



Thermodynamic Properties of Yttrium Based Cuprate Due to Electron-Cooper Pair Interaction Using BVT

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Abstract

Since the discovery of high temperature superconductivity (HTSC), there have been varied results concerning the high pairing energy in the unconventional superconductivity. In an attempt to unearth the mechanism behind the high pairing energy, we study a model in which an excited electron interacts with a Cooper pair. The interaction was studied earlier on using second quantization which depended on a wave function. We now use Bogoliubov-Valatini transformation (BVT) that is independent of the wave function to study the thermodynamic properties due to the interaction between an electron and a Cooper pair in a Yttrium based cuprate. The interaction energy increases with temperature and at $T = 93\text{ K}$; we record the interaction energy of 2.173 meV and the specific heat of $4.669\text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$. The entropy of this system is found to be $5.11\text{ mJ}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$. The Sommerfeld's coefficient is maximum at $T = \frac{2}{3}T_c$ where $\gamma = 62.4\text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$. It has also been observed, for the first time, that the thermodynamic quantities of YBCO123 are constant when temperature varies between 0 K and 18 K . Above 18 K , the thermodynamic quantities rise sharply. This observation has been attributed to the pairing of electrons in the singlet-s and singlet-p states.

Subject Areas

Chemical Engineering & Technology

Keywords

Energy Gap, Specific Heat, Entropy

1. Introduction

The microscopic theory of superconductivity, based on s-wave pairing, has been

used to explain conventional superconductivity [1]. However, the theory does not hold in the case of unconventional superconductivity [2]. The pairing mechanism in high temperature superconductors below the critical temperature remains unclear despite the enormous research carried out on HTSC [3]. There is need to develop consistence and consensus between the various theoretical approaches towards explaining the mechanism of HTSC. The energy gap plays a central role in explaining superconductivity, both conventional and unconventional. The energy gap in high temperature superconductor is non-uniform along the Fermi surface, characteristic of all cuprates [4].

YBa₂Cu₃O₇, with a T_c of 93 K, was discovered a year later after the landmark discovery of a lanthanum-based cuprate [5] [6]. Later on, Bismuth and Lanthanum based cuprates were discovered [7] [8] [9] [10]. Sulfur hydride, under extremely high pressure of about 200 GPa was found to undergo superconducting transition at a T_c of 203 K, the highest experimental T_c that has ever been achieved in the history of superconductivity [11]. High temperature superconductors have a wide range of applications ranging from the maglev trains, Superconducting Quantum Interface Devices (SQUIDs) up to Magnetic Resonance Imaging (MRI). Understanding the pairing mechanism in HTSC superconductors will enhance theoretical predictions, with precision, of the T_c 's as well as other thermodynamic properties of cuprates. This will open avenues for discoveries towards room-temperature superconductivity (RTS). Although many different HTSC cuprates have been discovered, theoretical as well as experimental studies are still conflicting with the observed properties [12] [13] [14]. Experimental studies have shown evidence of d-wave pairing in YBCO [2]. The Cooper pair in a high temperature superconductor has an angular momentum greater than zero, which implies the presence of nodes [15]. Electron-phonon interactions and spin fluctuations are central to the mechanism of superconductivity [16]. Spin fluctuations have sufficient strength to mediate the pairing interactions in high-temperature superconductivity except that the estimates of the strengths of this interaction differ widely [17]. Superconductivity majorly results from the formation of Cooper pairs, at the Fermi surface, at the critical temperature. However not all electrons at the Fermi surface form Cooper pairs, giving rise to a phenomenon in which Cooper pairs interact with electrons [3]. The interaction occurs between the copper oxide planes of the cuprate. When second quantization was applied on this model, the resulting entropy and specific heat of YBCO123 showed close proximity to the results from previously done experimental and theoretical work [14] [18] [19] [20]. However, the energy determined by the same method, varied from the previous experimental result [3] [21] [22]. This discrepancy might have been due to the method of second quantization used. In Bogoliubov-Valatini transformation (BVT), a Hamiltonian of interaction between the electron and the Cooper pairs is formed based on the kinetic energies of both the electron and the Cooper pair, the positive potential and the negative Coulombic potential. Row reducing the Hamiltonian leads to

energy of the system at condensate state. The entropy and specific heat of the system have been deduced from the expression of the system's energy.

2. Theoretical Formulation

The Hamiltonian, H_0 , of interaction between a Cooper pair in state k and electron in state q for unperturbed system is

$$H_0 = \sum_q \epsilon_q a_q^\dagger a_q + \sum_k \epsilon_k b_k^\dagger b_k \quad (1)$$

where a_q^\dagger (a_q) is the creation (annihilation) operator for an electron in state q , $b_k^\dagger = a_k^\dagger a_{-k}^\dagger$ ($b_k = a_{-k} a_k$) is the creation (annihilation) operator for the Cooper pair in state k , $a_q^\dagger a_q$ and $b_k^\dagger b_k$ are the number operators for an electron and a Cooper pair respectively; $\epsilon_q = \hbar k_q^2 / 2m_e$ is the kinetic energy for electron and $\epsilon_k = \hbar k_e^2 / 2m_c$ is the kinetic energy for the Cooper pair.

The Hamiltonian for the perturbation, H_P , is given by

$$H_P = \sum_{k,q} V_{k,q} a_q^\dagger a_q (b_k^\dagger - b_k) - \sum_{q,k} U_k a_q^\dagger a_q b_k^\dagger b_k \quad (2)$$

where $V_{k,q}(U_{k,q})$ is the interaction potential between electron and the Cooper pair.

Equations (1) and (2), when combined, give the Hamiltonian for a perturbed system as

$$H = \sum_q \epsilon_q a_q^\dagger a_q + \sum_k \epsilon_k b_k^\dagger b_k + \sum_{k,q} V_{k,q} a_q^\dagger a_q (b_k^\dagger - b_k) - \sum_{q,k} U_k a_q^\dagger a_q b_k^\dagger b_k \quad (3)$$

Equation (3) is then written in terms of Bogoliubov-Valatini operators, γ , using the relations $a_k = u_q \gamma_q + v_q \gamma_{-q}^\dagger$, $a_{-k} = u_k \gamma_{-k} - v_k \gamma_k^\dagger$, $a_k^\dagger = u_q \gamma_q^\dagger + v_q \gamma_{-q}$ and $a_{-k}^\dagger = u_k \gamma_{-k}^\dagger - v_k \gamma_k$. In this case, $|u_k|^2$ is the probability that the pair state $\{\mathbf{k}, -\mathbf{k}\}$ within a certain interval around the Fermi level is unoccupied and $|v_k|^2$ is the probability that the pair state $\{\mathbf{k}, -\mathbf{k}\}$ within a certain interval around the Fermi level is occupied (\mathbf{k} is the wave vector). Thus, Equation (4) gives the total Hamiltonian of the system.

$$\begin{aligned} H = & \sum_q \epsilon_q \left\{ u_q^2 m_q + v_q^2 (1 - m_{-q}) + u_q v_q (\gamma_q^\dagger \gamma_{-q}^\dagger + \gamma_{-q} \gamma_q) \right\} \\ & + \sum_k \epsilon_k \left\{ u_k^4 m_{-k} m_k - u_k^2 v_k^2 m_k (1 - m_{-k}) + u_k^2 v_k^2 (1 - m_k) m_k \right. \\ & + u_k^2 v_k^2 (1 - m_{-k}) m_{-k} - u_k^2 v_k^2 (1 - m_{-k}) m_k + v_k^4 (1 - m_{-k}) (1 - m_k) \\ & + \left. \left\{ u_k^3 v_k (m_{-k} + m_k) + v_k^3 u_k (2 - m_k - m_{-k}) \right\} (\gamma_k^\dagger \gamma_{-k}^\dagger + \gamma_{-k} \gamma_k) \right\} \\ & + \sum_{k,q} V_{k,q} \left\{ \left\{ u_q^2 m_q + v_q^2 (1 - m_{-q}) \right\} (\gamma_k^\dagger \gamma_{-k}^\dagger - \gamma_{-k} \gamma_k) \right\} \\ & - \sum_{k,q} U_k \left\{ u_k^4 u_q^2 m_{-k} m_k m_q + u_k^4 v_q^2 m_k (1 - m_{-q}) m_{-k} \right. \\ & + u_q^2 v_k^4 (1 - m_k) (1 - m_{-k}) m_q + v_q^2 v_k^4 (1 - m_{-k}) (1 - m_{-q}) (1 - m_k) \\ & + u_q^2 u_k^2 v_k^2 m_q \left[m_k (1 - m_k) - 2 m_k (1 - m_{-k}) + m_{-k} (1 - m_{-k}) \right] \\ & + \left. u_k^2 v_k^2 v_q^2 (1 - m_{-q}) \left[(1 - m_k) m_k - 2 (1 - m_{-k}) m_k + (1 - m_{-k}) m_{-k} \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + \left[u_k^3 u_q^2 v_k (m_{-k} + m_k) m_q + u_k^3 v_q^2 v_k (m_{-k} + m_k) (1 - m_{-q}) \right. \\
& + \left. v_k^3 u_q^2 u_k (2 - m_k - m_{-k}) m_q + v_k^3 v_q^2 u_k (1 - m_{-q}) (2 - m_k - m_{-k}) \right] (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \\
& + \left[u_k^2 v_k^2 u_q v_q (1 - m_{-k}) m_{-k} - 2 u_k^2 v_k^2 u_q v_q m_k (1 - m_{-k}) + u_k^2 v_k^2 u_q v_q (1 - m_k) m_k \right. \\
& + \left. u_k^4 u_q v_q m_{-k} m_k + v_k^4 u_q v_q (1 - m_{-k}) (1 - m_k) \right] (\gamma_q^+ \gamma_{-q}^+ + \gamma_{-q} \gamma_q) \} + 4\text{OT}
\end{aligned} \quad (4)$$

where 4OT are the fourth order terms.

2.1. Energy of the System

The diagonal part of the effective Hamiltonian represents the energy of the system at equilibrium. Therefore, at equilibrium the energy of the system is given by Equation (5).

$$\begin{aligned}
E_k = & \sum_q \epsilon_q \{ u_q^2 m_q + v_q^2 (1 - m_{-q}) \} + \sum_k \epsilon_k \{ u_k^4 m_{-k} m_k - u_k^2 v_k^2 m_k (1 - m_{-k}) \\
& + u_k^2 v_k^2 (1 - m_k) m_k + u_k^2 v_k^2 (1 - m_{-k}) m_{-k} - u_k^2 v_k^2 (1 - m_{-k}) m_k \\
& + v_k^4 (1 - m_{-k}) (1 - m_k) \} - \sum_{k,q} U_{k,q} \{ u_k^4 u_q^2 m_{-k} m_k m_q + u_k^4 v_q^2 m_k (1 - m_{-q}) m_{-k} \\
& + u_q^2 v_k^4 (1 - m_k) (1 - m_{-k}) m_q + v_q^2 v_k^4 (1 - m_{-k}) (1 - m_{-q}) (1 - m_k) \\
& + u_q^2 u_k^2 v_k^2 m_q [m_k (1 - m_k) - 2 m_k (1 - m_{-k}) + m_{-k} (1 - m_{-k})] \\
& + u_k^2 v_k^2 v_q^2 (1 - m_{-q}) [(1 - m_k) m_k - 2 (1 - m_{-k}) m_k + (1 - m_{-k}) m_{-k}] \}
\end{aligned} \quad (5)$$

At equilibrium, the quasi-particles represented by the operators γ are very few or do not exist and therefore, $m_k = m_{-k} = 0$ and $m_q = m_{-q} = 0$. Thus, Equation (5) becomes

$$E_k = \sum_q \epsilon_q v_q^2 + \epsilon_k v_k^4 - v_k^4 \sum_q U_{k,q} v_q^2 \quad (6)$$

For the electron to interact with the Cooper pair, they must be in the same state *i.e.* at the time of interaction we only consider the state k of the electron and neglect all the other states in q and therefore Equation (7) becomes,

$$E_k = \epsilon_q v_k^2 + \epsilon_k v_k^4 - v_k^4 U_{k,k} v_k^2 \quad (7)$$

For the three-electron interaction to take place, the cooper pair and the electron involved in the interaction must be present. Thus, $v_k = 1$ and $u_k = 0$,

$$E_k = \epsilon_q + \epsilon_k - U_{k,k} \quad (8)$$

To introduce temperature dependence, the energy E_k is multiplied by the thermal activation factor $\exp\left(\frac{-E_k}{K_B T}\right)$ where E_k is energy of the system and K_B is the Boltzmann constant. This produces a temperature dependent energy E_T given as

$$E_T = E_k e^{\left(\frac{-E_k}{K_B T}\right)} \quad (9)$$

The sum of kinetic energies ($\epsilon_q + \epsilon_k$) and $U_{k,k}$ for Y123 have been determined as 10.8 meV and 26.8 meV respectively [3] [23].

2.2. Specific Heat Capacity

The specific heat capacity of a system is given by

$$C_V = \frac{\partial E_T}{\partial T} \quad (10)$$

For the three electron system, we substitute 10 into 9 so that,

$$C_V = \left[\frac{E_k^2}{K_B T^2} \right] e^{\left(\frac{-E_k}{K_B T} \right)} \quad (11)$$

2.3. Sommerfeld's Coefficient

The electronic specific heat capacity (γ) is determined from the specific heat capacity using the formula

$$\gamma = \frac{C_v}{T} \quad (12)$$

Putting (9) into (12) we get

$$\gamma = \left[\frac{E_k^2}{K_B T^3} \right] e^{\left(\frac{-E_k}{K_B T} \right)} \quad (13)$$

2.4. Entropy

From the first law of thermodynamics temperature is defined as

$$\frac{1}{T} = \frac{ds}{dQ} \quad (14)$$

From which we have,

$$ds = \frac{dQ}{T} \quad (15)$$

But recalling that $dQ = C_v dT$ and integrating Equation (13), we have

$$S = \int \frac{C_v}{T} dT \quad (16)$$

Putting Equation (11) into Equation (14) to substitute for C_v , we have

$$S = \int \left[\frac{E_k^2}{K_B T^3} \right] e^{\left(\frac{-E_k}{K_B T} \right)} dT \quad (17)$$

So that the entropy becomes

$$S = \int -K_B \left\{ \left(\frac{E_k}{K_B T} - 1 \right) e^{\frac{E_k}{K_B T}} \right\} \quad (18)$$

3. Results and Discussions

3.1. Energy of the System

The total energy of a system results from the interaction between the particles of the system. The energy due to interaction between these particles increases with the temperature of the system. At T_O point the material changes from a super-

conducting to a normal state. **Figure 1** shows the total energy of YBCO123 as a function of temperature.

This half-stretched sigmoid curve has been obtained previously by other researchers when they were relating energy of the system to temperature [24] [25] [26] [27]. From the graph, it is observed that the energy of the system increases with temperature but not linearly. At $T=0$, the electrons are completely non-interacting and thus the energy due to interaction between electrons interaction, $E_T=0$. The rise in temperature of the system beyond 18.5 K causes a significant change in the energy of interaction within the system. This phenomenon is shown in **Figure 2**.

As the temperature rises from 0 K to 18.5 K, the Cooper pair formation is largely due to the singlet s-state because most of the electrons are in the ground state. The energy of a mole of YBCO123 within this temperature range is kept close to 0 K *i.e.* below 0.0007482 meV. When the temperature rises above 18.5 K, some electrons enter the first excitation state where Cooper pair start forming in the singlet p-state. The result is that the energy of the system starts to increase rapidly from below 0.0007482 meV. As the temperature increases towards the critical temperature, more electrons enter the first excitation state and more interactions between electrons in the singlet p-state increase leading to continued increase in the energy of the system. At $T=T_C$, the energy per unit mass for an

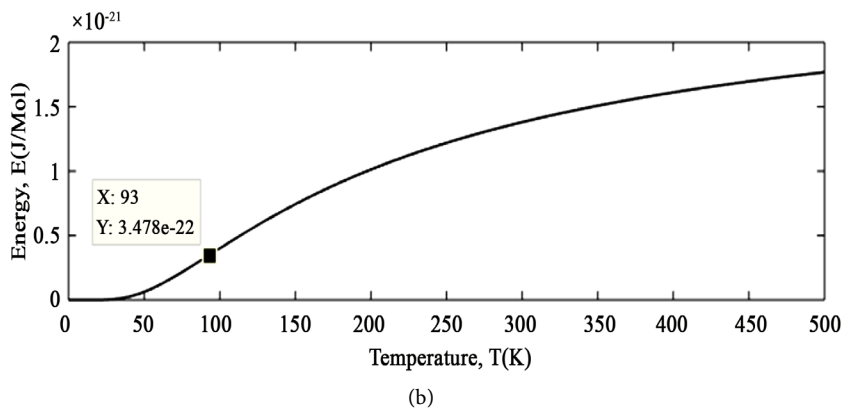
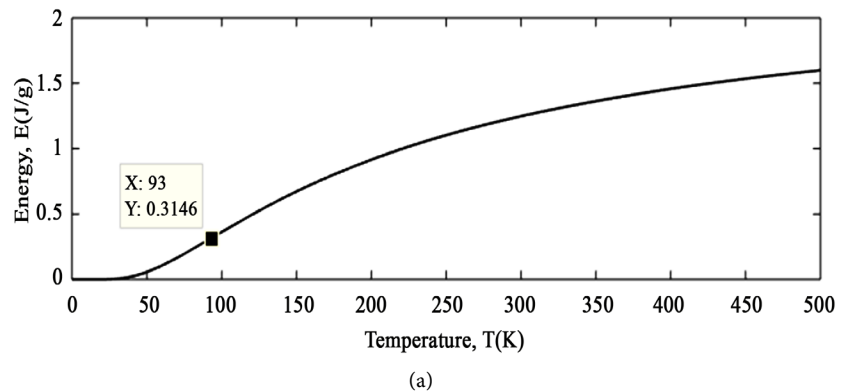


Figure 1. (a) Energy of a unit mass of Y123 as a function of temperature; (b) Energy of a mole of Y123 as a function of temperature.

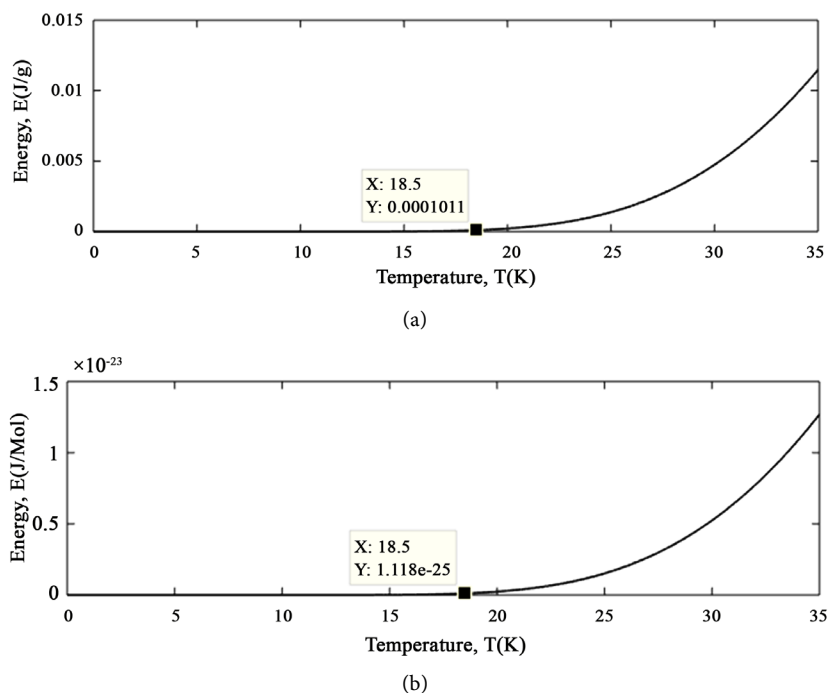


Figure 2. Energy in (a) $\text{J}\cdot\text{g}^{-1}$ and (b) $\text{J}\cdot(\text{Mol})^{-1}$ of the system as a function of temperature 0 K - 35 K.

electron interacting with a Cooper pair in Y123 is $314.7 \text{ mJ}\cdot\text{g}^{-1}$. This energy falls within the range for cuprates ($240 \text{ J}\cdot\text{kg}^{-1}$ - $375 \text{ J}\cdot\text{kg}^{-1}$) at T_c as provided by Odhiambo (2016). The energy of a mole of YBCO123 at T_c is 2.173 meV . This energy was determined at T_c using second quantization method as 2.168 meV [3].

The measured bulk energy for YBCO123 is 34 meV [22]. The bulk energy represents the energy of interaction between the particles within the superconducting material [3]. Other than electron-Cooper pair interactions, there are other interactions within the structure of YBCO123 that contribute to the bulk energy. Thus, the energy of interaction between an electron and a Cooper pair is just a fraction of the measured bulk energy.

3.2. Specific Heat Capacity

Specific heat capacity of a substance is the amount of energy required to change the temperature of a unit mass of substance by 1 K. The unit of specific heat is $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$. The specific heat of a substance depends on the temperature of the substance and is highest at the critical temperature. Figure 3 shows the specific heat as a function of temperature.

This shape concurs with those observed in previous research work [25] [27] [28]. From Figure 3, the specific heat capacity of YBCO123 increases with temperature of the system and attains its maximum at

$$T = T_c$$

where $C_V = 6.757 \text{ mJ}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ ($4.669 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$). Odhiambo (2016) gives the

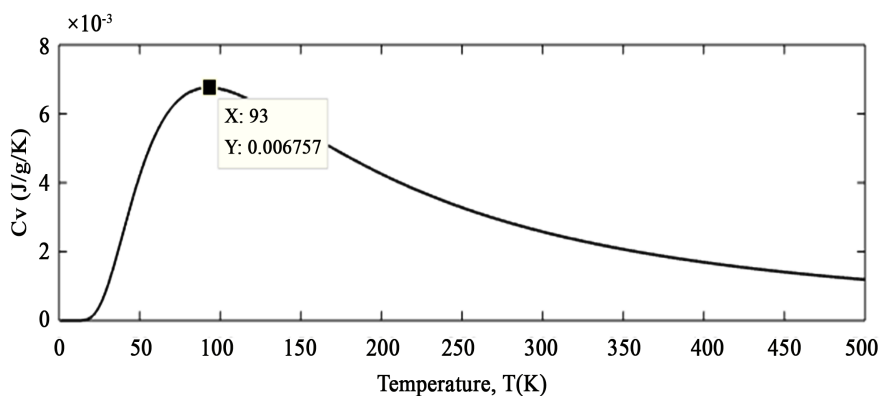


Figure 3. Specific heat capacity of a mole of YBCO123 as a function of T/T_C and (b) Specific heat capacity of a mole of Y123 as a function of T/T_C .

specific heat of YBCO123 as ($4.526 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$). A theoretical study the pairing symmetry of the singlet and triplet pairing reveals that specific heat capacity of a $3\text{He} - 4\text{He}$ mixture at T_C is $28.91 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ [29]. Experimentally, the specific heat for YBCO123 at $T_C = 91.68 \text{ K}$ is $127.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and the electronic contribution is about 1% - 2% of the phonon contribution to the total specific heat [19] [30]. Elsewhere, the contribution electrons to the total specific heat has been given as 3.86% [31]. Below T_C , the specific heat dependence on temperature follows a power law indicating that the energy gap at Fermi surface has nodes in certain directions implying anisotropy in the energy gap [32]. This kind of energy gap suggests a d-wave pairing in the energy gap.

3.3. Sommerfeld's Coefficient

The Sommerfeld's coefficient of a material relates the heat capacity of the material to a specific temperature. Figure 4 shows a graph of specific heat capacity of YBCO123 as a function of (a) temperature (b) T/T_C .

Using the graph, the Sommerfeld's coefficient increases with temperature and is optimum at $T/T_C = 0.6666$ where $\gamma = 0.09031 \text{ mJ}\cdot\text{g}^{-1}\cdot\text{K}^{-2}$, which upon conversion becomes $62.4 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$. This value is again close to $60.4 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ that was obtained by second quantization method [3]. On the other hand, a high resolution differential technique has given this value as $60 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ [19].

3.4. Entropy

Entropy of a system is the measure of disorder within the system. Increase in temperature of the system increases the agitation of the particles hence increase in entropy. When the entropy is very high, the enhanced disorder hence increased energy within the system destroys Cooper pairs. Consequently, the material changes from being superconducting state to a normal state or vice versa. The lower the entropy of a system, the higher the orderliness of its particles. Figure 5 shows the relationship between entropy of YBCO123 and its temperature.

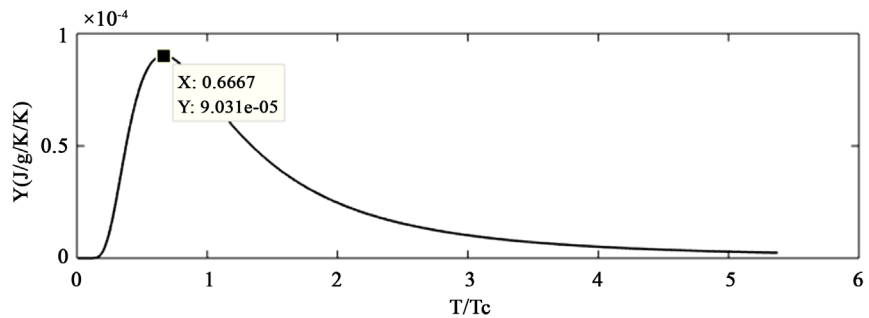


Figure 4. Sommerfeld's coefficient per unit mass of YBCO123 as a function of T/T_c .

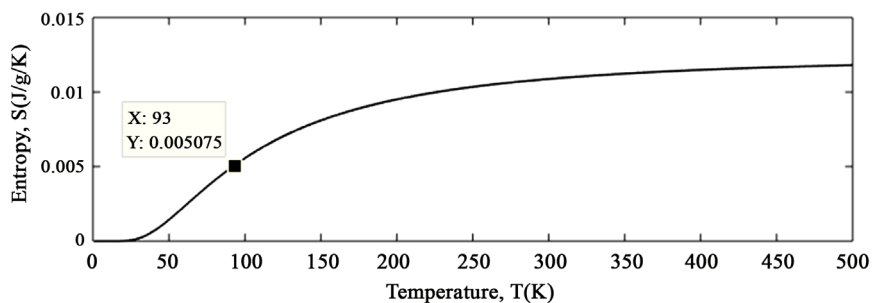


Figure 5. Entropy of a unit mass of Y123 as a function of temperature.

The entropy of the system decreases with temperature implying increase in the orderliness of the system with decrease in temperature. At lower temperature, the entropy is zero to imply that the system is highly ordered. Above this entropy, the increased energy of the system agitates the lattice particles and the superconductivity of the system is destroyed. The lower the entropy of a system, the higher the order of its particles. At $T = 0$, the entropy of the system is zero and the particles within the system, at this point, are highly ordered. **Figure 6** shows the change in the entropy as the temperature rises from 0 K to 35 K.

Within the temperature range $0 \leq T \leq T_c$, the entropy YBCO123 is maintained below $0.0002083 \text{ meV} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. When the temperature rises above 17.5 K, some electrons are excited into the first excitation state where electrons pair in the singlet p-state. At this point, disorder starts setting in. As the temperature increases up to the critical temperature, more electrons enter the first excitation state and more electrons pair up in the singlet p-state leading to continued decrease in the order of the system. Therefore, a singlet s-state is more ordered than the singlet p-state.

Similar curves were obtained by other authors [18] [20] [24]. **Figure 7** shows entropy as a function of T/T_c .

Figure 7 shows that at $T = T_c = 93 \text{ K}$ that the entropy $S = 5.075 \text{ mJ} \cdot \text{K}^{-1}$. Upon conversion, the entropy becomes $3.507 \text{ meV} \cdot \text{K}^{-1}$. The interaction of singlet and triplet state in a heavy fermion superconductor gives an entropy of $3.5 \times 10^{-21} \text{ J} \cdot \text{K}^{-1}$ [29] while dipole mediated t-J model (t-J-d) gives a maximum entropy of $(5.04694 \times 10^{-22} \text{ J} \cdot \text{K}^{-1})$ [20]. Loram *et al.*, (1993), experimentally determined entropy to range between $0.06 - 0.22 K_B (\text{Unit cell})^{-1}$ when holes were varied

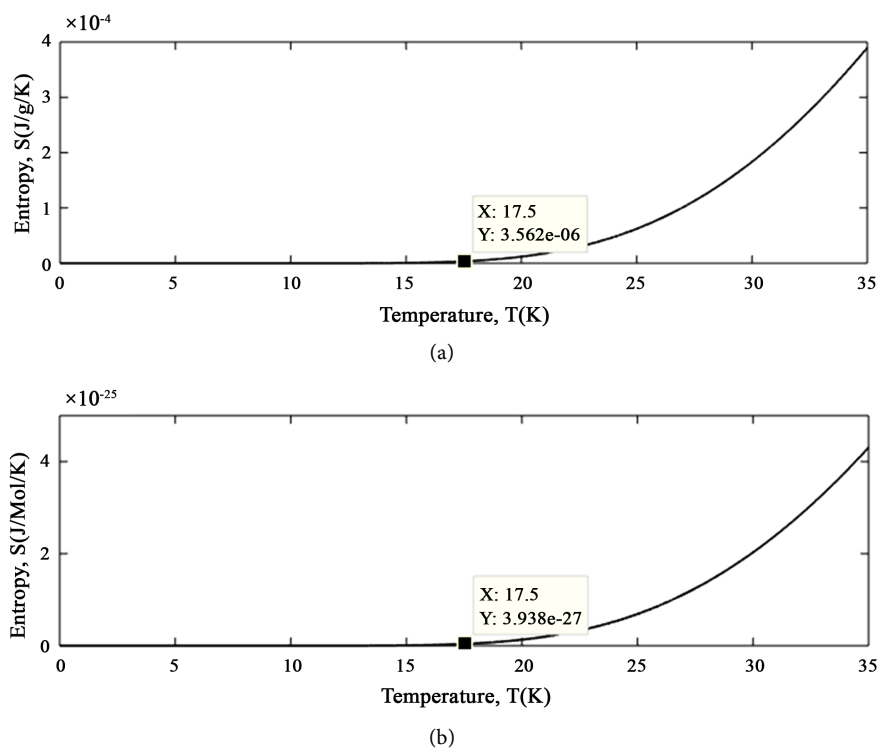


Figure 6. The entropy (a) $\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$; (b) $\text{J}\cdot(\text{Mol})^{-1}\cdot\text{K}^{-1}$ of the system between 0 K to 35 K.

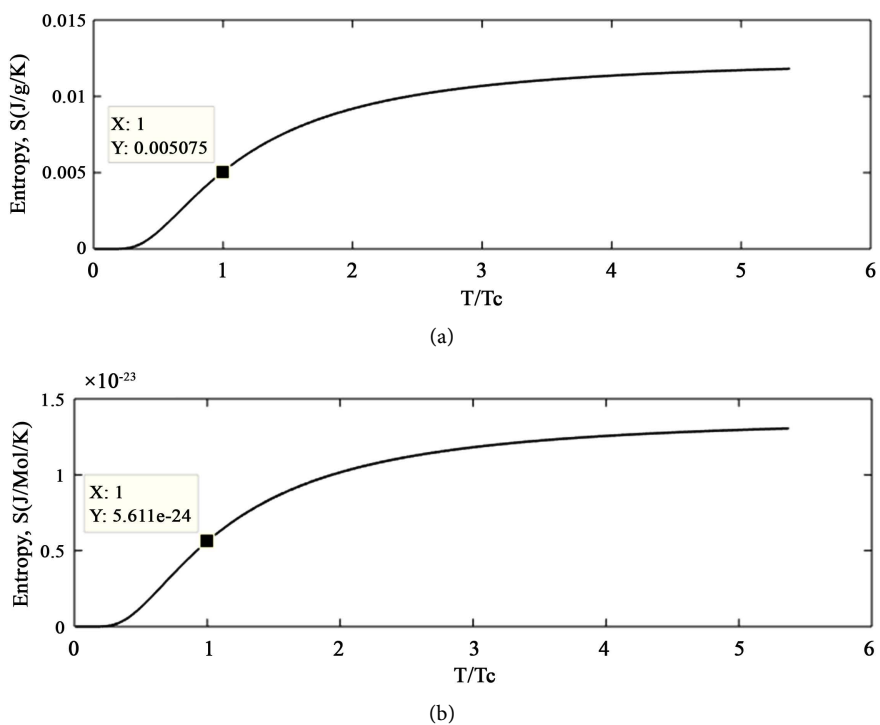


Figure 7. (a) Entropy per unit mass of YBCO123 as a function of T/T_C (b) Entropy of amole of YBCO123 as a function of T/T_C .

from $0.57 - 0.97 (\text{Unit cell})^{-1}$ [19]. This is an equivalent of $8.28 \times 10^{-25} - 3.036 \times 10^{-24} \text{ J}\cdot(\text{Unit cell})^{-1}\cdot\text{K}^{-1}$. When the temperature of a material rises above its T_C

the increased energy of the system agitates the lattice vibrations (increased disorder), leading to a higher entropy. In that condition, no Cooper pair exists and thus superconductivity of the material is destroyed. However, below this entropy, the system exhibits orderliness resulting into the formation Cooper pairs. **Figure 8** shows the change in the entropy as the temperature rises from 0 K to 35 K.

Within this range of temperature, the entropy YBCO123 is below $0.0002083 \text{ meV} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. When the temperature rises above 17.5 K, some electrons gain access to the first excitation state where electrons pair in the singlet p-state. At this point, disorder sets in slowly. As the temperature increases up to the critical temperature, more electrons enter the first excitation state and more electrons pair up in the singlet p-state leading to a less ordered system. Therefore, a singlet s-state is more ordered than the singlet p-state.

4. Conclusions

We note that the energy of interaction between a Cooper pair and an electron increases with temperature in the range $18 \leq T \leq T_c$. The energy of interaction within Y123 at $T = T_c$, as determined in this study, is $2.174 \text{ meV} \cdot \text{mol}^{-1}$. As the energy of the system increases from zero as the Cooper pairing changes from singlet s-state to singlet p-state. The energy of interaction between the electron and the Cooper pair determined in this study accounts for 6.39% of the total energy.

The specific heat of YBCO123 increases with temperature with the peak at

$$T = T_c$$

where $C_v = 4.669 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. In the region $T > T_c$, the specific heat decreases with increase in the temperature of the system. In the range $18 \leq T \leq T_c$, the Sommerfeld's coefficient increases with temperature and is highest at

$$T = \frac{2}{3} T_c$$

where $\gamma = 0.09036 \text{ mJ} \cdot \text{g}^{-1} \cdot \text{K}^{-2}$, which upon conversion becomes $62.4 \text{ mJ} \cdot \text{mol}^{-1} \cdot \text{K}^{-2}$. The entropy of YBCO123 at $T/T_c = 1$ was found to be $3.84 \text{ meV} \cdot \text{K}^{-1}$. The electron pairing is more ordered in singlet s-state (below 18 K) than in the singlet p-state (above 18 K).

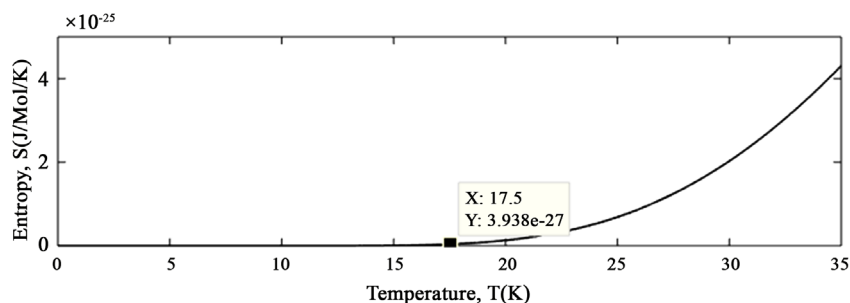


Figure 8. The entropy of the system between 0 K to 17.5 K.

This study has shown that the energy, specific heat, Sommerfeld's coefficient and entropy of YBCO123 remain almost constant (and close to zero) as temperature rises from zero to about 18 K due to electron pairing in the singlet-s state. Above $T = 18$ K the energy of YBCO123 rises sharply owing to the electron pairing in singlet-p state. In this region, high energy of up to 2.174 meV per Mole is involved. The change in electron pairing from a purely singlet-s environment to a combination of both singlet-s and singlet-p states might be an avenue to understanding high temperature superconductivity, owing to the variation of energy with temperature associated with the change in the pairing environment.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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