Role of LO Phonon on Pseudo-Gap Phase in High-$T_c$ Cuprate Superconductors

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Abstract. In analyzing the role of optical phonon on transition temperature $T_c$, the simplified extended BCS-like theory was tried in success and why Coulomb interaction must be large was understood. Oxygen (O) -isotope effect on $T_c$ was explained in good agreement with more than 120 experimental data. The superconductivity appears in itself due to Bose-condensation of bipolarons coupled with surrounding local distortion and the change is discussed basing on the relative movement of light O-atoms in high-$T_c$ oxides. From the present theoretical formula, LO phonon modes are made mainly at O-sites, and the mode couple to electrons changes from Z.B. type (under-doped region) to Z.C. type (over-doped region) at a doped point ($x=1/8$ in $La_{2-x}Ba_xCuO_4$). At optimally doped point, the vibration type of O-atoms exchanges through zero vibration, and therefore, the concentration takes the form of dip point of $T_c$. In over-doped region, LO-Z.C. mode with negative pressure dependence plays and condenses simultaneously at $T_c$, whereas in under-doped region, LO-Z.B. mode with positive pressure dependence couples to electrons to make charged boson at pseudo-gap phase, and condensed for $T$ under $T_c$. By introducing the strong electron correlation in addition to the conventional mechanism of superconductivity, $T_c$-equation would be derived for $d$-wave superconductors.

1. Introduction

Since the discovery of copper oxide superconductors with high transition-temperature ($T_c$), the mechanism and the role of phonons for the remarkable superconductivity remain a matter of primary concern. Although the evidence for electron-phonon coupling was reported by the angle-resolved photoemission spectroscopy (ARPES) some years ago [1], afterward, the contribution of phonons to superconductivity is regarded as small as ever from recent tunneling spectroscopy, etc. [2]

In this paper, therefore, we study the role of acoustic and optical phonons in perovskite-type and the reduced type oxides. We introduce the strong electronic correlation in addition to the conventional BCS formula to make the mechanism for $d$-wave superconductivity. After taking into account the common feature to superconductors and ferroelectrics with the perovskite structure, we study the role of optical phonons on high-$T_c$ superconductivity and explain Oxygen (O) -isotope effect on $T_c$ for many experimental data in these substances. Furthermore, the difference between under-doped and over-doped regions is discussed from the importance of the longitudinal optical (LO) phonon modes playing for the pseudo-gap phase.
2. Bose-condensation of bipolaron

2.1. Energy gap in BCS formula
First, we stand on the viewpoint of superconducting mechanism due to Bose-condensation of quasi-particles, and try to give the simplified formula of high-$T_c$ Cu-oxides. In the theory of superconductors, an idea of small-polaron pairs as quasi-particles was introduced successfully by Alexandrov and Ranninger [3] before the discovery of copper-oxides by Bednorz and Müller [4]. They considered the BCS formula for the energy gap:

$$\Delta \cong 2\hbar \omega \exp \left(-\frac{1}{\lambda}\right), \quad (1)$$

with $\lambda = VN(0)$, $V$ being the electron-phonon interaction. $T_c$ is given by

$$k_B T_c \cong \hbar \omega \exp \left(-\frac{1+\lambda}{\lambda}\right), \quad (2)$$

which remains fairly low (< 40 K) for metallic superconductors ($\lambda = 0.3$), and obeys the condition of $\lambda \sim 1$ for polaron formation. All the carriers form polarons, where acoustic phonons change the form to surrounding local distortion. In two polarons with the same sign repelling each other, an attractive force works when the polarized regions overlap especially in two-dimensional systems. This superconducting model due to Bose-condensation of polaron-bound pairs (bipolarons) can be applied in SrTiO$_3$ and other similar materials [5].

2.2. Superconductivity in perovskite-like oxides
In this section, we study some kinds of optical phonons in perovskite-type (Ba(Pb$_{1-x}$Bi$_x$)O$_3$ (BPBO) ($T_c$=13K) and (Ba$_{1-x}$K$_x$)BiO$_3$ (BKBO) ($T_c$=30K) ) and the reduced type oxides La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) ($T_c$=40K), YBa$_2$Cu$_3$O$_7$ (YBCO) ($T_c$=90K) and Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi2212) ($T_c$=92K) ) with various $T_c$, and in the next section, we will explain O-isotope effect on $T_c$ for many experimental data in these substances.

In Fig. 1, we show four types of optical phonon modes made by Cu-O (or Bi-O) in-plane motion; ($Q_1$ and $Q_3$: LO mode, $Q_2$ and $Q_4$: TO mode; $Q_1$ and $Q_2$: Z.C. type, $Q_3$ and $Q_4$: Z.B. type).

In perovskite-oxides with ferroelectric transition point $T_a$, it is observed without exception that the substances with softening of Z.C. type ($q=0$) TO phonon corresponds to negative pressure dependence on $T_a$, and Z.B. type ($q=\pi/a$) to positive pressure dependence on $T_a$ [6]. From the comparison with pressure-dependence of transition point coming from various O-vibration modes in perovskite-oxides, it will be concluded that perovskite-like oxides with superconducting $T_c$, are classified into Z.C. type with $dT_c/dp < 0$ and Z.B. type with $dT_c/dp > 0$ for LO phonon mode.

The nature of $dT_c/dp > 0$ are found in La214 (ex. La$_{1.88}$Sr$_{0.12}$CuO$_4$), Y124 (YBa$_2$Cu$_3$O$_8$), and Y123 (YBa$_2$Cu$_3$O$_7$), and on the other hand, of $dT_c/dp < 0$ in BKBO, Bi2212 and Tl2201 (Tl$_2$Ba$_2$CuO$_{6+y}$) [7]. The substance NCCO (Nd$_{1.85}$Ce$0.15$CuO$_4$) without apical O shows no pressure dependence on $T_c$. Taking into account that the effect of pressure will be more sensitive for vertical displacement of apical O, applying pressure is expected to strengthen the planar O-vibration modes in the existence of both upper and lower apical O (ex. La214, BKBO).

Here we adopt the site representation formalism developed by Appel and Kohn [8], and set up a homogeneous integral equation for the vertex part $\Gamma$ from which the critical temperature $T_c$ is calculated [9]:
\[ \Gamma(\omega) = -\beta^{-1} \sum_{\omega'} \Gamma(\omega') F(\omega') \left[ I(\omega', \omega) + U \right] , \quad (3) \]

where the Coulomb interaction part is put as \( U \). A crucial point in the present problem is that bipolaron-Green’s function and O-optical phonon Green’s function are assumed to be separable in real space. Then interaction vertex part \( I \) takes on a form such that the roles played by bipolaron and optical phonon may be separated as \( I = (V_{bp}, V_o) \) according to the effective energy range.

3. Role of LO phonon

3.1. Oxygen-isotope effect on \( T_c \)

In this section, let us consider the role of optical phonon given for the relative movement of light O-atoms. O-isotope effect has been measured on the in-plane penetration depth in LSCO [10] and on ARPES nodal dispersion in Bi2212 [11]. Although an overall trend for anomalous oxygen (\(^{16}\text{O} - ^{18}\text{O} \)) isotope effect on \( T_c \) presented in an early stage for LBCO, YBCO, etc. [12] was tried to explain by using the theoretical model of small bipolaron [13], subsequent experimental results suggest the contribution of LO phonon associated with the movement of O-atoms.

Here, by considering LO phonon made mainly at O-sites, we discuss the role of LO phonon playing on the bipolaron-based superconductivity. In the site-representation formalism, we present the generalized BCS-like equation for \( T_c \):

\[ T_c \propto \theta_{bp} \exp \left[ -1 / N(0)V_{eff} \right] , \quad (4) \]

\[ V_{eff} = V_{bp} + \frac{V_o - U^*}{1 - (V_o - U^*) N(0) \ln(\omega_o / \omega_a)} , \quad (5) \]

\[ U^* = \frac{U}{1 + N(0)U \ln(\omega_F / \omega_o)} . \quad (6) \]

This derivation is based on the technique explained successfully in Ref.[9], which is the similar form to equation given by Allender-Bray-Bardeen for an exciton model [14]. Within the weak-coupling theory, we introduced the effective electron-electron interaction vertex \( V_{eff} \) which is enhanced by optical phonon interaction \( V_o \) (cutoff frequency \( \omega_o \)) and by a factor \( \ln(\omega_o / \omega_a) \) in the denominator, and is reduced by Coulomb repulsion (cutoff frequency \( \omega_k \)). It is easily guessed that optical phonon due to oxygen vibration contributes to \( T_c \), and the O-mass \( (M) \) dependence is introduced through only \( \omega_o \). Oxides with large \( U^*/V_o \) exhibits the importance of strong electron-electron correlation to enhance \( T_c \).

In Fig.2, \( T_c-\alpha \) relation \( (T_c \propto M^{-\alpha} ) \) with \( \alpha = - d \ln T_c / d \ln M \) is described for some parameters of \( U/V_o \) in good agreement with more than 120 experimental data of high-\( T_c \) superconductors [12], where \( N(0)V_o = 0.3 \) estimated for YBCO, \( \omega_o = 50 \) meV and \( \omega_a = 10 \) meV are assumed for the calculation of \( \alpha \). \( \theta_{bp} = 600 \) K is presumed for a characteristic temperature forming bipolaron condensation. The solid line is the curve depicted for a parameter \( U^*/V_o = 1.0 \) which is the case of best fit to most of experimental data.
The parameters with \( \frac{U'}{V_o}>0.5 \) are realized when strong electron-electron correlation exceeds the half of the contribution of optical phonon playing on \( T_c \). When \( \frac{U'}{V_o} \) exceeds 0.5, \( \alpha \) becomes positive, and induce anomalous \( T_c-\alpha \) relation with both \( \alpha>0.5 \) and \( \alpha<0.5 \). It means that the optical phonon makes the overall behavior of \( \alpha>0.5 \) (for lower \( T_c \)) and \( \alpha<0.5 \) (for higher \( T_c \)) in oxide superconductors with large Coulomb repulsion. For \( \frac{U'}{V_o}=0.5 \), no Isotope effect would be expected for the appearance of \( T_c \). If \( \frac{U'}{V_o} \) becomes smaller than 0.5, \( \alpha-T_c \) behavior becomes similar to it in BCS-like metal superconductors derived by Morel-Anderson [15] where \( \alpha \) reduces from 0.5 (BCS-value) with decreasing \( T_c \). The negative value of \( \alpha<0 \) is realized in dash and dotted line for only one experimental example in Fig. 2.

3.2. Difference between under-doped and over-doped regions
In the previous theoretical formula, we had the result that optical phonon contributes to induce anomalous O-isotope effect. Basing on the pressure-dependence of \( T_c \), we present the prospect that the LO phonon mode to couple to electrons changes from Z.B. type in under-doped region to Z.C. type in over-doped region. The \( T-x \) phase diagram is shown in Fig. 3 schematically, where \( x \) called as hole-concentration corresponds to the density of bipolarons in the present model. It is expected that in coherent overlapping region of Bose-condensed bipolarons, Cooper pairs will be formed which is also discussed as a crossover from Bose-condensation to BCS state in bixiton model [16].

By taking into account \( d \)-wave symmetry, in under-doped region of LBCO, Z.B. type LO phonon (half-breathing stretching mode around \((\pi,0)\): \( Q_0 \) in Fig. 1) with \( dT_c/d\rho>0 \) couples to electrons, whereas in over-doped region, Z.C. type (full-breathing stretching mode around \((\pi,\pi)\): \( Q_1 \) in Fig.1) LO phonon with \( dT_c/d\rho<0 \). The existence of apical O is meaningful to make the stretching modes in Cu-O in-plane motion, and thus high-\( T_c \) oxides are realized in perovskite-like structure.

Now it will be analyzed the origin of superconductivity for both under-doped and over-doped regions. In under-doped region, we would be able to explain that optical mode \( Q_0 \) plays a role to make incoherent charged boson at \( T_c<T<T^* \) (pseudo-gap region), and condenses for \( T<T_c \). In over-doped region, \( Q_1 \) mode plays and condenses simultaneously at \( T_c \).

4. Discussion
In this approach, the simplified extended BCS-like theory is in success in analyzing explicitly the role of optical phonon on \( T_c \), from which it would be explained why Coulomb interaction \( U' \) should become large to some degree in perovskite-like oxide superconductors.

We propose a model that LO phonon mode to couple to electrons changes from Z.B. type (under-doped region) to Z.C. type (over-doped region) at an optimal doped point (\( x=1/8 \) in LBCO). However, at the change point, the vibration-type of O-atoms exchanges through zero vibration, and therefore, an optimally doped point takes the form of dip point of \( T_c \).

Finally, as the appearance of \( T_c \) might be decided as Bose-condensation of small bipolaron made by acoustic phonon, we exchanged Debye temperature \( \Theta_D \) to a characteristic temperature forming small bipolaron \( \Theta_{bp} \), and also \( V \) to polaron-polaron attraction \( V_{pp} \) to describe charged boson in Eq. (5). Thus we had to introduce the strong electronic correlation in addition to the conventional mechanism of superconductivity. Furthermore, the derivation of \( T_c \)-equation for \( d \)-wave superconductivity should be published in detail with energy gap \( \Delta(k)=\Delta(\cos k_x-\cos k_y) \) in the forthcoming paper.
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Figure Captions

Fig. 1 Four kinds of Optical phonons: $Q_1$, $Q_2$, $Q_3$ and $Q_4$-mode ($Q_1$: LO- Z.C., $Q_2$: TO- Z.B., $Q_3$: LO- Z.B., $Q_4$: TO- Z.C.).

Fig. 2 $T_c-\alpha$ relation predicted theoretically for many perovskite-like oxide superconductors; solid line: $U^*/V_c=1.0$, dotted line: 0.8, broken line: 0.6, dash and dotted line: 0.4. Experimental data are plotted as the symbols $\Box$, $\triangle$, $\blacksquare$, $\bigcirc$ corresponding to LSCO, YBCO, Bi2212 and EuBa$_2$Cu$_{1-x}$Zn$_x$O$_7$-$\delta$ respectively [12].

Fig. 3 Schematic $T$-$x$ phase diagram in Cu-oxide superconductors LBCO.
Fig. 1

(a) $Q_1$ mode
(b) $Q_2$ mode
(c) $Q_3$ mode
(d) $Q_4$ mode
**Fig. 2**

The figure shows a plot of $\alpha$ versus $T_c$ in Kelvin, with different lines representing various $U^*/V_o$ values: 1.0, 0.8, 0.6, and 0.4. The data points are indicated by different symbols for each $U^*/V_o$ value.
$$\frac{dT_c}{dT} < 0$$

$$\frac{dT_c}{dP} > 0$$

$T^*$

under-doped

over-doped

Fig. 3