Sommerfeld's Coefficient Of Boson-Fermion Pair Condensate In Optimally-Doped Cuprates

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Abstract—**High temperature superconductivity has shown dependence on the interaction between a finite momentum Cooper-pair boson and a fermion. The occurrence of a superconducting energy gap in cuprates is defined by collective excitation of boson-fermion pair condensates (BFPC) above the ground state. The ground state energy of the system represents its total internal and has been used to determine Sommerfeld's coefficient of a BFPC in high temperature superconductor's. Atypically, the study is furthered by linking the theory to experiments, through extrapolations, leading to high-precision results both in cuprates and iron-based superconductors. For instance, the Sommerfeld's coefficients of the model in $YBa_2Cu_3O_7$ and $Ca_{0.33}Na_{0.67}Fe_2As_2$ are found to be $30.36 mJmol^{-1}K^{-2}$ and $114.1 mJmol^{-1}K^{-2}$ respectively while the empirical ranges in these materials are $30 \pm 5 mJmol^{-1}K^{-2}$ and $105 \pm 5 mJmol^{-1}K^{-2}$ respectively.**

Keywords—Boson-fermion Pair Condensate, Ground-state energy, Specific heat, Sommerfeld's Coefficient

I. INTRODUCTION

The electronic specific heat of a system is derived from its total internal energy. Theoretically, the total internal energy is represented by the temperature-dependent ground state energy of a system. In high temperature superconductors, the electronic specific heat in superconducting state of a material increases with temperature up to near T_c [1]. At T_c, the condensate system breaks down, paving way for another form of electronic interactions thereby causing a significant variation in the specific heat of the electron gas. The phenomenon of high temperature superconductivity is driven by the collective rather than single-particle behaviour of boson-fermion pairs [2][3].

A jump in specific heat per unit temperature has been observed in cuprates and iron-based superconductors [4][5][6]. The jump is expressed, in terms of the applied external magnetic field using the Rutgers' formula, as [7].

$$\frac{C_S}{T_c} - \frac{C_n}{T_c} = \frac{1}{4\pi}\left[\left(\frac{dH}{dT}\right)^2\right]_{T=T_c} \quad (1)$$

Where, H is the external applied field, $\frac{C_S}{T_c}$ is the maximum electronic specific heat in superconducting state and $\frac{C_n}{T_c}$ is the electronic specific heat in the normal state of a material. The difference in equation (1) is the Sommerfeld's coefficient.

Increase in the hole content (δ) causes a drop in the Sommerfeld's coefficient [4]. The change (ΔC) in specific heat during transition is about 1-2% of the total specific heat [4][5]. Elsewhere the contribution by ΔC to the total specific heat has been estimated at 3.86% [6]. The quality of a sample influences the Sommerfeld's coefficient of a sample. Poor quality samples produce lower values while good quality samples possess higher values of Sommerfeld's coefficient [7][8].

Annavarapu [9] submits that contributions from electrons and plasmons may open up a new insight into the thermodynamic properties of cuprates. Recent studies have shown that the collective excitation of plasmon-mediated BFPC is in tandem with the measured energy gaps in high temperature superconductors. The model has also shown anisotropy due to Coulomb attraction. In this paper, we study the Sommerfeld's coefficient of a BFPC in cuprate iron-based superconductors using the ground state and then extrapolating the electronic specific heat to critical temperature (T_c).

II. THEORETICAL FORMULATIONS

The

2.1 Electronic Specific Heat of a Boson-fermion Pair Condensate

Mukubwa and Makokha [3] have shown that the ground state energy of a group I high temperature superconductors is given by

The average temperature-dependent total ground state energy is given as

$$E_0 = -\eta_{ph} N E_k \exp\left(-\frac{2T_c}{T}\right) \qquad (2)$$

The molar specific heat of a BFP becomes

$$C_v = 2\eta_{ph}\left(\frac{T_c}{T^2}\right) N_A N E_k \exp\left(-\frac{2T_c}{T}\right) \qquad (3)$$

Where N is the number density of particles. In group I superconductors, N is given by

$$N = \begin{cases} -\frac{1}{q}(2k_B T_c \times 10^{-3}); & \text{due to } V_+ \\ -\frac{1}{q}\left(\frac{4}{3}k_B T_c \times 10^{-3}\right); & \text{due to } V_- \end{cases} \qquad (4)$$

The first value of N represents the ground state energy due to the potential V_+ in the positive direction while the second one is that due the negative potential V_-. In the case of group II superconductors,

$$N = \begin{cases} -\frac{1}{q}(2\exp(2) \times 10^{-3}); & \text{due to } V_+ \\ -\frac{1}{q}\left(\frac{4}{3}\exp(2) \times 10^{-3}\right); & \text{due to } V_- \end{cases} \qquad (5)$$

The specific heat in this case is due to the boson-fermion pair condensate (BFPC) in the superconducting state of a material. However, during transition at $T = T_c$ in optimally doped materials, the BFPC system disintegrates to other electronic systems in the normal state of the material. The values of specific heat of the electron systems in the two states are different leading to a 'jump'. The specific heat per unit temperature of a BFPC system can be expressed as

$$\frac{C}{T} = \frac{1}{N}\left(\frac{C_v}{T}\right) \qquad (6)$$

In this case, the electronic specific heat, $C_e = \frac{C}{T}$ is dependent on properties of single-particle-like system of electrons rather than their collective behaviour. Substitution of equation (4) into equation (5) gives the molar C_e as

$$= 2\eta_{ph}\left(\frac{T_c}{T^3}\right) N_A E_k \exp\left(-\frac{2T_c}{T}\right)$$

$$C_e = \frac{C}{T} \qquad (7)$$

Earlier studies have shown that the Electronic specific heat is maximum at $T = \frac{2}{3}T_c$ [10].

2.2 Linking the theory to Experiments – Extrapolations

Figure 1 shows a typical experimental graph of $\frac{C}{T}$ as a function of T.
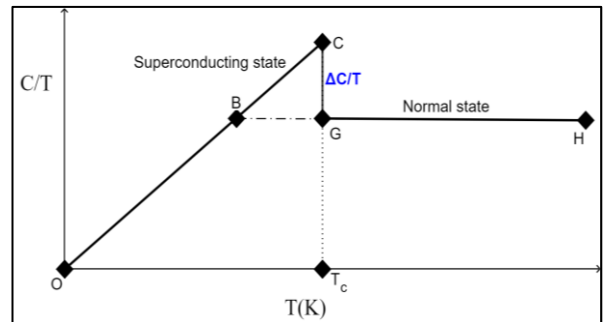

Figure 1: Dependence of Sommerfeld's coefficient of an IBSC on temperature. The horizontal line GH represents the average $\frac{C_n}{T_c}$ in the normal state while the diagonal line OC is an extrapolation to $\frac{C_s}{T_c}$(at C) through the origin. Lines OC and GH (extrapolated) meet at some point B along OC in the superconducting state. The point B can be viewed as a point of divergence to points G and C representing $\frac{C_n}{T_c}$ and $\frac{C_s}{T_c}$ respectively.

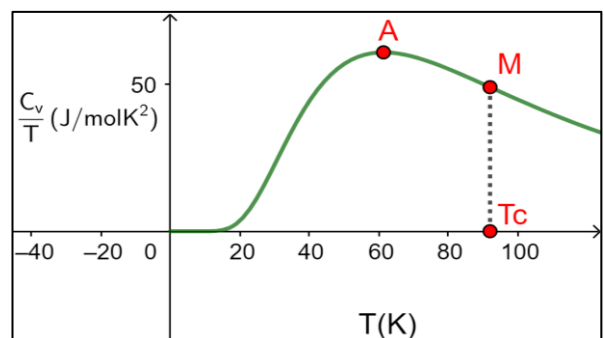We compare **Figure 1** to a theoretical curve of $\frac{C}{T}$ as a function of temperature in **Figure 2**.

Figure 2: Key points on a $\frac{C}{T} = f(T)$ curve: Points A is a theoretical maximum of $\frac{C}{T}$ at $T = \frac{2}{3}T_c$ and M, a theoretical minimum at $T = T_c$.

Point A can sufficiently be estimated each as a point of divergence of the projections to $\frac{C_s}{T_c}$ of the superconducting state and $\frac{C_n}{T_c}$ of the normal state.

The horizontal extrapolation leads to the average path of $\frac{C_n}{T_c}$ while the diagonal extrapolation through the origin leads to the maximum $\frac{C}{T}$ labelled $\frac{C_s}{T_c}$. The difference between $\frac{C_n}{T_c}$ and $\frac{C_s}{T_c}$ is the Sommerfeld's coefficient, that is,

$$\gamma = \frac{\Delta C}{T_c} = \frac{C_s}{T_c} - \frac{C_n}{T_c} \qquad (8)$$

Figure 3 shows the relationship between the electronic specific heat and the Sommerfeld's coefficient of a BFPC system in a superconductor material.
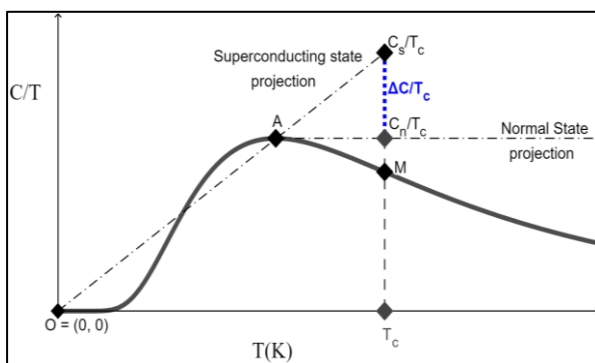

Figure 3: *Extrapolations of $\frac{C}{T}$ curves to obtain Sommerfeld's coefficients of cuprate and iron-based superconductors. Extrapolation from maximum point A produces the Sommerfeld's coefficient. The horizontal extrapolation through A leads to the average path of $\frac{C_n}{T_c}$ while the extrapolation through the origin leads to the maximum $\frac{C}{T}$ labeled $\frac{C_s}{T_c}$. In some materials, the horizontal extrapolation is lower than A (at point M). The difference between $\frac{C_n}{T_c}$ and $\frac{C_s}{T_c}$ is the Sommerfeld's coefficient.*

The BFP condensate does not exist beyond the critical temperature and therefore, any plot of $\frac{C}{T}$ beyond the critical temperature cannot be explained using the condensate system. Generally, the drop from $\frac{C_s}{T_c}$ to point A results into a larger $\frac{\Delta C}{T_c}$ and is common among group I superconductors while a drop to point A produces a smaller $\frac{\Delta C}{T_c}$ and is common among group II superconductors.

Odhiambo *et al.,* (2016), has shown that at point A, $T = \frac{2}{3} T_c$. From the foregoing, it follows that at $T = T_c$, the minimum electronic specific heat is

$$\frac{C_n}{T_c} = \begin{cases} \frac{27}{4} \eta_{ph} \left(\frac{1}{T_c^2}\right) N_A E_k \exp(-3); \text{ group I} \\ 2\eta_{ph} \left(\frac{1}{T_c^2}\right) N_A E_k \exp(-2); \quad \text{group II} \end{cases} \qquad (9)$$

The first part of Eq. (9) is the electronic specific heat through point A extrapolated to the normal state (by a horizontal line) while the second part is the electronic specific heat in the normal state at M. The maximum electronic specific heat in the superconducting state is
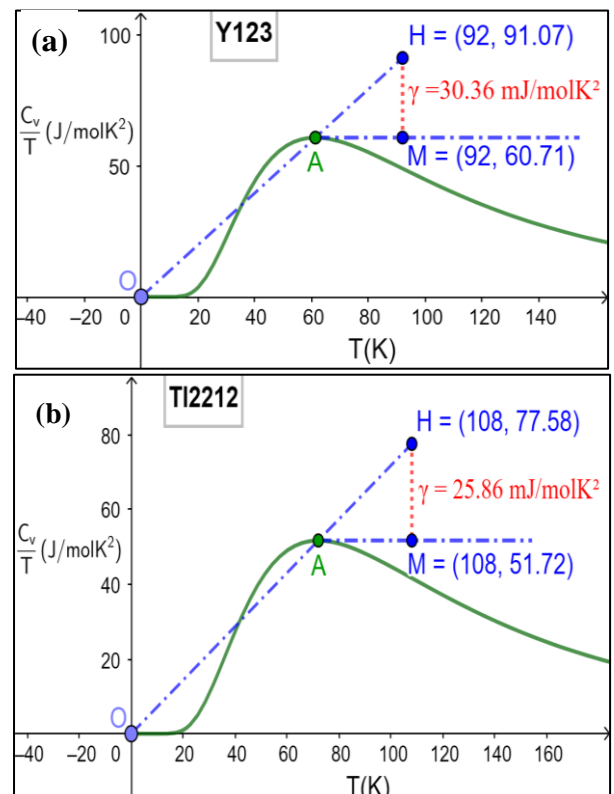
$$\frac{C_s}{T_c} = \frac{3}{2} C_e \text{ at A} = \frac{81}{8} \eta_{ph} \left(\frac{1}{T_c^2}\right) N_A E_k \exp(-3) \qquad (10)$$

Consequently, substituting Eqs. (9) and (10) into Eq. (8), the Sommerfeld's coefficient at $T = T_c$ becomes

$$\gamma = \begin{cases} 0.336 \eta_{ph} \left(\frac{N_A k_B}{T_c}\right); \text{ group I} \\ 0.467 \left(\frac{N_A k_B}{T_c}\right); \quad \text{group II} \end{cases} \qquad (12)$$

III. RESULTS AND DISCUSSIONS

Figure 4 shows the Sommerfeld's coefficients obtained from extrapolations of $\frac{C_s}{T_c}$ and $\frac{C_n}{T_c}$.
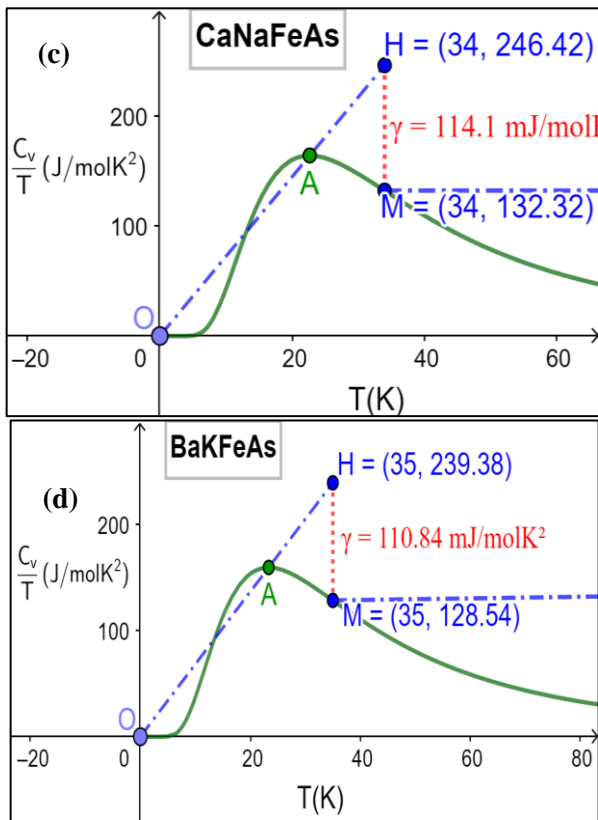
Figure 4: Sommerfeld's coefficient of a BFPC as a function of temperature in group I superconductors (Y123 and Tl2212) and group II superconductors (CaNaFeAs and BaKFeAs).

The Sommerfeld's coefficient of a BFPC is in proximity with the experimental values for the same materials. For instance, the Sommerfeld's coefficient of the model in Y123, from the graph is $30.36 \, \text{mJmol}^{-1}\text{K}^{-2}$ while the experimental processes on Y123 material have shown that $\gamma = 30 \pm 5 \, \text{mJmol}^{-1}\text{K}^{-2}$ [11]. Bessergeven *et al.* notes that the experimental Sommerfeld's coefficient of Y123 lies in the range $25 - 30 \, \text{mJmol}^{-1}\text{K}^{-2}$ while Shaviv *et al.* records the measurement as $28.2 \pm 10 \, \text{mJmol}^{-1}\text{K}^{-2}$ [12][13]. The discrepancy between Sommerfeld's coefficients arises from different extent of imperfections in samples of cuprates used, as well as from inaccurate normalization that arises from imprecise oxygen composition determination [12].

In the case, of Tl2212, three different samples based on the number of thallium atoms were considered: $2.10, 1.94$ and 1.82 with T_c's of $104\text{K}, 96\text{K}$ and 89K [17]. The corresponding Sommerfeld's coefficients are $25, 29$ and $24.7 \, \text{mJmol}^{-1}\text{K}^{-2}$ respectively. The Sommerfeld's coefficient of a BFPC system in Tl2212 is $25.5 \, \text{mJmol}^{-1}\text{K}^{-2}$. These results are summarized in **Table 1**.

Table 1: Comparison between Model and Experimental values of γ

Superconductor	T_c(K)	γ (J/molK) Model	Exp	Ref.
Group I				
$YBa_2Cu_3O_7$	93	30.4	30 ± 5	[10]
$Tl_2Ba_2CaCu_2O_8$	108	25.5	25	[16]
Group II				
$Ca_{0.33}Na_{0.67}Fe_2As_2$	34	114.5	105 ± 5	[18]
$Ba_{0.6}K_{0.4}Fe_2As_2$	35	110.8	100	[7]

The variations in the experimental values are attributed to the sample quality of the superconductor materials – poor quality samples produce lower values while good quality samples possess higher values of Sommerfeld's coefficient [7]. The Sommerfeld's coefficient of BFP condensate in layered superconductors compares closely with the experimental values of the respective samples (see Table 1).

The Sommerfeld's coefficient, based on the corrected phonon term, is found to vary depending on the oxygen concentration [14]. These variations with the oxygen content are only observed specifically at $T = T_c$, below which the Sommerfeld's coefficient is independent of the oxygen content. When the hole-concentration in the phonons is varied between 0.8 amd 0.92, the Sommerfeld's coefficient varies between $14.4 \text{mJmol}^{-1}\text{K}^{-2}$ and $59.8 \, \text{mJmol}^{-1}\text{K}^{-2}$ with $T_c = 92$ K respectively for an optimally oxygen-doped sample [14]. On the other hand, electron doping lowers the Sommerfeld's coefficient. For example, when y is raised from 0 to 0.07 in $YBa_2\left(Cu_{(1-y)}Zn_y\right)_3O_7$, the Sommerfeld's coefficient drops from $41 \text{mJmol}^{-1}\text{K}^{-2}$ to $10 \, \text{mJmol}^{-1}\text{K}^{-2}$ [4].

Materials with higher $T_c's$ are characterized by smaller Sommerfeld's coefficient while smaller T_c give rise to larger values of Sommerfeld's coefficient. The BFPC in cuprates breaks down at A into other electronic systems. However, the system iron-based superconductors persist below point A (at point M) before breaking down into constituent particles. Increased hole-doping up to optimal doping is accompanied by a rise in T_c which produces a consequent decrease in the Sommerfeld's coefficient. Conversely, electron doping lowers T_c of a material and presents a larger value of Sommerfeld's coefficient.

The electronic term, however, shows a different trend from that of the Sommerfeld's coefficient. For instance, the term increases with the electron-doping content in $La_{2-x}Sr_xCuO_4$ [15]. In the same way, when the hole-doping content in $Tl_2Ba_2CuO_{6+\delta}$ is increased from 0 to 0.1 , the coefficient drops from about $13 \, mJmol^{-1}K^{-2}$ to nearly zero [16].

The electronic specific heat is directly dependent on the ground state energy of the BFPC model. Increasing the hole content raises the ground state of a BFPC towards the Fermi surface thereby reducing both its ground state energy and electronic specific heat at T_c . Conversely, electron doping lowers the ground state of the system which leads to an enlarged energy gap and an increase in the electronic specific heat of the condensate at T_c

CONCLUSION

The interaction energy between bosons and fermions at ground state increases with temperature and hence a rise in the electronic specific heat of the system. The BFPC system breaks down during transition, at constant temperature, leading to another form of electronic system. The former has a higher electronic specific heat than the latter necessitating a 'jump' in the electronic specific heat – Sommerfeld's coefficient. The Sommerfeld's coefficient of bosons-fermion pair condensate in cuprates concurs with the empirical values.

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