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The Specific Heat of a Spin-Fluctuated Cuprate superconductors with strong electronic-Phonon Correlations

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Abstract
Strongly correlated electronic models such as the Hubbard, are often used to describe the properties of cuprates. In most cases, the projected Hubbard operators are normally used to study this models. The Hubbard operators normally give rise to a specific kinematical interaction of electrons with spin and charge fluctuations. These interaction is induced by the intraband hopping with a coupling parameter, W=8t, of the order of the kinetic energy of electrons which is much larger than the antiferromagnetic exchange interaction J induced by the interband hopping. This study presents a theoretical approach to specific heat of a spin fluctuated superconductivity in electron-doped Niodium Cellenium Copper Oxide ($Nd_{2-x}Ce_xCuO_4$ -NCCO) and Praseodymium Cellenium Copper Oxide ($Pr_{2-x}Ce_xCuO_4$-PCCO) and hole-doped Yitrium Barium Copper Oxide (YBa_2CuO_7-YBCO) and Lanthanum Strontium Copper Oxide ($La_{2-x}Sr_xCuO_4$-LSCO) where these interactions are taken into account within the Hubbard operator technique. The low-energy spin excitations are considered for the Heisenberg model, while the electronic properties are studied using the two-dimensional Hubbard-Holstein model.

Keywords: Specific Heat, Electronic Correlations, Cuprate

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I. Introduction

The role of the electron–phonon interaction (EPI) in condensed matter physics of High-Tc cuprate superconductors has been under study for decades (1,2) with no agreed upon theory. With the role of EPI in superconductivity being under debate, its strong manifestations were shown clearly in numerous other phenomena in high-Tc materials (3,4). One of the observation is that strong EPI effects seen in spectroscopic data of undoped and weakly doped compounds become less pronounced with hole doping (5,6) and hence, the understanding of how the EPI effects change the specific heat of hole-doped cuprate superconductors is fundamental in understanding the nature of unconventional superconductors where studies are hampered by the strong electron-phonon problem. A number of experiments have suggested that electron-phonon coupling may not be relevant to understand cuprate superconductors (7). However, Migdal and Eliashberg investigated the low-temperature phonon-mediated superconductors in their theory of phonon-electron interactions (8,9). Anderson (10) proposed that strong electron-electron correlation is a possible mechanism of cuprate superconductors. This was applauded as an attractive approach of d-wave pairing which is a natural consequence in superconductivity. Furthermore, the cuprate superconductors evolved from antiferromagnetic insulating compounds reveal strong electron-electron interactions.

Experimental investigations on cuprate superconductors have detailed information concerning the physical properties of cuprates. However, theoretically, no accepted theory has been accepted concerning superconductivity in cuprates. The two most commonly discussed mechanisms of cuprate superconductors are the electron-phonon pairing (11,12) and the spin-fluctuation mediated pairing [13,14]. Neutron scattering experiments have suggest a strongly temperature-dependent contributions arising from critical fluctuations within the energy range $K_B T$. However, the challenge has been if such fluctuations arises due to spin or charge (15,16). Magnetic resonant inelastic x-ray scattering (RIXS) experiments have revealed that spin fluctuations in cuprate superconductors normally persist with a similar dispersion and comparable intensity in a large family of cuprate superconductors even in the overdoped region (17). These experiments shows that spin fluctuations have sufficient strength to mediate high-temperature superconductivity in cuprate superconductivity can be used to explain some physical properties of cuprate materials such as, the “kink” phenomenon observed in the electronic spectrum by the angle-resolved photoemission spectroscopy (18). Therefore, we can conclude that the spin-fluctuation mediated and the electron-phonon pairing plays major role in superconductivity of cuprate superconductors. The main problem in a theoretical study of the cuprate superconductors is the lack of a single model that takes into account the spin-fluctuation dynamics and electron-phonon pairing. In view of this problem, the Hamiltonian of the extended Hubbard (Heisenberg-Hubbard-Holstein) model is developed. This model is so unique such that it considers the spin-fluctuation mediated pairing and the electron-phonon interactions at the same time. The Heisenberg-Hubbard-Holstein (H-H-H) model is then used to study the physical property mainly the specific heat of the hole-doped cuprates.

II. Formalism

Heisenberg-Hubbard-Holstein Model

It is worth noting that doping a superconductor allows for the modulation of conductivity. The Fermi level is normally required to add an electron to the system. The spin-fluctuations in cuprates are best described by the Heisenberg model whereas the electron-phonon interaction is described by the Hubbard-Holstein model. The model Hamiltonian of the H-H-H can be given by;

$$H_{H-H-H} = \left[\sum_{ij} J\left(S_i S_j - \frac{1}{4} n_i n_j\right)\right] + \left[-t\sum_{k,-k}(C_k^+ C_k + H.c) + \omega_0 \sum_k b_k^+ b_k + \mathrm{g}\omega_0 \sum_{ij\sigma} n_k (b_k + b_k^+) + Uknk\uparrow+nk\downarrow \right. \quad (1)$$

Where H_{H-H-H} is the Heisenberg-Hubbard-Holstein Hamiltonian, S_i and S_j are the electrons spin operators in the ith and jth locations respectively, J is the spin exchange energy whereas n_i and n_j are the electron occupation number operators, $C_k^+$is the fermionic creation operator for itinerant spin σ and electrons at the site *j* with hopping integral *t*, *H.c* is the hermitian conjugate and $C_k$is the fermionic annihilation operator, the number operator $n_k \equiv C_k^+ C_k$, b_k^+ is the corresponding bosonic creation operator, b_k is the bosonic annihilation operator characterized by the dispersionless phonon frequency ω_0 with *U* and *g* representing the strengths of on-site electron-electron (*e-e)* and electron-phonon (*e-ph)* interactions respectively.

This Hamiltonian is diagonalized by both fermionic and bosonic canonical transformations resulting into the diagonalized Hamiltonian as;

$$H_{diag} = \sum_{k,-k} J\left\{\frac{3}{4}V_k^2 - \frac{1}{4} - \frac{1}{2}V_k^4 - \frac{1}{2}U_k^2 V_k^2\right\} + 2U_k^2 V_k^2 - U_k V_k - U_k^3 V_k^2 - U_k^2 V_k^3 \quad (2)$$

On solving equation (2), we obtain;

$$U_k = \sqrt{2} \text{ and } V_k = \sqrt{1} \quad (3)$$

Inorder to obtain the ground state energy of the cuprate superconductors, equation (3) was substituted back to equation (2) to get;

$$E_o = J + 2t - 2\omega_0 - 2g\omega_o + 2U \quad (4)$$

By multiplying the ground-state energy of the system,E_o, at any temperature with the thermal activation factor, $e^{-\frac{\Delta\in}{kT}}$, where k is the Boltzmann constant and $\Delta\in$ is the energy gap which is equal to $\Delta\in = \frac{E_o}{100}$,gives the ground state energy as;

$$E = (J + 2t - 2\omega_0 - 2g\omega_o + 2U).e^{-\left(\frac{J+2t-2\omega_0-2g\omega_o+2U}{100kT}\right)} \quad (5)$$

The specific heat capacity at constant volume, C_v of the system was determined from the first derivative of the energy of the system as follows;

$$C_v = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\left\{(J + 2t - 2\omega_0 - 2g\omega_o + 2U).e^{-\left(\frac{J+2t-2\omega_0-2g\omega_o+2U}{100kT}\right)}\right\}$$

$$=\frac{(J+2t-2\omega_0-2g\omega_o+2U)^2}{100kT^2}.e^{-\left(\frac{J+2t-2\omega_0-2g\omega_o+2U}{100kT}\right)} \quad (6)$$

Equation (6) is the expression for determining the specific heat of the cuprate superconductors

III. Results And Discussions

The total specific heat of the cuprate is the sum of bosonic and fermionic specific heat contributions. As a bulk measurement technique, specific heat is very powerful method used to study the physical properties in condensed matter physics (19). The specific heat values are based on derived equation (6). In Fig. 1.1, we plot the specific heat, Cv, as a function of temperature for electron-doped cuprates (NCCO and PCCO). The parameters used are t=0.42 eV, U=5.04 eV, J = 0.168 eV, g=0.03 and ω_0=0.12 K for NCCO and t=0.38 eV, U=4.56 eV, J = 0.152 eV, g=0.027 and ω_0=0.10 K for In Fig. 1.2, PCCO, we plot the specific heat, Cv, as a function of temperature for hole-doped cuprates (YBCO and LSCO). The parameters used are t=0.38 eV, U=5.16 eV, J = 0.176 eV, g=0.54 and ω_0=0.2 K for YBCO and t=0.44 eV, U=5.16 eV, J = 0.152 eV, g=0.037 and ω_0=0.14 K for LSCO. The graphs for specific heat as a function of temperature are shown in figures (1.1) and (1.2). This graphs are skewed Gaussian shaped curves.

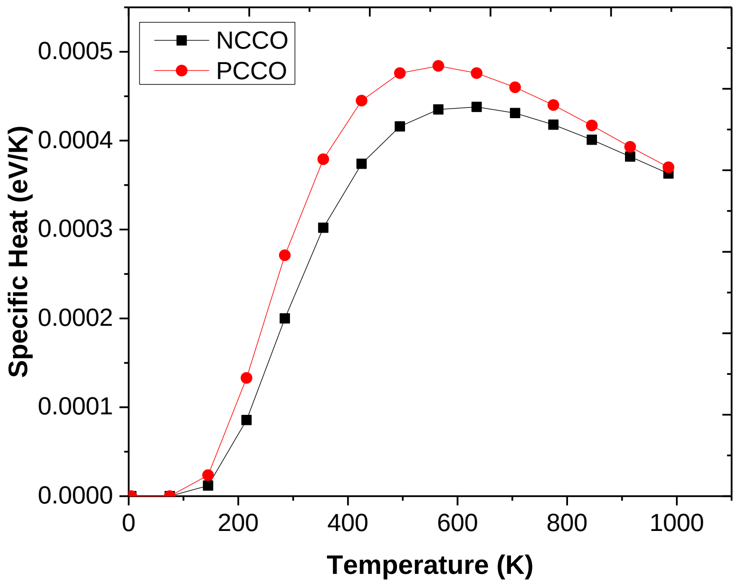

Figure 1.1: Variation of Specific Heat with Temperature for NCCO and PCCO for Heisenberg-Hubbard-Holstein model

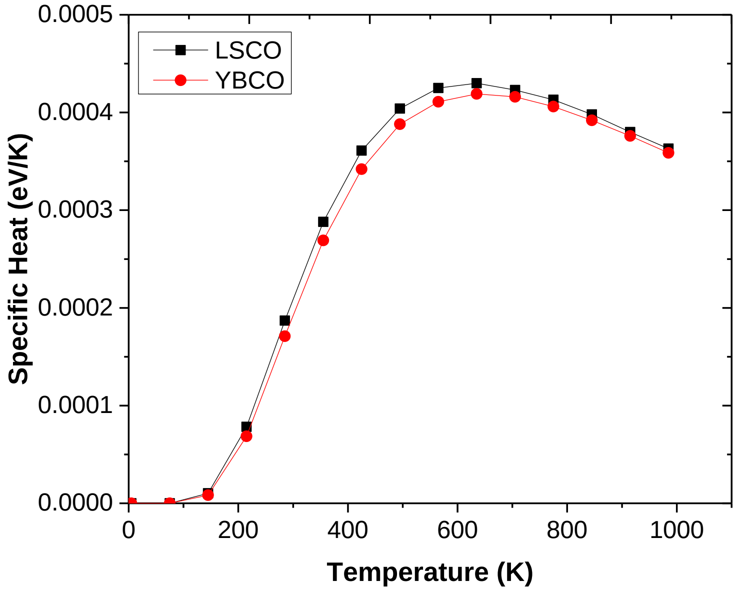

Figure 1.2: Variation of Specific Heat with Temperature for LSCO and YBCO for Heisenberg- Hubbard-Holstein model

For all the four cuprates, the specific heat is seen to drop exponentially with temperature from a given peak value. The maximum value of specific heat for the cuprates was maintained at $4.7 \times 10^{-3} eV/K$ $(7.530 \times 10^{-22} J/K)$. The highest values of specific heat for NCCO, PCCO, LSCO and YBCO are $4.663 \times 10^{-3} eV/K$ $(7.470 \times 10^{-22} J/K)$,$4.662 \times 10^{-3} eV/K$ $(7.469 \times 10^{-22} J/K)$, $4.669 \times 10^{-3} eV/K$ $(7.480 \times 10^{-22} J/K)$, $4.672 \times 10^{-3} eV/K$ $(7.485 \times 10^{-22} J/K)$ respectively. It was observed that the interaction between electron-electron and electron-phonon gave a constant value of specific heat of $4.6 \times 10^{-3} eV/K$ $(7.37 \times 10^{-22} J/K)$ for the four cuprates under study. Peak specific heat occurred at the transition temperature. (20) used Bogoliubov Valatin transformation to study interaction of two electrons, one in singlet and the other in triplet state. He found the value of specific heat at T_C as $4.8 \times 10^{-23} J/K$. (21) while studying thermodynamic properties of Mercury based cuprate due to Cooper pair-electron interaction noted that the heat

capacity was $7.472\times10^{-24} J/K$ at Tc. Our results therefore are in close agreement with other scholars, the small discrepancy is that in our case we considered interactions between electron-electron and electron-phonon.
This type of Gaussian shaped curves relating specific heat to temperature has been observed by other scientists while investigating relationship between specific heat and temperature for varied materials under varied conditions (22, 23, 24,25)

IV. Conclusions

In this work, Heisenberg-Hubbard-Holstein model Hamiltonian was diagonalized using Bogoliubov-Valatin transformation inorder to obtain the values of cuprate superconductors namely: NCCO, PCCO, LSCO and YBCO. We have shown that the H-H-H model can also be used to study the specific heat, being a bulk phenomena, of cuprates. The peak value of the Gaussian curves of specific heat represents the superconducting transition temperature of the cuprates. At this point, a condensate is formed and specific heat remains fairly constant. This shows that the system is unstable at the peak and a second order phase transition occurs due absence of latent heat. The fermionic specific heat is normally driven by electrons while bosonic specific heat is driven by phonons and plasmons and is used to infer the strength of electron-phonon coupling. The work on fermionic specific heat will be published later.

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