Sommerfeld Coefficient for Hole- And Electron-Doped Cuprates

Michael Nakitare Waswa[1] and Horace E. Kibe[2]

[1]*University of Kabianga, Department of Physical Sciences P.O Box, 2030-20200 Kericho, Kenya*
[2]*Masinde Muliro University of Science & Technology, Department of Physics, P.O Box, 190 Kakamega, Kenya*

Abstract: **We have reflected on the ratio of specific heat and temperature (γorC_{el}) of selected electron and hole doped high-Tccuprates. The electronic specific heat rises slowly and there is a sudden drop at the critical temperature and then it gradually decreases for temperatures above T_C. The behavior of electronic specific heat below T_C is in good agreement with the BCS result for d-wave superconductor. The electronic contribution to the total specific heat of these materials is less than 1 %.The relevance to high-Tc superconductivity in the cupratesis discussed.**

Keywords: **Electronic specific heat, Critical temperature, Electron-doped and Hole-doped**

I. INTRODUCTION

High transitional temperature (Tc) superconductors are commonly categorized into two groups: hole-doped (p-type) and electron-doped (n-type) cuprates. To the former category belong, for example, the first high-Tc material $La_{2-x}Ba_xCuO_4$[1], $YBa_2Cu_3O_7$, $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$and the superconductor with the highest critical temperature $HgBa_2Ca_{n-1}Cu_nO_{2n+2}$. The latter category is formed by the materials $Ln_{2-x}Ce_xCuO_4$, with Ln = La, Nd, Pr, Eu, or Sm [2]

A. Hole-Doped Cuprate Superconductors

Cuprates exhibiting high-temperature superconductivity have been intensively studied in the last roughly three decades. All series of high-$T_C$cuprates, La-214, Y-123, Bi2212, etc, have the parent compounds which are anti-ferromagnetic (AF) Mott insulators. In the hole-doped cuprates, doping of hole carriers into the parent compound destroys an AF order quickly, and then, the superconductivity appears. With increasing hole-doping, T_C is raised in the under-doped regime and exhibits the maximum in the optimally doped regime. With further doping, T_C turns into a decrease in the over-doped regime, and finally the superconductivity disappears in the heavily-over-doped regime where the system becomes a metal. Experiments [3]have shown that there exist AF fluctuations in the superconducting reegime, suggesting that AF fluctuations are a glue to form superconducting electron pairs. In the non-heavily-over-doped regime, theories and experiments have suggested the existence of ferromagnetic fluctuations or itinerant carriers [4].

B. Electron Doped Cuprate Superconductors

Electron-doped high-$T_C$cuprates were first discovered by Tokura in 1989 [5]. There are pronounced different features from those in the hole-doped cuprates. Here, the current or charge carriers are electrons, and to obtain superconductivity in electron-doped cuprates, it is absolutely necessary to have reduction annealing. The doping of electrons into the parent compounds weakens the AF order, but the AF order is maintained around the optimally doped regime. The superconductivity with the maximum T_C appears around the optimally doped regime and is monotonically suppressed with over-doping. Since AF fluctuations were observed around the optimally doped regime, the electron pairing mediated bu AF fluctuations is also believed to be the case in the electron-doped cuprates. However, the mechanism of the un-doped superconductivity is still unclear, whereas there seems to be an intimate relation between the superconductivity and AF fluctuations, whether the cuprates are hole-doped or electron-doped.

The thermodynamics of superconductors at low temperatures is determined by the excitation of two quasi-particles. In the conventional superconductors with BCS type pairing, the energy gap is isotropic, and the temperature dependence of the heat capacity has exponential form $\approx \exp -\Delta / k_B T$, where Δ is the superconductor's gap. In superconductors with anisotropic pairing, the temperature dependence of the heat capacity has power character, namely, T^n. The appearance of such temperature dependences is related to that of the superconductor's gap which has zeros on the Fermi surface. The development of a model to explain the thermodynamics of high-temperature superconductors remain unsolved [6].

The electronic specific heat capacity C_{el} of $La_{2-x}Sr_xCuO_4$ (La214) was measured over a wide range and then, U_o evaluated from C_{el}. In highly doped samples, U_o agreed with the BCS value but it was significantly reduced in the under-doped region [7]. [8] in their research on the temperature dependence of specific heat capacity for $BaFe_{1.8}CO_{0.2}AS_2$, clearly showed a specific heat discontinuity below T_C peaking at 20 K. The fitted sommerfeld coefficient, γ was 0.471mJ/K^{2}mol.The superconducting properties for the $Sr_{1-x}La_xFBiS_2$ system [9]have been studied. An anomaly relevant to the superconducting transition was discernible at

T=3 K in the zero-field curve, reflecting the bulk superconductivity in this compound. The data for the normal state, on the other hand, were well fitted to the conventional relation:$C/T = \gamma_n + \beta T^2$. The best-fitted result gave the normal-state specific-heat coefficient of γ_n=1.6 mJ/molK^2. After subtracting the phononic contribution (βT^2), the electronic specific heat C_{el}showed a clear jump which manifested itself at the superconducting transition. Taking the entropy balance into consideration, T_C=3.0 K was obtained and the specific-heat jump of $\Delta C/\gamma_n T_C$=1.1. This value of specific-heat jump is less than that of the BCS weak-coupling limit (=1.43), but it can be comparable to the BCS value when considering the apparent shielding fraction.

In this work we deduce the electronic specific heat, γ of selected hole and electron doped cuprates in the framework of Bose-Fermi-Hubbard model. The electron-doped compounds Nd_{2-x} Ce_xCuO_4 (NCCO) and Pr_{2-x} Ce_xCuO_4 are studied and compared with YBa_2CuO_7 (Y123) and La_{2-x} Sr_xCuO_4 (LSCO)-hole-doped materials by using Bogoliubov-Valatin transformation technique.

II. MODEL AND APPROACH

The effective Hamiltonian, in the context of Bose-Fermi-Hubbard model system in a strong coupling regime is given by [10];

$$H = -J\sum_{\langle k,-k\rangle}(b_k^{\dagger}b_k + b_{-k}^{\dagger}b_{-k}) - \mu\sum_k b_k^{\dagger}b_k + \frac{U}{2}\sum_k b_k^{\dagger}b_k(b_k^{\dagger}b_k - 1)$$
$$-t\sum_k c_k^{\dagger}c_k - U\sum_{k,-k} c_{k\uparrow}^{\dagger}c_{-k}^{\dagger}c_{-k\downarrow}c_{k\uparrow} - \mu\sum_k c_k^{\dagger}c_k - U\sum_k c_k^{\dagger}c_k b_k^{\dagger}b_k \quad (1.1)$$

This Hamiltonian is diagonalized by both fermionic and bosonic canonical transformations resulting into ground state energy of the system from which specific heat is ascertained[10].

The quotient of specific heat and temperature results intosommerfeld coefficient (electronic specific heat)[10]given by;

$$\text{Cel} = \left[\frac{(t + 1.4\Delta - 2\mu + 2J + U)^2}{100kT^3}.e^{-\left(\frac{(t+1.4\Delta-2\mu+2J+U)}{100\,kT}\right)}\right] \quad (1.2)$$

III. RESULTS AND DISCUSSION

The specific heat is a bulk thermodynamic measurement that probes all excitations in a system. In order to extract the excitations arising only from the electronic quasi-particle density of states, we have considered the contributions by the electrons to the specific heat. Using data generated from expression (1.2), we have estimated the electronic specific heat of the high T_C superconductors and drawn the variation of electronic specific heat of hole- and electron-doped materials in the temperature interval 0 K−500 K (figure 1.1 and 1.2). It is observed that the electronic specific heat rises slowly and there is a sudden drop at the critical temperature and then it gradually decreases for temperatures above T_C. The hump-like feature of γ or C_{el} is in good agreement, in both shape and size, with the BCS result for d-wave superconductor i.e LSCO [11]. The C_{el} is maximum at the peak (T_C) and exponentially reduced below T_C. Such behavior indeed resembles the work reported by [9],[12], [13][14],and [15]. Narrowing of the peak (curve for LSCO) at T_C might characterize the phase transition into the second order type. This conforms to the work reported by [16], in which case the narrowing of the peak is related the conventional superconductivity scenario with Cooper pairs becoming more effective.

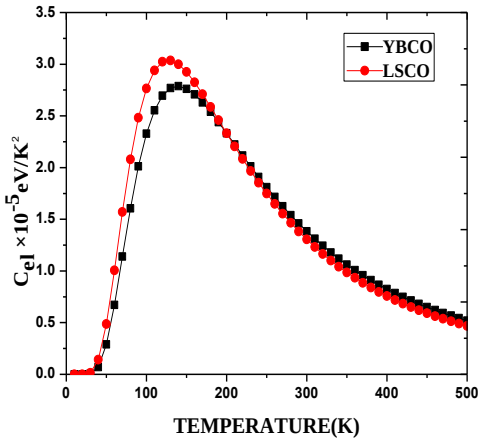

Figure 1.1: Variation of electronic specific heat with temperature for YBCO and LSCO.

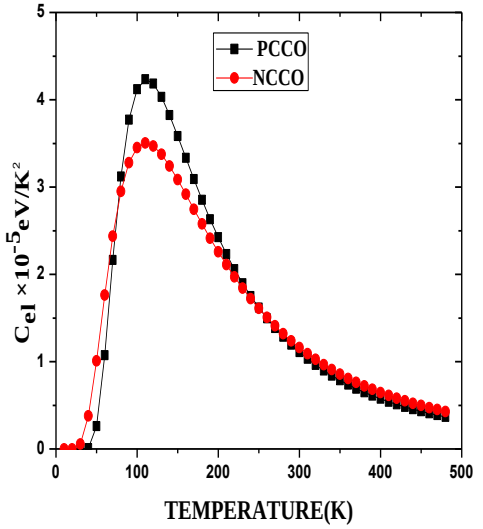

Figure 1.2: Variation of electronic specific heat with temperature for NCCO and PCCO.

In Figure (1.1), the electronic specific heat is higher for LSCO between 0-190 K after which YBCO records higher values.

This observation perhaps signify that C_{el} is dominated with other contributions (perhaps plsamons, phonons and magnetism) being insignificant for LSCO within the specified temperature ranges. The higher C_{el} for LSCO, could be attributed to the higher effective mass of LSCO hence increased population of the density of states. The maximum electronic specific heat for YBCO is $2.769 \times 10^{-5} eV/K^2$ ($\sim 4.43 \times 10^{-24} JK^{-1}$), occurring at $T_C \approx 130$ K and for LSCO is $3.037 \times 10^{-5} eV/K^2$ ($\sim 4.89 \times 10^{-24} JK^{-1}$) at 130 K. At approximately 190 K, both cuprates have $C_{el}=2.459 \times 10^{-5} eV/K^2$ ($\sim 3.93 \times 10^{-24} JK^{-1}$).

From figure 1.2, we deduce the maximum C_{el} to be $3.505 \times 10^{-5} eV/K^2$ ($\sim 5.61 \times 10^{-24} JK^{-1}$) at T=170 K and $4.234 \times 10^{-5} eV/K^2$ ($\sim 6.77 \times 10^{-24} JK^{-1}$) at T=110 K for NCCO and PCCO, respectively. [14], while studying the gap structure in the electron-doped Iron-Arsenide superconductor $Ba(Fe_{0.92}CO_{0.08})_2As_2$ using the phonon part of C_V obtained C_{el} of $18 mJ/molK^2$ ($\sim 2.99 \times 10^{-26} JK^{-2}$). [15], in his work on the interaction of Cooper pair and an electron found (γ) or C_{el} of $\gamma=60.4$ $mJ/molK^2$ ($\sim 1.0 \times 10^{-25} JK^{-2}$) for Y123 at T=62 K. Similar findings for Y123 were reported by [12] and [17] who obtained an electronic specific heat of 60 $mJ/molK^2$ ($\sim 9.96 \times 10^{-26} JK^{-2}$) and 56 $mJ/molK^2$ ($\sim 9.3 \times 10^{-26} JK^{-2}$), respectively, while using different techniques and conditions. [18]obtained an electronic C_V ~45 $mJ/molK^2$ ($\sim 7.47 \times 10^{-26} JK^{-2}$), while working on the specific heat of underdopedcuprate superconductors from a phenomenological layered Boson-Fermion model. Indeed, our results agree in principle with the findings from other authors.

IV. CONCLUSION

We have examined the ratio of specific heat and temperature in the context ofBose-Fermi-Hubbard model and we infer that the electronic contribution to specific heat is lower for electron-doped cuprates compared to hole doped cuprates. This could be due to rare Earth magnetism in electron-doped cuprates which give rise to anomalies at low temperatures hence making extraction of C_{el} difficult. Besides, the presence of apical oxygen in electron-doped cuprates may alter the order of crystal structure of these materials there by suppressing the density of states. Clearly, the maximum contribution by electrons to the total specific heat occurs at lower critical temperatures. The maximum electronic contribution to the total specific heat of these materials is nearly 0.006 %.Above T_C, the values decrease gradually and finally at 300 K it is about 0.0033 % for the four cuprates. Our % electronic contribution to the total C_V concurs with that reported by [18]who noted that the electronic specific heat contributes less than 2 % to the total specific heat. Perhaps a large contribution to the total specific heat could be from bosons and plasmons which need to be explored.

ACKNOWLEDGEMENTS

We extend our heartfelt gratitude to University of Kabiangaand Masinde Muliro University of Science and Technology for the conducive atmosphere to carry out the research .

REFERENCES

[1] Bednorz, J. and Muller, K. . (1986). Possible High Temperature Superconductivity in the Ba-La-Cu-O System. *Nature Physics., 64* (2), 189-193.

[2] Brinkman, A., &Hilgenkamp, H. (2005). Electron-hole coupling in high-Tccuprate superconductors. *Physica C: Superconductivity, 422*(3-4), 71-75.

[3] Koike, Y., & Adachi, T. (2012). Impurity and magnetic field effects on the stripes in cuprates. *Physica C: Superconductivity, 481*, 115-124.

[4] Adachi, T., Kawamata, T., & Koike, Y. (2017). Novel electronic state and superconductivity in the electron-doped high-Tc T'-superconductors. *Condensed Matter, 2*(3), 23.

[5] Tokura, Y., Takagi, H., Uchida, S. (1989). A Superconducting Copper Oxide Compound with Electrons as the Charge Carriers. *Nature, 337*, 345-347.

[6] Kruchinin, S. P. (2014). Physics of High-Tc Superconductors. *Reviews in Theoretical Science, 2*(2), 1-22.

[7] Loram, W., Mirzaa A., Cooper, R., Liang, Y., Wade, J. (1994). Electronic Specific Heat of TI2Ba2CuO6 from 2 K to 300 K. *Journal of Superconductivity, 7*(243), 261-264.

[8] Sefat, A., McGuire, M., Sales, B., Jin, R., Howe, J., Mandrus, D. (2008). Superconductivity at 22 K in Co-doped BaFe2As2 Crystals. *Phys. Rev. Lett, 101*, 117004.

[9] Sakai, H., Kotajima, D., Saito, K., Wadati, H., Wakisaka, Y., Mizumaki, M., & Ishiwata, S. (2013). Insulator-to-Superconductor Transition upon Electron Doping in a BiS2-Based Superconductor Sr1− x La x FBiS2. *Journal of the Physical Society of Japan, 83*(1), 1-19.

[10] Waswa, M.N., Ayodo, Y.K., Sakwa, T.W., and Ndinya, B. (2017). Specific Heat of Doped High-T_CCuprate Superconductors within the Bose-Fermi-Hubbard Model. *Journal of Multidisciplinary Engineering Science and Technology (JMEST), 4*(2), 7020-7025.

[11] Momono, N., Toshiaki, M., Miguku, O., Masayuki, I. (2002). Superconducting Condensation Energy and Pseudogap. *Journal of Physical Society of Japan, 71*(12), 2832-2835.

[12] Loram J. W., Mirza K. A., Cooper J. R., and Liang W. Y. (1993). Electronic specific heat of Y123 from 1.8 to 300 K. *Phys. Rev. Lett, 71*, 1740-1743.

[13] Capogrosso-Sansone, B; Prokof ev, N; and Svistunov , B. (2007). Phase diagram and thermodynamics of the three-dimensional. *Physics Department Faculty Publication Series, 1172*, 1-11.

[14] Gofryk, K., Sefat, A. S., Bauer, E. D., McGuire, M. A., Sales, B. C., Mandrus, D., and Ronning, F. (2010). Gap structure in the electron-doped iron–arsenide superconductor Ba (Fe0. 92Co0. 08) 2As2: low-temperature specific heat study. *New Journal of Physics, 12*(2), 023006.

[15] Odhiambo J. O., Sakwa T. W., Rapando B.W., and Ayodo Y. K. (2016). Thermodynamic properties of Mercury based cuprate due to Cooper pair - electron interaction. *Journal of Multidisciplinary Engineering Science and Technology (JMEST), 3* (7), 1-8.

[16] Abdullaev, B., Park, C. H., Park, K. S., and. Kang, I. J. (2016). Metal-insulator (fermion-boson) crossover origin of pseudogap phase of cuprates I:anomalous heat conductivity, insulator resistivity boundary, nonlinear entropy. *Physics, Chemistry and Mathematics , 6* (804), 1-8.

[17] Cooper J. R., Loram J. W., Kokanovic I., Storey J. G., and Tallon J. L. (2014). Pseudogap in YBa2Cu3O6+δ is not bounded by a line of phase transitions: Thermodynamic evidence. *Physical Review B, 89*, 201104R.

[18] Salas, P., Fortes, M., Solis, M. A., and Sevilla, F. J . (2016). Specific heat of Underdoped cuprate superconductors from a phenomenological layered Boson-Fermion model. *Physica C, 524*, 37-43