CHINESE PHYS. LETT.
Vol.4, No.9(1987)

CHINESE PHYSICS LETTERS
Science Press, Beijing
Springer-Verlag

MECHANISM OF HIGH T_c SUPERCONDUCTIVITY IN Ba-La-Cu-O*

LIU Fusui, SHENG Yi, DAI Yuandong
刘福绥 盛毅 戴远东
(Department of Physics, Peking University, Beijing)

(Received 11 February 1987; revision received 24 April 1987)

It is proposed that the high T_c superconductivity in Ba-La-Cu-O system comes from the phonon cloud mediated Fröhlich polaron pair. The T_c should be lower than the transition tmeperature of small polaron into large polaron. Estimated value of T_c is also given based on the mechanism proposed by the authors.

Bednorz and Müller have found that the highest superconductivity onset temperature in Ba-La-Cu-O system was in 30K range from resistivity experiment[1]. It was also observed in the measurement of magnetic susceptibility[2]. The high T_c in Ba-La-Cu-O is realized in the K_2NiF_4 type structure from the X-ray analysis[3]. Even much more high T_c was observed in Ba-La-Cu-O[4,5].

Some mechanisms which possibly concern the Ba-La-Cu-O superconductivity were proposed. It includes the bipolarons (small) superconductivity[6] and LO polar modes superconductivity in $SrTiO_3$ (ref.7).

Our mechanism of high T_c in Ba-La-Cu-O is phonon cloud mediated Fröhlich (large) polaron pair superconductivity. At first we indicate some instructions coming from experiments. Then some derivation and numerical estimates are given. At last we make some discussions.

There is clearly an exponential increase part before the onset of superconductivity in the curves of temperature dependence of resistivity in some samples of Ba-La-Cu-O[1,5]. The exponential increase looks like the behavior of small polaron. It will be shown in the following that the small polaron can translate into Fröhlich polaron, when the temperature goes down. Considering the small polaron which does not benefit the superconductivity for the localization and there is no exponential increase for another samples, we guess that the carrier of superconductivity is Fröhlich polaron. The reasons of enhancement of phonon mediated interaction between Fröhlich polarons are: (1) the Ba-La-Cu-O system exhibits a number of oxygen-deficient phases with mixed valent copper constituents, i.e. with itinerant electronic states between the non-J.T.Cu^{3+} and J.T.Cu^{2+}, thus was expected to have considerable electron-phonon coupling[1]; (2) Fröhlich polaron motion produces phonon cloud, the phonon number of which can be larger than one, so the phonon cloud me-

* This work was supported by the Science Fund of the Chinese Academy of Sciences.

diated superconductivity will have higher T_c than the one phonon mediated superconductivity.

The Hamiltonian of small polarons is[8]

$$H=J\sum_{j\delta} C^+_{j+\delta}C_j + \sum_{q} \omega_q a^+_q a_q + \sum_{j\vec{q}} C^+_j C_j e^{i\vec{q}\cdot\vec{R}_j} M_{\vec{q}}(a_{\vec{q}}+a^+_{-\vec{q}}) , \tag{1}$$

where C_j is the destruction operator for an electron on site R_j, and a_q is the phonon destruction operator. The Hamiltonian is solved in the position space without resorting to collective coordinates. By the following canonical transformation the last two terms of the Hamiltonian (1) can be diagonalized. M_q is the electron-phonon matrix element in Wannier representation.

$$S=-\sum_{j\vec{q}} n_j e^{i\vec{q}\cdot\vec{R}_j}(a_{\vec{q}}-a^+_{-\vec{q}}) ,$$

$$\bar{H}=e^S He^{-S}=J\sum_{j\delta} C^+_{j+\delta}C_j X^+_{j+\delta}X_j + \sum_{\vec{q}} \omega_q a^+_q a_q - \sum_j n_j \Delta ,$$

$$\Delta=\sum_{\vec{q}} \frac{M^2_{\vec{q}}}{\omega_{\vec{q}}} \tag{2}$$

$$X_j=\exp[\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_j}\frac{M_{\vec{q}}}{\omega_{\vec{q}}}(a_{\vec{q}}-a^+_{-\vec{q}})] .$$

The effective band energy is

$$\vec{\varepsilon}_{\vec{q}}=J\sum_{\delta} e^{i\vec{q}\cdot\vec{\delta}}\, e^{-S_T} ,$$

$$e^{-S_T}=\langle i|X^+_{j+\delta}X_j|i\rangle=\exp[-\sum_{\vec{q}}(\frac{M_{\vec{q}}}{\omega_{\vec{q}}})^2(1-\cos(\vec{q}\cdot\vec{\delta}))(\frac{2}{e^{\beta\omega_{\vec{q}}}-1}+1)] . \tag{3}$$

So, when temperature decreases, the effective band energy also increases, i.e. the Fröhlich polaron occurs at lower temperature than the small polaron. Holstein[8] estimated the transition temperature between Fröhlich polaron and small polaron to occur around 40% of Debye temperature for some materials. For Ba-La-Cu-O system we can not calculate the transition temperature for lack of data. But we can say from the above exact derivation that our guess on the Fröhlich polaron superconductivity does not contradict the theory.

The Fröhlich polaron causes the lattice deformation which have discrete amounts, i.e. phonons. The average number of phonons in polaron, i.e. phonon cloud, can be calculated as follows. From the first order perturbation the wave function of the electron is

$$\Psi_{\vec{p}}(\vec{r})=|\vec{p}\rangle+\sum_{\vec{p}'} \frac{|\vec{p}'\rangle\langle\vec{p}'|V|\vec{p}\rangle}{\varepsilon_p-\varepsilon_{p'}+\omega_0}$$

$$=\frac{1}{V^{\frac{1}{2}}}\left[e^{i\vec{p}\cdot\vec{r}}|0\rangle+\frac{M_0}{V^{\frac{1}{2}}}\sum_{\vec{q}}\frac{1}{q}\frac{e^{i(\vec{p}+\vec{q})\cdot\vec{r}}a_{\vec{q}}^{+}|0\rangle}{\varepsilon_p-\varepsilon_{p+q}-\omega_0}\right], \quad (4)$$

where $|0\rangle$ is the phonon vacuum, ω_0 is the LO mode frequency. The total number of phonons in the phonon cloud is found by taking the expectation of the phonon number operator with this state

$$Nu(p)=\int d^3r\Psi_{\vec{p}}^{+}(\vec{r})\sum_{\vec{k}}a_{\vec{k}}^{+}a_{\vec{k}}\Psi_{\vec{p}}(\vec{r})=\frac{\alpha}{2}\left(\frac{\omega_0}{\omega_0-\varepsilon_p}\right)^{\frac{1}{2}}, \quad (5)$$

where $\alpha=(e^2/\hbar)(m/2\hbar\omega_0)^{0.5}(1/\varepsilon_\infty-1/\varepsilon_0)$. The estimated value of α for strong coupling theory, i.e. small polaron, is $\alpha\geq 5$ (ref.9). We assume the value of α does not change when the small polaron translates into Fröhlich polaron.

Assuming the average electron energy ε_p is $\omega_0/2$, then $Nu(p)\geq 3.5$. When the Fröhlich polaron exchanges phonon cloud, the indirect attractive interaction, v, will be 3.5 times, at least, stronger than the general one phonon indirect attractive interaction. From the formular $T_c=1.14\ \omega_0\exp(-1/N(E_F)v)$, we can see that the '3.5 time' has a big effect. For example, if a sample's T_c is 0.019K, $\omega_0\tilde{=}500K$, then we get $N(E_F)v=0.097$. But, if $N(E_F)v=3.5\times 0.097=0.34$, then $T_c=30K$! If we consider also the J.T. enhancement of electron-phonon coupling, then we have no difficulty in understanding the high T_c superconductivity in Ba-La-Cu-O system.

In principle our mechanism can be used also for acoustic phonon polaron. The key quantity of our mechanism is the number in phonon cloud which is proportional to α.

The authors are grateful to Professor HAN Rusan, Professor YIN Daole, and Professor GAN Zizhao for the discussions of this problem.

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