Thermodynamic Properties Of YBCO-123 Superconducting Materials With S-Wave And P-Wave Singlet Admixture

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***Abstract*—The first truly high temperature ceramic superconductor is composed of Yttrium, Barium, Copper and Oxygen (YBCO).The copper oxide networks play a major role for the occurrence of superconductivity. We present a possible pairing mechanism in YBCO-123 materials. Different models like; Resonance valence bond ,spin fluctuation and t-j models have been used to explain superconductivity but have not fully explained the behavior of these materials in the superconducting state. At present there exists no alternative model that can predict maximum critical temperature in these materials. The thermodynamic properties of YBCO-123 have been studied using the Bogoliubov-Valatin formalism approach. In this research s-wave singlet and p-wave singlet pairing admixture has been studied. Two jumps in the specific heat were noted at T_C = 65K and T_C = 284K. Specific heat for the admixture was found to be 5.9x10^{-27} J/K at T_C .These measurements are important in understanding the electronic excitations close to quantum phase transitions. This study is a step towards realizing room temperature (T_C = 298k) superconductors which will bring in great technological advancement.**

Keywords—High temperature superconductivity, Specific heat, Transition temperature

I. INTRODUCTION

In 1986, Bednorz and Muller discovered superconductivity in lanthanum-based cuprate whose transition temperature was 35K. Later, Chu and Wu found that replacing the lanthanum with Yitrium, i.e. making a superconductor YBCO, raised the critical temperature to 92K, and this was important since liquid nitrogen could be used as a refrigerant (its boiling point is 77 at atmospheric pressure). Such superconductors whose transition temperature is greater than 90K are called high-T_C superconductors. Properties of these superconductors cannot be described by the BCS theory.

Until 1986, the transition temperature for a superconductor was 23K [1].In that year, Bednorz and Muller synthesized [2] the compound La_2CuO_4 which remains superconducting up to 30K, and soon afterwards cuprate materials were discovered with even higher transition temperatures. $YBa_2Cu_3O_{7-}\delta$(YBCO) has a critical temperature of 92K, which is significant because it's greater than the boiling point of liquid nitrogen at atmospheric pressure [3]. Bi-Sir-Ca-Cu-O,Tl-Ba-Ca-Cu-O [5] and Hg-Ba-Ca-Cu-O [4]. Some of the compounds with higher critical temperature are shown in the table below

Table 1: Transition temperatures of some high T_C. superconducting compounds.

Material	Tc (K)
$YBa_2Cu_3O_{7-8}$	92
$Bi_2Sr_2CaCu_2O_8$	85
$Bi_2Sr_2Ca_2Cu_3O_{10}$	110
$TiBa_2Ca_2Cu_3O_9$	123
$HgBa_2Ca_2Cu_3O_g$	135

All these high temperature superconductors have highly anisotropic crystal structures containing layered CuO_2 planes in which the superconducting charge carriers are to be localized.

YBCO Materials

The unit cell of YBCO is based on a stack of three perovskite cells in the figure 1 and the lattice type is either tetragonal or orthorhombic, depending on the oxygen content. perovskite cell contains a Y atom, sandwiched between CuO_2 planes. Adjacent to the CuO_2 planes are layers of BaO_2 and at the top and bottom of the cell there are Cu-O chains which have variable oxygen content dependent upon the overall oxygenation level of the material.

Thus the crystal structure may be represented as in figure 1. Each square base pyramid has O atoms at its apices and a Cu atom at the centre of the base. The square CuO_2 sheets have an O atom at each corner and a Cu atom at the centre. Note that in order to show two complete blocks of CuO_2

planes, the origin of figure 1 ,is shifted by (0, 0, and 0.5) relative to the conventional cell

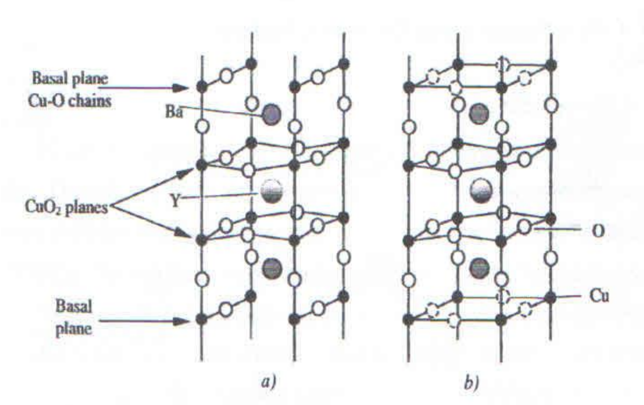

Figure 1: Unit cell of a) $YBa_2Cu_3O_7$ and b) $YBa_2Cu_3O_{7\text{-}8}$. The dashed circles indicate oxygen sites which are partially filled [6]

The variation of the oxygen content in the YBCO is extremely important in determining the superconducting properties. The effect of reducing the oxygen content below 7 atoms per unit cell is shown in figure 2. An optimum critical temperature of 93K is obtained for δ=0.08,but if more oxygen is removed from the structure critical temperature falls rapidly and for δ=0.56,YBCO is not superconducting. Also important for the superconducting properties of YBCO is the existence of chains of CuO_2 atoms, which have metal like electrical properties and reduce the anisotropy of the superconductor.

The variation of the unit cell parameters of YBCO with oxygen is shown in figure 2, which demonstrates the tetragonal-orthorhombic transition at around δ=0.6. Although the superconducting phase of YBCO is orthorhombic, in practice it's not possible to distinguish "a" and "b" directions in a microscopic sample due to twinning on a fine scale.

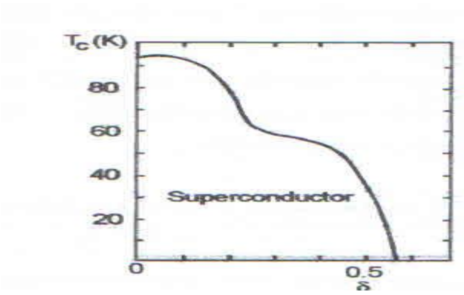

Figure 2: The effect of oxygen content on the Tc of $YBa_2Cu_3O_{7\text{-}8}$. [6]

II. FORMALISM

A. Model Hamiltonian

The description of thermodynamic properties of YBCO-123 is done by considering the pairing mechanism. Starting from the BCS Hamiltonian,

$$H_{BCS} = K.e + P.e \tag{1}$$

According to [8] the BCS Hamiltonian is given as;

$$H_{BCS} = \sum_K \varepsilon_k (C_k^+ C_k + C_{-k}^+ C_{-k}) - \sum_{kk'} V_{kk'} C_{k'}^+ C_{-k'}^+ C_{-k} C_k \tag{2}$$

In this research we are considering S-wave singlet and P-wave singlet admixture as the possible pairing mechanism.

In this research we are considering S-wave singlet and P-wave singlet admixture as the possible pairing mechanism. In the S-wave singlet state, the electrons have opposite spins. The negative sign shows that the interactions are attractive.

B. S-wave singlet Hamiltonian

$$H_S = \sum_k \varepsilon_k (c_k^+ c_k + c_{-k}^+ c_{-k}) - \sum_{kk'} v_{kk'} c_{k'}^+ c_{-k'}^+ c_{-k} c_k \tag{3}$$

In the P-wave singlet the electrons interact with their spins facing in the same direction hence the interaction is repulsive. The Hamiltonian becomes;

$$H_P = \sum_l \varepsilon_l (c_l^+ c_l + c_{-l}^+ c_{-l}) + \sum_{ll'} v_{ll'} c_l^+ c_l^+ c_{-l'} c_{-l'} \tag{4}$$

Bogoliubov-Valatin transformations are used to transform equations (3) and (4). This is achieved by defining two new operators related to the fermion creation and annihilation operators and later applying inverse transformation of the equation (4) as follows ;

$$\gamma_k = u_k c_k - v_k c_{-k}^+ , c_k = u_k \gamma_k + v_k \gamma_{-k}^+ \tag{4a}$$

$$\gamma_{-k} = u_k c_{-k} + v_k c_k^+ , c_{-k} = u_k \gamma_{-k} - v_k \gamma_k^+ \tag{4b}$$

$$\gamma_k^+ = u_k c_k^+ - v_k c_{-k} , c_k^+ = u_k \gamma_k^+ + v_k \gamma_{-k} \tag{4c}$$

$$\gamma_{-k}^+ = u_k c_{-k}^+ + v_k c_k , c_{-k}^+ = u_k \gamma_{-k}^+ - v_k \gamma_k \tag{4d}$$

The effective Hamiltonian according to equation (1) is written as;

$$H_T = \sum_k \varepsilon_k \{2V_k^2 + (U_k^2 - V_k^2)(m_k - m_{-k}) + 2U_k V_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} - \sum_{kk'} V_{kk'} \Big\{ U_{k'} V_{k'} U_k V_k \big((1 - m_{-k} - m_{k'})(1 - m_{-k} - m_k) \big) + U_{k'} V_{k'} (1 - m_{-k} - m_{k'})(U_k^2 - V_k^2)(\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k) \Big\} + 4OT \tag{5}$$

C. Parametric Expressions for U_k and V_k for S-wave Singlet State.

At the lowest energy state of this system both m_k and m_{-k} are zero. Carrying out Bogoliubov-Valatin transformation for a superconductor in its ground state m_k and m_{-k} are set to zero and 4OT neglected since the non-diagonal terms vanish from equation (5)

$$\sum_k 2\varepsilon_k U_k V_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k) - \sum_{kk'} V_{kk'} (U_k^2 - V_k^2)(\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k) = 0 \tag{6}$$

Applying the condition;

$$U_k^2 + V_k^2 = 1 \tag{7}$$

By defining a single variable χ such that, $U_k^2 = \frac{1}{2} - \chi_k$ and $V_k^2 = \frac{1}{2} + \chi_k$ and expressing a quantity Δ_k as;

$$\Delta_k = \sum_{kk'} V_{kk'} \sqrt{\left(\frac{1}{4} - \chi_k^2\right)} \tag{8}$$

The result is

$$\Delta_k^2 = \pm \sum_{kk'} V_{kk'} \sqrt{1 - \left(\frac{\varepsilon_k^2}{\varepsilon_k^2 + \Delta_k^2}\right)} \tag{9}$$

which is the gap parameter equation.

D. P-wave Singlet Hamiltonian

In the P-wave singlet the electrons interact with their spins facing in the same direction hence the interaction is repulsive. The Hamiltonian becomes;

$$H_P = \sum_l \varepsilon_l (c_l^+ c_l + c_{-l}^+ c_{-l}) + \sum_{ll'} v_{ll'} c_l^+ c_l^+ c_{-l'} c_{-l'} \tag{10}$$

The effective Hamiltonian is written according to equation (1) as;

$$H_{Tp} = \sum_l \varepsilon_l \{2V_l^2 + (U_l^2 - V_l^2)(m_l - m_{-l}) + V_l(\gamma_l^+\gamma_{-l}^+ + \gamma_{-l}\gamma_l)\} - \sum_{kk'} V_{ll'} \{U_{l'}V_{l'}U_lV_l((1 - m_{-l} - m_{l'})(1 - m_{-l} - m_l)) + U_{l'}V_{l'}(1 - m_{-l} - m_{l'})(U_l^2 - V_l^2)(\gamma_l^+\gamma_{-l}^+ + \gamma_{-l}\gamma_l)\}$$
(11)

E. Energy of the Assembly

$$E_{SP} = 2\varepsilon_k V_k^2 - U_k V_k \Delta_k + 2\varepsilon_l V_l^2 + U_l V_l \Delta_l \quad (12)$$

The total energy is multiplied by the thermal activation factor $e^{-\frac{E_T}{K_BT}}$ where K_B is Boltzmann's constant.

$$E_T = \{2(\varepsilon_k V_k^2 + \varepsilon_l V_l^2) + (U_l V_l \Delta_l - U_k V_k \Delta_k)\} \times e^{-\frac{E_T}{K_BT}} \quad (13)$$

This is the total energy of the admixture i.e the p-wave singlet and s-wave singlet states.

F. Specific Heat Capacity of HTSC cuprate-123 system

The specific heat capacity at constant volume C_V of the system is determined using the following relation

$$C_V = \frac{\partial E_T}{\partial T} \quad (14)$$

$$C_V = \frac{\{2E_T(\varepsilon_k V_k^2 + \varepsilon_l V_l^2) + E_T(U_l V_l \Delta_l - U_k V_k \Delta_k)\} \times e^{-\frac{E_T}{K_BT}}}{K_B T^2} \quad (15)$$

This is the specific heat capacity equation for HTSC cuprate-123 system.

G.Transition Temperature for HTSC cuprate-123 system

The transition temperature of the system is obtained from the condition that,

$$\left(\frac{\partial C_V}{\partial T}\right)_{T=T_c} = 0 \quad (16)$$

$$T_c = \frac{E_T}{2K_B} \quad (17)$$

Equation (17) is the expression for determining the transition temperature for HTSC cuprate-123 system.

H. Entropy of HTSC cuprate-123 System

Entropy of the system is determined from the relation,

$$\int \partial s = \int_1^2 \frac{\partial Q}{\partial T} = \int_1^2 \frac{mC_V \partial T}{T} \quad (18)$$

$$S = m\left(\frac{2E_T(\varepsilon_k V_k^2 + \varepsilon_l V_l^2) + E_T(U_l V_l \Delta_l - U_k V_k \Delta_k)\}}{K_B}\right).\left(\frac{K_B}{TE_T}.e^{-\frac{E_T}{K_BT}} + \frac{3K_B^2}{E_T^2}.e^{-\frac{E_T}{K_BT}} + \frac{6K_B^3 T}{E_T^3}.e^{-\frac{E_T}{K_BT}} + \frac{6K_B^4 T^2}{E_T^4}e^{-\frac{E_T}{K_BT}}.\right) \quad (19)$$

where 'm' is the mass of the electron.

III.RESULTS AND DISCUSSION

One of the characteristics quantities in the thermodynamic properties of HTSC cuprate-123 system is the system energy, which can be obtained by using the essential parameters of the internal energy in equation (13). In Fig. 1, we plot the system energy as a function of temperature for HTSC cuprate-123 system.

The parameters used for HTSC cuprate-123 system are $\varepsilon_k = h\omega_D = 0.03eV$, $\varepsilon_l = h\omega_D = 0.006eV$, $U_K = 0.707221$ and $V_K = 0.541090$ for s-wave ,$U_l = 0.707144$ and $V_K = 0.54116$ for p-wave according to [7] and [8].

A.Total Energy of the System of S-wave and P-wave Mixture.

A graph depicting the variation of system energy versus temperature is as shown in figure 3

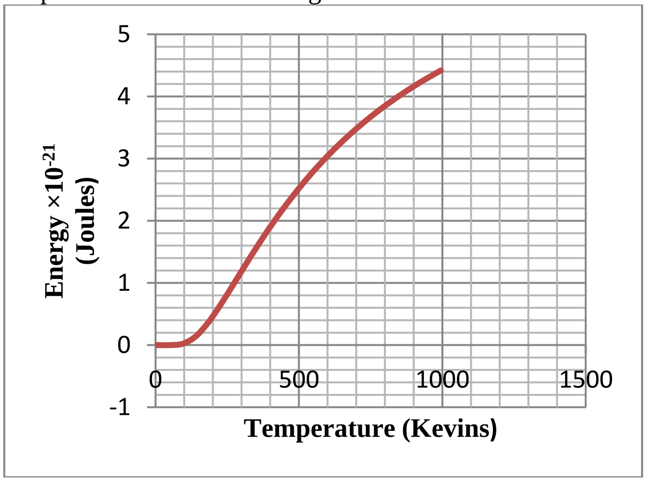

Figure 3: Variation of energy against temperature

The value of E decreases below T_C (K) and goes to zero at T=0 K and this is consistent with the nature of super-fluid state. The total energy of the system increases with increase in temperature of the system.

Total energy increases with increase in temperature of the system. It's noted that the graph can attain a plateau like phase at very high temperatures implying energy saturation with no more thermal agitation on the electrons. Similar results relating energy and temperature have been noted by other scientists. [9], [10], and [11].

B. Specific Heat Capacity of HTSC cuprate-123 system

A graph depicting the variation of Specific Heat Capacity versus temperature is as shown in figure 4

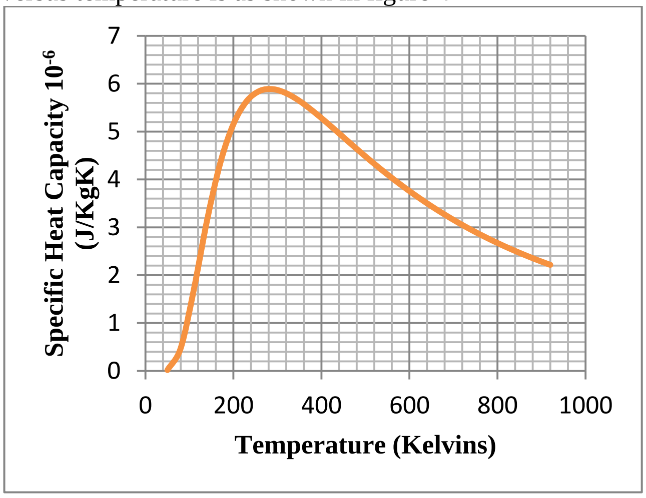

Figure 4: Variation of specific heat against the temperature

Specific heat capacity per unit volume drops exponentially with temperature from peak .At the peak-maxima $\left(\frac{\partial C_V}{\partial T}\right)_{T=T_c} = 0$,corresponds to the critical temperature which is 280k. This is in agreement with other researchers for apical oxygen [7], This shows that room temperature superconductivity is possible. Similar results relating specific heat and temperature have been noted by other scientists [13], [9], [10] and [11]). The variation of specific heat capacity against temperature shows two phase transitions, one at T_C = 65K and the other at 280K. The later transition lies at 280K thereby establishing the contribution from a mixture of s-wave singlet and p-wave singlet that could lead to a superconducting transition in YBCO. Such a transition has been observed experimentally previously [3]. Moreover, two superconducting gaps have also been observed in the Cu-based family of superconductors and hence our observation is in agreement with observed trends [12].

C. Entropy of HTSC cuprate-123 System

A graph depicting the variation of Entropy versus temperature is as shown in figure 5

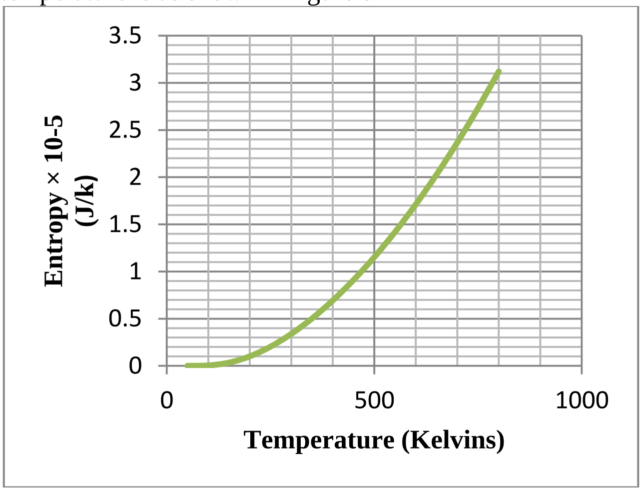

Figure 5: Variation of entropy against temperature

The results show exponential growth of entropy with temperature for YBCO-123 compounds. The variation of entropy against temperature shows that the entropy is almost zero up to 200K, and then it starts increasing almost linearly. Thus the transition temperature is greater than 200K, and this is what is indicated in the variation of specific heat against temperature. Zero entropy corresponds to second order phase transition (Latent heat = 0). Similar shapes of curves relating entropy and temperature have been noted by other scientists [9], [13], [10] and [11].

CONCLUSIONS

This work considered an admixture of the s-wave and p-wave as contributing to superconductivity in YBCO-123 materials. We have explicitly demonstrated that superconductivity is a bulk phenomenon as exhibited by a hump-like feature on the specific heat Figure 4. The peak value of the Gaussian curves of specific heat represents the superconducting transition temperature of the YBCO-123 compounds. At this point, a condensate is formed and C_v remains fairly constant. This depicts that the system is unstable at the peak and a second order phase transition (normal metal to superconducting state) occurs due to absence of latent heat. In general, the total specific heat of any system is the sum of several different excitations. Specific heat need to be explored in order to unravel the magnitude of different contributions to the total specific heat. Many experiments on high-T_C superconductors lead to the simultaneous existence of electron-phonon and electron-electron interactions.

Whereas s-wave singlet and p-wave triplet combinations have been explored, s-wave singlet and d-wave combination could also contribute to this phenomenon. Such calculations can be advanced to determine their contribution to high temperature superconductivity.

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REFERENCES

[1] Gavaler, J. R. (1973) *sciencedirect.com*. Retrieved August 30, 2016, from Science Direct www.sciencedirect .com/science/article/pii/0375960183908514.

[2] Bednorz.J.G, Muller (1986). Possible high temperaure superconductivityin Ba-la-Cuo system. *Zeitschrift fur physik B,Vol.64* , 189-193.

[3] Stoyanova-Ivanova, A., Blagoev, B., Georgieva, S., Kovacheva, D. (2018) Superconductivity and Magnetic Studies of Bulk Y123/$BaCuO_2$ Composite *Romanian Journal of Physics*1-18.

[4] Hogg, M. J., Kahlmann, F., Tarte, E. J., & Barber, Z. H. (1999). Vortex Channeling and the VI Characteristic of $YBa_2Cu_3O_7$ Low Angle Grain Boundaries.

[5] Parkin, S. S., Lee, V. Y., Engler, E. M., Nazzal, A. I., Huang, T. C., Gorman, G., (1988). Bulk Superconductivity at 125 K.

[6] Cryot. (1995). Superconductivity:the new high critical temperature supercoductors. *Cryogenic society of America,Inc.*

[7] Mourachkine.A (2004).*Room-Temperature superconductivity.* 7 Meadow Walk, Great Abington, Cambridge, U.K: Cambridge International Sciences Publishing.

[8] Khanna, K.M (2008). *Inaugural lecture on SUPERCONDUCTIVITY.* (Vol. 7).Moi University Eldoret,, Kenya: Moi University Press.

[9] Rapando B. W., Khanna K. M., Tonui J. K., Sakwa T. W., Muguro K. M., Kibe H.,Ayodo Y. K and Sarai A (2015).The dipole mediated t-J model for high-Tc superconductivity. International Journal of Physics and Mathematical Sciences. 2015, Vol. 5 Issue 3 Pp 32 – 37.

[10] Odhiambo J.O, Sakwa T.W, Ayodo Y.K, Rapando B.W, (July 2016).Thermodynamic properties of Mercury based cuprate due to Cooper pair-electron interaction. Journal of Multidisciplinary Engineering Science and Technology. ISSN: 2458-9403. Vol 3, Issue 7.

[11] Kibe,H.E, Sakwa T. Khanna K.M. (2018). Specific heat of the integrated S-wave and P-wave pairing in uranium based heavy-fermion superconductors. *International journal of physics and mathematical sciences ISSN:2277-2111* , 6.

[12] Adroja, D., Bhattacharyya, A., Biswas, P., Smidman, M., Hillier, A., Mao, H., Luo, H., Cao,G.,Wang, Z., Wang, C.(2017) Multigap Superconductivity in ThAsFeN Investigated using µSR Measurement *Physical Review B 96*144502-1-*96*144502-7.

[13] Sakwa T. W., Ayodo Y. K., Sarai A.Khanna K. M, Rapando B. W. and Mukoya A. K.(2013).Thermodynamics of a Grand-Canonical Binary System at Low Temperatures, International Journal of Physics and Mathematical Sciences.2013, Vol. 3 Issue 2 Pp 87-98.