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Research Article

Theory of Isotope Effect in $YBa_2Cu_3O_{7-\delta}$

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This paper is the first to demonstrate that a pure nonphonon mechanism can quantitatively explain all isotope effect experiments in $YBa_2Cu_3O_{7-\delta}$ (YBCO) and to conclude that the influence of zero-point oscillation on the two local spin-mediated interaction (TLSMI) causes the isotope effects in YBCO. This paper is the first to calculate the doping dependence of exponents of oxygen isotope effect for all quantities of YBCO, such as T_c, T^*, pseudogap at T_c, gap at 0 K, and number density of supercurrent carriers at 0 K. This paper points out that the observed inverse isotope effect of T_c comes also from zero-point oscillation.

1. Introduction

Understanding the high-temperature superconductivity in cuprate superconductors is at the heart of current research in solid-state physics. However, the pairing mechanism responsible for high-T_c is still controversial [1–7]. The isotope effect is an important experimental probe in revealing the underlying pairing mechanism of superconductivity. When high-T_c superconductivity was discovered in cuprates, the oxygen isotope exponents, defined by $\alpha_{T_c} = -\mathrm{dln}Tc/\mathrm{dln}M$, with M being the oxygen isotopic mass, were promptly measured [8–17]. In [1, 7] the authors think that such elaborate isotope effects strongly suggest that high-T_c superconductivity should be of phonon mechanism. Although [3] proposes a t-J model including phonons, it cannot explain the isotope effect quantitatively. Therefore, until quite recently, there are still two problems which have not yet been solved. The first problem is that there is not a unified microscopic theory for both isotope effect and all other properties of the high-T_c cuprates. The second problem is that there is not a quantitative theory of the isotope effect, which is based on a pure electron mechanism. This paper tries to solve those two problems.

The two local spin-mediated interaction (TLSMI), which is a pure electron mechanism, of high-T_c cuprates was proposed in [18] and can explain nearly all experiments except the isotope effect [6]. An electron mechanism similar to that in [18] is also proposed in [19, 20]. Therefore, isotope effect is a key criterion for the correctness of theory in [6, 18–20]. This paper uses TLSMI to explain quantitatively isotope effects and to give a series of predictions related to the isotope effect. The TLSMI is introduced briefly in Section 2. In Section 3, we take the zero-point oscillation of ^{18}O and ^{16}O as the origin of isotope effect in YBCO and make numerical calculations for the oxygen isotope effects of all quantities such as T_c, T^*, pseudogap at T_c, gap at 0 K, and number density of supercurrent carriers at 0 K. Based on the quantitative comparisons between theory and experiments, Section 4 makes conclusions and discussions.

2. Two Local Spin-Mediated Interaction

The effective Hamiltonian of Hubbard-Emery d-pσ model to describe the CuO_2 plane of high-T_c cuprates is [6]

$$H = -\sum_{i\alpha\beta s} T_{\alpha\beta} p^+_{\alpha s} p_{\beta s} + J_K \sum_{i\alpha\beta ss'} \hat{\mathbf{S}}_i \cdot \vec{\sigma}_{ss'} p^+_{\alpha s} p_{\beta s'} + J \sum_{i \neq j} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \tag{1}$$

where the summation over α and β is for the oxygen sites around ith Cu^{++} site, $p_{\alpha s}$ annihilates $O_{p\sigma}$ hole with spin s at site α, $\hat{\mathbf{S}}_i$ is the local spin operator of Cu^{++} at site i, $\vec{\sigma}$ Pauli matrix vector, and i and j are the nearest neighbors. Expand $p_{\alpha s}$ in $\mathbf{k}$ space. Here, $\mathbf{k}$ is the wave vector in Brillouin zone of the oxygen lattice in the CuO_2 plane. The second term in (1) is Kondo Hamiltonian, H_K, which implies that the $O_{p\sigma}$ holes with $\mathbf{k}\uparrow$ and $-\mathbf{k}\downarrow$ can have interactions with the local spins of Cu^{++} at sites i and j, respectively. The third term in

(1) is Heisenberg interaction, H_H, between the two nearest neighbor local spins at sites i and j. $J \propto t^4$, $J_K \propto t^2$, and t is the hopping integral between site of Cu^{++} and O^{--} ions. The effective interaction between the two $O_{p\sigma}$ holes with $\mathbf{k} \uparrow$ and $-\mathbf{k} \downarrow$, mediated by two nearest neighbor local spins at i and j, is called TLSMI.

Using the extended Abrikosov's pseudo-Fermion method in [6], the expression of TLSMI $U_{\mathbf{kk}'} = -A(T)F_{\mathbf{kk}'}$ is

$$U_{\mathbf{kk}'} = -A(T)F_{\mathbf{kk}'}, \tag{2}$$

$$A(T) = \frac{JJ_K^2 N'' / N' w(J/T)}{T^2 + 64JJ_K^2 \sum_{\mathbf{kp}} g(\mathbf{k},\mathbf{p}) / \left\{1 + 32\pi^2 J_K^2 [N(E_F)]^2 \overline{h(\mathbf{q})}\right\}}, \tag{3}$$

$$g(\mathbf{k},\mathbf{p}) = \left(\frac{1}{2N_{\mathrm{Cu}}}\right)^2 \frac{f[\epsilon(\mathbf{k}) - E_F]F_1(\mathbf{k})F_1(\mathbf{p})F_5(\mathbf{k})F_5(\mathbf{p})}{\epsilon(\mathbf{p}) - \epsilon(\mathbf{k})} \times e^{i(\mathbf{k}-\mathbf{p})\cdot(\mathbf{R}_{i'} - \mathbf{R}_i)}, \tag{4}$$

where $h(\mathbf{q}) = [\cos(q_x a/2)\cos(q_y a/2)]^4$, $F_{\mathbf{kk}'} = \sum_{i=1}^{4} \cdot F_i(\mathbf{k})F_i(\mathbf{k}')F_5(\mathbf{k})F_5(\mathbf{k}')$, $F_1(\mathbf{k}) = \cos(k_x a)\cos(k_y a)$, $F_2(\mathbf{k}) = \sin(k_x a)\sin(k_y a)$, $F_3(\mathbf{k}) = \sin(k_x a)\cos(k_y a)$, $F_4(\mathbf{k}) = \cos(k_x a)\sin(k_y a)$, $F_5(\mathbf{k}) = \cos^2(k_x a/2)\cos^2(k_y a/2)$, $f(x)$ is Fermi distribution, $\epsilon(\mathbf{k})$ energy of $O_{p\sigma}$ holes, E_F Fermi energy, $N(E_F)$ density of states, N' the number of Cu^{++} in a cluster with antiferromagnetic short-range order in the CuO_2 plane, N'' the number of Cu^{++} in the nearest-neighbor position in the same cluster, and $\mathbf{R}_{i'} - \mathbf{R}_i$ are any position vectors of two local spins in nearest neighbor. The bar represents the average on Fermi surface. $w(J/T)$ is the transformation factor in the extended Abrikosov's pseudo-Fermion method [6].

3. Oxygen Isotope Effect in YBCO

Reference [21] estimated the effect of zero-point oscillation on the hopping integral t, and gave an isotope mass (M)-dependent formula of the hopping integral, which is $t = t(a_\circ)(1 + 3.71 \times \hbar \times 10^{16}/(2M\omega_\circ 1.6^2))$, and $\omega_\circ$ is circular frequency of optical mode, $\omega_\circ = 500\,\mathrm{K}$. According to our estimation, ${}^{18}t/{}^{16}t = 0.99952$. From (3) and [22], we see that TLSMI is nearly proportional to t^6, and thus, a small value of ${}^{18}t/{}^{16}t$ can have obvious isotope effect. Taking TLSMI as Cooper pairing potential, considering that the Fermi surface in the CuO_2 plane has nesting structure [6], and using the values of parameters given in [6], we obtain the following theoretical doping evolutions of the isotope effects for all quantities of YBCO.

The definition of exponent of oxygen isotope effect of T_c is

$$\alpha_{T_c} = -\frac{\ln^{18} T_c - \ln^{16} T_c}{\ln 18 - \ln 16}. \tag{5}$$

The result of numerical calculations for YBCO is given in Figure 1. The theoretical results fit the data well. The physical origin of the nonmonotonic x-dependence in Figure 1 is as follows. Both the experimental data and theoretical calculations show that the x-dependence of T_c is nonmonotonic [6, 11]. For example, $T_c = 0$ at $x = 0.05$, 0.27, and the maximum value of T_c is at $x = 0.16$. Because the values of T_c at $x \cong 0.05$ and $\cong 0.27$ are very small, even a very small effect of isotope substitution will lead to large exponent of isotope effect. On the contrary, because the value of T_c at $x = 0.16$ is maximum, even the same effect of isotope substitution, as that at $x \cong 0.05$ and $\cong 0.27$, occurs at $x = 0.16$ will lead to the small exponent of isotope effect.

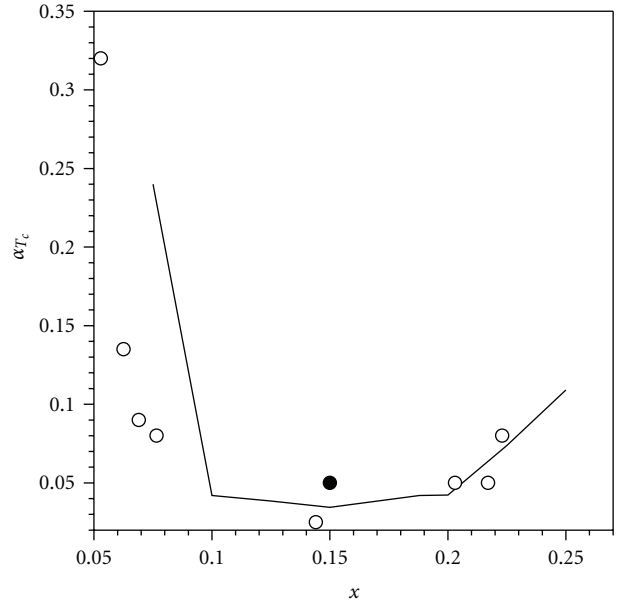

Figure 1: Theoretical curve of α_{T_c} versus x. x is the number of oxygen hole per cell of Cu lattice in the CuO_2 plane of YBCO. The filled circle is from [10]. The open circle is from [1, 11].

The definition of exponent of oxygen isotope effect of the pseudogap at T_c is

$$\alpha_{\Delta(T_c)} = -\frac{\ln^{18}\Delta(T_c) - \ln^{16}\Delta(T_c)}{\ln 18 - \ln 16}. \tag{6}$$

The result of numerical calculations for YBCO is given in Figure 2. There are no data in Figure 2. For reference, we give the data of $YBa_2Cu_4O_8$ [12]. The result of experiment in [12] is $\alpha_{\Delta(T_c)} < 0.01$. Although our theoretical results are not less than 0.01, the values of $\alpha_{\Delta(T_c)}$ is only one third of the values of α_{T_c} for YBCO. The physical origin of the nonmonotonic x-dependence in Figure 2 is nearly the same as that for Figure 1.

The definition of exponent of oxygen isotope effect of the gap at 0 K, $\Delta(0)$ is

$$\alpha_{\Delta(0)} = -\frac{\ln^{18}\Delta(0) - \ln^{16}\Delta(0)}{\ln 18 - \ln 16}. \tag{7}$$

The result of numerical calculations for YBCO is given in Figure 3. There are no data in Figure 3. Therefore, Figure 3 is a prediction for YBCO. The physical origin of the monotonically increasing x-dependence in Figure 3 is

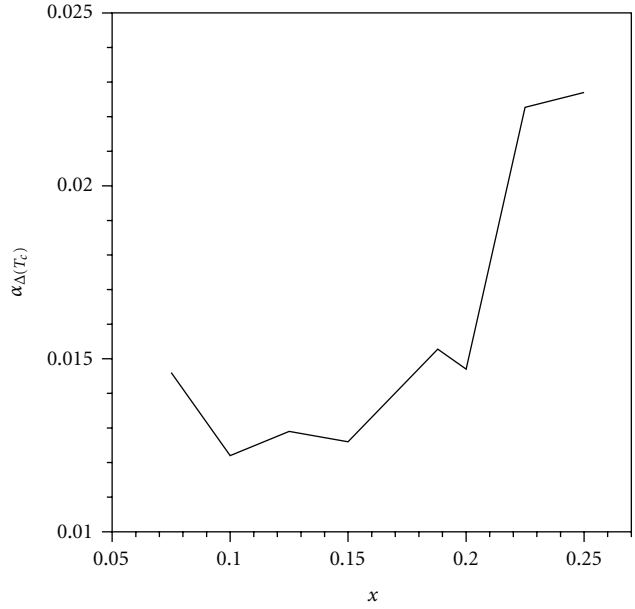

Figure 2: Theoretical curve of $\alpha_{\Delta(T_c)}$ versus x for YBCO.

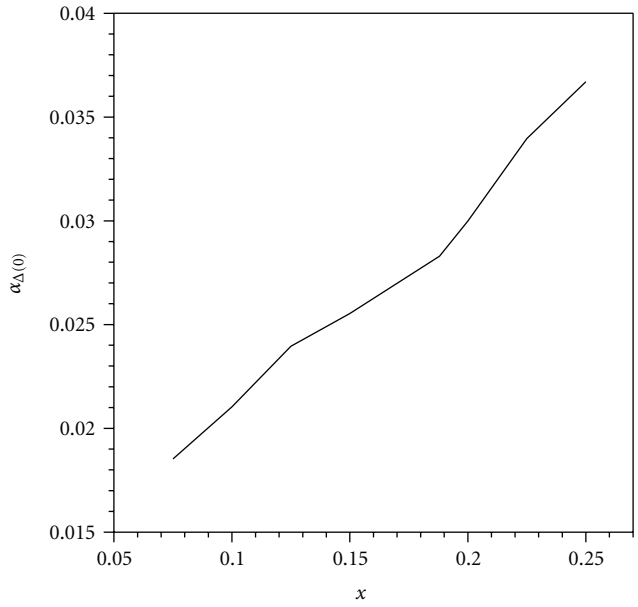

Figure 3: Theoretical curve of $\alpha_{\Delta(0)}$ versus x for YBCO.

as follows. Our numerical calculations indicate that the potential of Cooper pairs is a monotonically reducing x-dependence (e.g., from 7000 K at $x = 0.07$ to 4500 K at $x = 0.25$). The scale of potential of Cooper pairs determines directly the scale of the gap at 0 K. Therefore, even if the effects of isotope substitution are the same, the exponent of oxygen isotope effect of the gap at 0 K and small value of x will be less than that at large value of x.

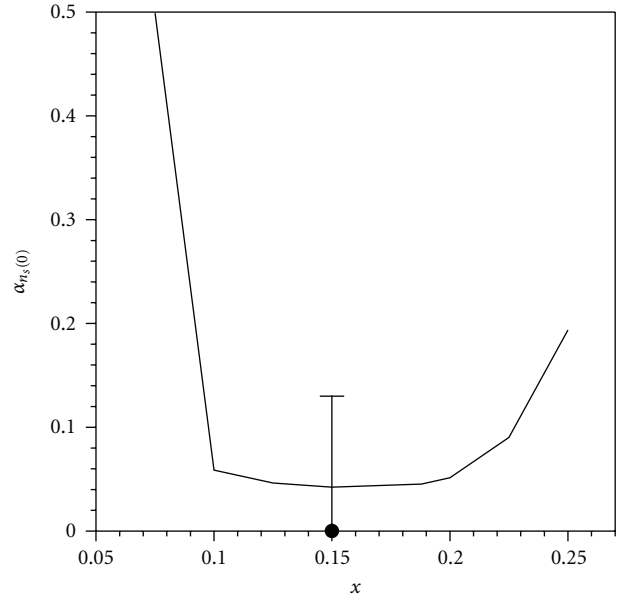

Figure 4: Theoretical curve of $n_s(0)$ versus x for YBCO. The data are from [10].

The definition of exponent of oxygen isotope effect of the number density of supercurrent carriers at 0 K is

$$\alpha_{n_s(0)} = -\frac{\ln^{18} n_s(0) - \ln^{16} n_s(0)}{\ln 18 - \ln 16}. \tag{8}$$

The result of numerical calculations for YBCO is given in Figure 4. The data are from [10].

As is well known, the number density of supercurrent carriers at 0 K determines directly the value of T_c. Therefore, the physical origin of the nonmonotonic x-dependence in Figure 4 is the same as that for Figure 1.

The definition of exponent of oxygen isotope effect of the temperature T^*, at which the pseudogap begins to open, is

$$\alpha_{T^*} = -\frac{\ln^{18} T^* - \ln^{16} T^*}{\ln 18 - \ln 16}. \tag{9}$$

The result of numerical calculations for YBCO is given in Figure 5. The data are for $YBa_2Cu_4O_8$ [13]. Therefore, Figure 5 is a prediction for YBCO. $\alpha_{T^*} > 0$ is in Figure 5. However, $\alpha_{T^*} < 0$ is a theoretical result in [3]. The physical origin of the oscillatory and increasing x-dependence in Figure 5 comes from many factors. Both the experimental data and our numerical calculations show that the value of T^* is monotonically reducing from small value of x ($x = 0.05 T^* = 350$ K) to large value of x ($x = 0.27 T^* = 20$ K). Note that the range of variation of the values of T^* is very high. If we just consider the value of T^*, then the exponent of oxygen isotope effect of the temperature T^* will tend to be monotonic increasing. However, the scale of T^* is determined by the potential of Cooper pairs. This potential is given by (3). From (3), we see that the potential is very sensitive to temperature T through the T^2 factor in denominator and the $w(J/T)$ factor in the numerator. The variation of T^* means the variation of T. The x-dependence

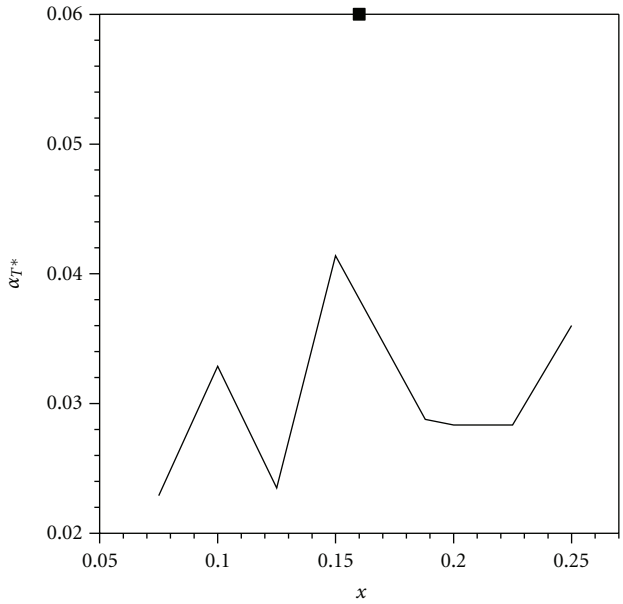

FIGURE 5: Theoretical curve of α_{T^*} versus x for YBCO. The data are for $YBa_2Cu_4O_8$ [13].

of the potential in (3) is more complicated, because the J, J_K, E_F, and so on in (3) are x-dependent. Many factors determine the oscillatory and increasing x-dependence.

The definition of exponent of oxygen isotope effect of effective mass in the CuO_2 plane, m^*_{ab}, is

$$\alpha_{m^*_{ab}} = -\frac{\ln^{18} m^*_{ab} - \ln^{16} m^*_{ab}}{\ln 18 - \ln 16}. \tag{10}$$

The experiment in [10] is $\alpha_{m^*_{ab}} = -0.061$, which means that ${}^{18}m^*_{ab} > {}^{16}m^*_{ab}$. The explanation for this result is as follows. The carriers in YBCO are polaronic oxygen holes. According to [4], The mass of polaronic oxygen holes are oxygen isotope mass (M) dependent. $m^*_{ab} \propto \exp(a\sqrt{M})$, and $a > 0$. Therefore, ${}^{18}m^*_{ab} > {}^{16}m^*_{ab}$.

The experiments in [14, 16] pointed out that the inverse isotope effect of α_{T_c} was observed in some magnetic superconductors. The theory in Section 3 can have inverse isotope effect in principle. The reason is as follows. It is possible that $t = t(a_\circ)(1 - 3.71 \times \hbar \times 10^{16}/(2M\omega_\circ 1.6^2))$ [21]. In this case, the larger the M is, the larger the hopping integral t is. From (2) and (3), we see that the larger the t is, the larger the TLSMI is, and, thus, the larger the T_c is.

4. Conclusions and Discussions

From [6] and this paper, we know clearly that the mechanism in Section 2 for the high-T_c cuprates, that is, the TLSMI between two polaronic oxygen holes that causes the high-T_c superconductivity in YBCO, can explain many experimental findings including oxygen isotope effects of YBCO quantitatively. Right now, the theoretical curves in Figures 2, 3, and 5 are pure predictions for YBCO. If all the predictions can be verified by future experiments, then the mechanism in [6] for the high-T_c YBCO might be a correct unified microscopic theory for both isotope effect and all other properties of the high-T_c cuprates.

Although the theory in this paper cannot yet explain the following two experiments, we know the reasons. (1) Upon oxygen isotope substitution (${}^{16}O$ versus ${}^{18}O$), T_c and T^* are shifted from 79 K and 170 K to 78.5 K and 220 K for $HoBa_2Cu_4O_8$, respectively, by means of inelastic neutron scattering [15]. However, this huge isotope shift of T^* is absent in NMR and NQR experiments for the same material [15]. We guess that the formula of neutron cross-section, based on which [15] analysis experiment data, is wrong. Because [23, 24] pointed out that the Fermi golden rule, which is used to derive the formula in [15], is not correct. (2) The huge oxygen isotope effect of T_c in $La_{2-x}Sr_xCuO_4$ [17] cannot be explained by the theory in this paper. We guess that this huge oxygen isotope effect comes from inhomogeneous distribution of carriers in its stripe phase [4, 25].

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