CHINESE PHYS. LETT.
Vol.5, No.2(1988)

CHINESE PHYSICS LETTERS
Science Press,Beijing
Springer-Verlag

THE THEORETICAL STUDY OF SUPERCONDUCTIVITY IN OXIDE $BaPb_{1-x}Bi_xO_3$

WANG Wenguo, MA Benkun
王文国　　马本堃
(Department of Physics, Beijing Normal University, Beijing)

(Received 3 July 1987)

A local Hamiltonian is introduced to study $BaPb_{1-x}Bi_xO_3$. The usual CPA method is used to deal with the substitutional disorder effect. The superconducting $T_c \sim x$ relation is calculated and the result is in agreement with experiments. Some remarks on the characteristics of oxide superconductivity are presented.

The oxide superconductor $BaPb_{1-x}Bi_xO_3$ (or BPB) was discovered in 1975[1]. The crystal structure of ABO_3 type of BPB was verified at low temperature. The highest T_c of BPB is 13K with x=0.3. the magnetic penetration depth is 2.1-2.3μm, twice larger than the values in dirty limit[2]. Then the coherence length should be quite short, and it is reasonable to introduce the following local Hamiltonian for the electron system of BPB

$$H=\sum_{i,j,\sigma} t_{ij}c^+_{i\sigma}c_{j\sigma}+\sum_{i,\sigma} V_i c^+_{i\sigma}c_{i\sigma}-\sum_i \lambda_i n_{i\uparrow}\cdot n_{i\downarrow} , \tag{1}$$

where i,j denote lattice sites; $V_i=V_A$ or V_B(A refers to $BaPbO_3$ and B to $BaBiO_3$); $t_{ij}=t(|\vec{R}_i-\vec{R}_j|)$ is hopping matrix element; $\lambda_i(>0)$ is local BCS interaction parameter.

Model Hamiltonian (1) may be linearized as follows,

$$H'=\sum_{i,j,\sigma} t_{ij}c^+_{i\sigma}c_{j\sigma}+\sum_{i,\sigma} V_i c^+_{i\sigma}c_{i\sigma}-\sum_i [\Delta_i c^+_{i\sigma}c^+_{i\bar{\sigma}}+\text{H.C.}+|\Delta_i|^2/\lambda_i] , \tag{2}$$

where the spatially varying order parameter Δ_i can be determined by minimizing the free energy corresponding to H':

$$\Delta_i=\lambda_i\cdot\langle c_{i\downarrow}c_{i\uparrow}\rangle . \tag{3}$$

By introducing field operators(N is the total number of electrons)

$$\phi_i=\begin{pmatrix} c_{i\uparrow} \\ c^+_{i\downarrow}\end{pmatrix} , \quad \phi^+_i=(c^+_{i\uparrow}\ c_{i\downarrow}) , \quad \psi^+=(\phi^+_1\phi^+_2\cdots\phi_N) \tag{4}$$

and a Hamiltonian of matrix form

$$\mathcal{H}=\begin{pmatrix} H_0+V & -\Delta \\ -\Delta^+ & -H_0-V\end{pmatrix} , \tag{5}$$

where $(H_0)_{ij}=t_{ij}$; $(V)_{ij}=V_i\delta_{ij}$; $(\Delta)_{ij}=\Delta_i\delta_{ij}$;

we have $H'=\psi^+\cdot\mathcal{H}\cdot\psi$. (6)

Now define the Green's function

$$G_{ij} = \begin{pmatrix} \langle c_{i\uparrow};\ c^{+}_{j\uparrow} \rangle & \langle c_{i\uparrow};\ c_{i\downarrow} \rangle \\ \langle c^{+}_{i\downarrow};\ c^{+}_{j\uparrow} \rangle & \langle c^{+}_{i\downarrow};\ c_{j\downarrow} \rangle \end{pmatrix}, \tag{7}$$

which obeys the equation of motion(z is frequency variable)

$$(z-\mathcal{H})\cdot G(z) = 1 \tag{8}$$

For a given x, there are many atomic configurations which may be realized with nearly equal probabilities. When eq.(8) is configuration-averaged, it becomes

$$\begin{pmatrix} z - H_0 - \varepsilon(z) & \Delta(z) \\ \Delta^{+}\ (-z^{+}) & z + H_0 + \varepsilon^{+}(-z^{+}) \end{pmatrix} \bar{G}(z) = 1 , \tag{9}$$

here $\varepsilon(z)$ and $\Delta(z)$ are translationally invariant self-energy terms. $\bar{G}$ may be related to G by the scattering matrix T:

$$G = \bar{G} + \bar{G}\cdot T\cdot \bar{G} ; \tag{10}$$

when averaged again, this relation requires

$$\bar{T} = 0 . \tag{11}$$

With the usual Coherent-Potential-Approximation (CPA), equation (11) may be replaced by the following single site scattering condition[3]

$$\bar{T}_i = 0 . \tag{12}$$

This equation will determine $\bar{G}$, and then the physical quantities of the electron system.

BPB exhibits an M-I phase transition near x=0.35, which has been discussed already by Rice and Sneddon[4]. We will consider mainly the metal regime with x<0.35.

When the superconducting critical point is approached, we have

$$\Delta_i \to 0 , \quad \Delta(z) \to 0 , \quad (T \to T_c) . \tag{13}$$

Let $z\to 0$, and the energy constant be

$$\varepsilon_0 \equiv \varepsilon(z)\big|_{z\to 0} = (V_A + V_B)/2 ,$$

then condition (12) will be reduced to the following equation

$$(V_B - V_A)^{-1}\ (1-2x) = \int_0^{\infty} d\omega \cdot \rho(\omega, x)\ (\varepsilon_0 + \omega)^{-1} \qquad (0<x<0.35) , \tag{14}$$

where $\rho(\omega,x)$ is the distribition function of probability

$$\rho(\omega, x) = \rho_1(\omega)\cdot \rho_2(\omega)\cdot \rho_3(x) \tag{15}$$

$\rho_1(\omega) = (1+e^{\beta\omega})^{-1}$ is the Fermi function, $\beta = 1/k_B T_c$; $\rho_2(\omega) = e^{-\omega^2/D^2}$ is the integral cutting off factor of Gauss type, which corresponds to the square approximation of BCS type,

$$V_{kk'} = \begin{cases} V & E_F - \omega_P \leq E_k ,\ E_{k'} \leq E_F + \omega_P ; \\ 0 & \text{other cases} \end{cases} \tag{16}$$

and finally, $\rho_3(x) = N_F(x)$ is the density of states at Fermi level.

The electronic structure of BPB, especially the specific form of N_F (see fig.1), has been calculated by Mattheiss et al[5,6]. And their result will be used directly in our calculation.

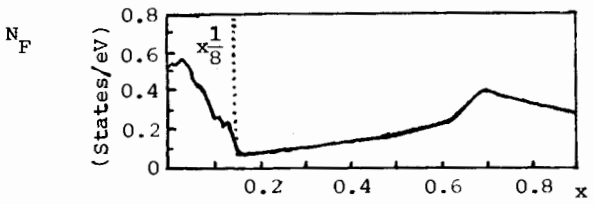

Fig.1 N_F as a function of x (from ref.6).

We have solved equation (14) by computer. The Gauss width D is set to be 0.01eV; the parameters $V_B \pm V_A$ are determined by the experimental data[1]

$$T_c = 9K \quad (x=0.05) \; ; \quad T_c \to 0 \quad (x=0.35) \; ,$$

then we get

$$V_B - V_A = 0.192eV \; ; \quad V_B + V_A = 2\varepsilon_0 = 0.796eV$$

The result of our calculation is presented in fig.2, and an agreement with that of experiments can be seen.

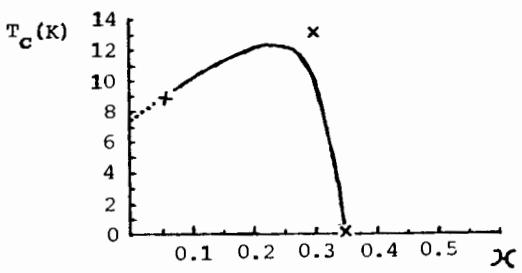

Fig.2 The calculated $T_c \sim x$ relation.
"x" represent experimental points.

Now we would make several remarks on the characteristics of oxide superconductors, including both BPB and Y-Ba-Cu-O system which has the highest T_c of 95K at present.

1. The mechanism of superconductivity in oxide systems is still that of phonon-induced Cooper-pair-condensation, but the average radius of Cooper pairs is quite short. This feature lowers the requirement for crystal perfection, and leads to a large magnetic penetration depth;

2. Barium has the lowest ionization energy among all II A elements

in the periodic table. In oxide state Ba has the tendency to stabilize itself by releasing two electrons of opposite spin directions, and this is favorable to the production of Cooper pairs and to the prevention of structural phase transitions;

3. The existence of valence-changing elements (such as Bi^{+3}, Bi^{+5} in BPB and Cu^{+1}, Cu^{+2}, Cu^{+3} in Ba-Y-Cu-O) make it difficult to satisfy the saturation and directionality of valence bonds. Then the electron system remains in the Cooper-pairing state instead of turning in to the localized valence-bonding state even though the electron-phonon interaction becomes quite strong;

4. The major difference between BPB and Ba-Y-Cu-O is that the latter includes rare earth element Y which has the electronic state $4d^1 5s^2$. The active 4d orbit of Y hybridizes strongly with the 2p orbit of O, and this results in many equivalent electronic orbits. Therefore N_F increases and so does T_c greatly.

The authors wish to thank Professor ZHANG Liyuan and Professor CAI Jianhua for helpful discussions.

REFERENCES

1. A.W.Sleight et al., Solid State Commun.17(1975)27.
2. T.Murakami, Jpn.J.Appl.Phys.24-2(suppl)(1985)10.
3. A.Weinkauf and J.Zittarz, Solid State Commun.14(1974)365.
4. T.M.Rice and L.Sneddon, Phys.Rev.Lett.47(1981)689.
5. L.F.Mattheiss and D.R.Hamann, Phys.Rev.B28(1983)4227.
6. L.F.Mattheiss, Jpn.J.Appl.Phys.24-2(suppl)(1985)6.