{\sigma \bar{k}}|^2} \quad \text{and} \quad \tilde{\epsilon}_{\bar{k}} = \sqrt{\epsilon_{\bar{k}}^2 + E_g^2(\mathbf{k})}$$

where  $e$  and  $ep$  are the electronic and phononic contributions respectively. The above equation can be written as  $2 \times 2$  matrix and can be used to find the expression of isotope effect (the limit of  $T \rightarrow T_c$ ) as

$$\alpha = \frac{\omega_p}{2T_c} \frac{dT_c}{d\omega_p} \Rightarrow \frac{\omega_p}{2T_c} \frac{dT_c}{d\omega_p} = \frac{d\omega_p}{dT_c} \quad \dots(3)$$

The final expression for isotope effect ( $\alpha$ ) is obtained as

$$\alpha = \frac{V_p \{V_e L_0(\omega_e) - 1\} \omega_p \frac{\partial L_0(\omega_p) / \partial(\omega_p)}{2T_c}}{\left[ V_e \{1 + V_p (2L_0(\omega_e) - L_0(\omega_p))\} F_e + V_p \{1 - V_e L_0(\omega_e)\} \left\{ F_p + G_p \frac{dE_g^2}{dT_c} \right\} \right]}$$

.....(4)

where,  $F_a = \frac{\partial L_0(\omega_a)}{\partial T_c}$  and  $G_a = \frac{\partial L_0(\omega_a)}{\partial E_g^2}$ , ( $a=e$ , or  $p$ )

$$L(\omega_a) = \frac{1}{4N} \sum_{\bar{k}'} |\chi(\bar{k}')|^2 \frac{\tanh\left(\frac{\beta \epsilon_{\bar{k}'}}{2}\right)}{E_{\bar{k}'}} \left( \frac{dE_g^2}{dT_c} \right)_{T=T_c} = \frac{dE_g^2}{dT_c} = -2E_g^2 \left( 1 - \frac{T_c}{T^*} \right) \quad \text{and}$$

$$L_0(\omega_a) = \frac{1}{8\pi} \sum_p \int_0^{2\pi} d\theta \int_{-\omega_a}^{\omega_a} d\epsilon \eta(\epsilon) \frac{\cos^2(2\theta)}{2} \frac{\tanh\left(\frac{\beta \tilde{\epsilon}_{kp}}{2}\right)}{\tilde{\epsilon}_{kp}}$$

$$\tilde{\epsilon}_{kp} = \tilde{\epsilon}_{\bar{k}} + p t_\perp \quad \text{and} \quad p = \pm 1,$$

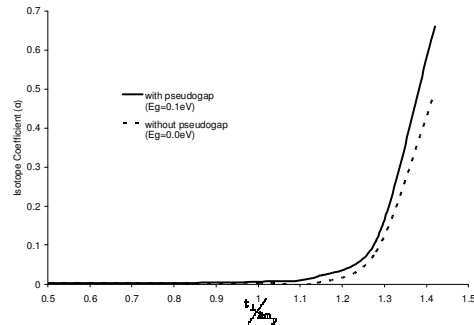
where pseudogap is parameterized as-

$$E_g(\theta) = E_g(T) \cos(2\theta) \quad \text{and} \quad E_g(T) = E_g(0) \left( 1 - \frac{T}{T^*} \right)$$

### III. RESULTS AND DISCUSSION

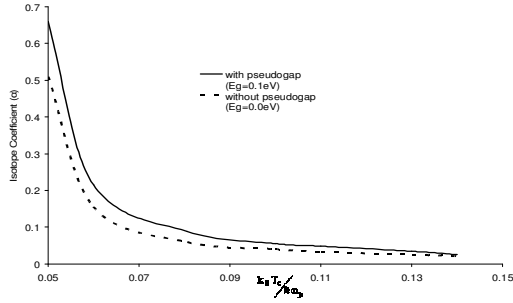
The isotope effect coefficient ( $\alpha$ ) has been calculated numerically from equation (4) as a function of transition temperature  $T_c$ , interlayer coupling ( $t_\perp$ ) and pseudogap  $E_g(\mathbf{k})$ . In Fig (1), we plot  $\alpha$  vs. renormalized interlayer coupling  $\tilde{\epsilon}_\perp = \left( \frac{t_\perp}{\hbar \omega_p} \right)$  keeping

other parameter fixed. One can see from Fig (1) that the isotope effect increases with  $\tilde{\epsilon}_\perp$ . The inclusion of pseudogap ( $E_g=1\text{eV}$ ) further enhances the rate of increase in  $\alpha$ .



**Fig. 1.**  $\alpha$  vs  $\tilde{\epsilon}_\perp$  keeping other parameter fixed ( $T_c=60^0$  K,  $T^\oplus=0.07968\text{eV}$ ,  $\omega_p=0.07\text{eV}$ ), without electronic contributions.

In Fig (2) we have shown the variation of  $\alpha$  with renormalized transition temperature  $\tilde{T} = \left( \frac{k_B T_c}{\hbar \omega_p} \right)$  with and without pseudogap parameter.



**Fig. 2.**  $\alpha$  vs  $\tilde{T}$  keeping other parameter fixed ( $t_{\perp}=0.09\text{eV}$ ,  $T_c=60\text{K}$ ,  $T^{\oplus}=0.07968\text{eV}$ ,  $\omega_p=0.07\text{eV}$ ), without electronic contributions.

The isotope effect decreases as we increase renormalized transition temperature  $\tilde{T}$ . Therefore, we concluded that the presence of pseudogap enhances the isotope effect ( $\alpha$ ). While  $\alpha$  found to be increased with  $\tilde{\epsilon}_{\perp}$  (coupling between the  $\text{CuO}_2$  planes) in high-  $T_c$  cuprates.

The pseudogap enhances the isotope coefficient. In the present analysis, we have taken the constant electronic density of states around the Fermi level. It will be interested to improve these results by introducing energy dependent density of the states around the Fermi level. These studies will be planned in near future.

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