Journal of Multidisciplinary Engineering Science and Technology (JMEST)
ISSN: 2458-9403
Vol. 6 Issue 10, October - 2019

Specific Heat Of A Square Lattice YBCO And LSCO Cuprates

Simon Mwatulo Lusamamba
Department of Science, Technology and Engineering,
Kibabii University, P.O BOX 1699-50200,Bungoma,Kenya.
Email: simonlusamamba@gmail.com

***Abstract*— The study of superconductivity arising from doping a Mott insulator has been an area of intense research in the area of superconductivity. Within the framework of electron-electron mechanism, the specific heat of a square- lattice in LSCO and YBCO are discussed. It is shown that a sharp peak in the specific-heat appears at the superconducting transition temperature, T_C and then the specific heat varies exponentially as a function of temperature for the temperatures $T < T_C$ due to the absence of d-wave gap nodes at the charge-carrier Fermi surface In particular, quantitatively, we report a specific heat value 1.33×10^{-3}eV/K for $YBa_2Cu_3O_6$ (YBCO), 1.031×10^{-3}eV/K for $La_{2-x}Sr_xCuO_4$ (LSCO), at their respective T_C values which are in favorable agreement with other recent research findings.**

Keywords—Specific Heat; Transition Temperature, Mott insulator

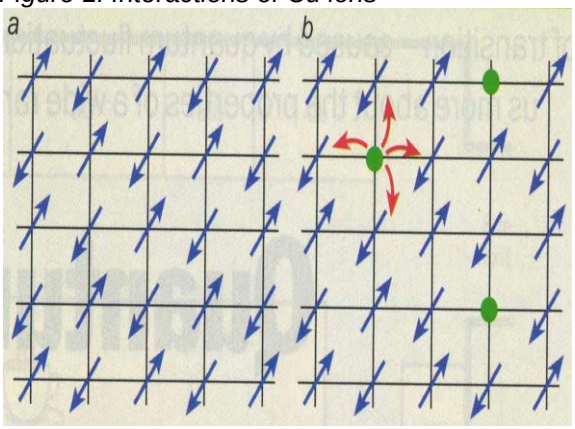
I. INTRODUCTION

Superconductivity in parent compounds of cuprates arises due to strong electron-electron repulsion [1]. Superconductivity is then obtained by adding charge-carriers to insulating parent compound [2]. Since the discovery of superconductivity in cuprate superconductors, the search for the superconducting (SC) mechanism has been an area of great research [3]. In the cuprate superconductors, Cu ions in a square array are ordered antiferromagnetically, and then spin fluctuations are thought to play a crucial role in the charge-carrier pairing [1]. Experimental studies in $La_{2-x}Sr_xCuO_{4+\delta}$ (LSCO) and $YBa_2Cu_3O_x$ (YBCO) , using small angle neutron scattering (SANS) succeeded to measure a well-ordered vortex lattice (VL) structure at all doping regimes of LSCO. In the optimally to overdoped regime a field-induced transition from hexagonal to square coordination is reported at around H = 0.4 T with the square lattice oriented along the anti-nodal direction of the d-wave superconducting gap [4]. In a recent experiment, [5] observed a similar phase transition in the YBCO superconductor, however with two main differences: first, the critical field at which the transition occurs is at least an order of magnitude higher than in LSCO; second, the square VL in YBCO is oriented along the nodal direction of the d-wave gap function. The heat capacity measurement of the specific heat can be used to study bulk properties of superconductors which are used to investigate low-energy quasiparticle excitations like the charge-carrier symmetry [1]. For conventional superconductors, lack of quasiparticle excitation results to an exponential specific heat at low temperatures since they are gaped at the Fermi surface. For Square lattice cuprates in LSCO and YBCO, experimental results have shown that Angle-Resolved Photo-Emission Spectroscopy (ARPES) in underdoped (hole-doped) cuprates generically observe open-ended lines of the Fermi surface known as Fermi arcs and accompanied by angle-dependent pseudogap [6]. At the same time, the observations of quantum oscillations indicate the presence of small closed Fermi surfaces. This phenomenology hinted at the possibility that the Fermi arcs originate from closed Fermi surfaces in a smaller Brillouin zone (BZ) emerging as a result of some kind of periodically modulated background. Such interpretations based on one-dimensional stripe-like or two-dimensional checkerboard-like charge modulations have indeed been proposed [7]. Spin modulations have mostly been omitted in these interpretations because of the absence of the experimental evidence of static spin response in YBa_2Cu_3Oy (YBCO) and other cuprate families exhibiting quantum oscillations [6].

One of the reason for the hexagonal-square lattice transition is the coupling of charge/stripe fluctuations or Fermi velocity anisotropies [8]. It should be noted that d-wave scenario favours a square VL aligned along the nodal direction (as observed in YBCO [5]), an anisotropy of the Fermi velocity would result in a VL aligned along the anti-nodal direction (as observed in LSCO [9]).

Here, the goal is to develop a model of non-interacting fermions of spin-1/2 on a square lattice coupled through spins to local fields. According to Heisenberg, when copper oxide is doped to half-filling level and increasing the onsite Coulomb energy to large values, the cuprate system becomes anti-ferromagnetic with neighboring electrons acquiring opposite spins; hence an electron would gain energy in hoping to the neighbor site where the other electron has opposite spin. This leads to pairing of electrons forming Cooper pairs that facilitate the process of superconductivity. The pairing electrons were found to exchange spins and as a result there exists exchange energy, J.

Figure 1: Interactions of Cu ions



(a)The lattice of copper ions in a single layer of La_2CuO_4. Each ion has a free spin, and at zero temperature these spins exhibit antiferromagnetic order.

(*b*) The addition of strontium ions has the effect of introducing "holes" into the spin lattice. These holes can hop between lattice sites, as indicated by the red arrows

FORMALISM

The Heinsberg Hamiltonian for a square lattice was expressed interms of spin exchange integral, J, the electron spin operators S_i and S_j in the neighboring sites as

$$H_{Heinsberg} = J\sum_{ij} S_i.S_j \quad (1)$$

Here, we impose a fermion constraint

$$\not{f}_{i\uparrow}^{+}\not{f}_{i\uparrow} + \not{f}_{i\downarrow}^{+}\not{f}_{i\downarrow} = 1 \quad (2)$$

The Heisenberg exchange term is now written in terms of fermion operators as [10];

$$S_i.S_j = -\frac{1}{4}\not{f}_{i\sigma}^{+}\not{f}_{j\sigma}\not{f}_{j\beta}^{+}\not{f}_{i\beta} - \frac{1}{4}(\not{f}_{i\uparrow}^{+}\ \not{f}_{j\downarrow}^{+} - \not{f}_{i\downarrow}^{+}\not{f}_{j\uparrow}^{+})(\not{f}_{j\downarrow}\not{f}_{i\uparrow} - \not{f}_{j\uparrow}\not{f}_{i\downarrow}) + \frac{1}{4}(\not{f}_{i\sigma}^{+}\not{f}_{i\sigma}) \quad (3)$$

Substituting equation (2) back to equation (1) gives

$$H_{Heinsberg} = J\sum_{ij} -\frac{1}{4}\not{f}_{i\sigma}^{+}\not{f}_{j\sigma}\not{f}_{j\beta}^{+}\not{f}_{i\beta} - \frac{1}{4}(\not{f}_{i\uparrow}^{+}\ \not{f}_{j\downarrow}^{+} - \not{f}_{i\downarrow}^{+}\not{f}_{j\uparrow}^{+})(\not{f}_{j\downarrow}\not{f}_{i\uparrow} - \not{f}_{j\uparrow}\not{f}_{i\downarrow}) + \frac{1}{4}(\not{f}_{i\sigma}^{+}\not{f}_{i\sigma}) \quad (4)$$

Let the new operators, $\gamma_{i\sigma}$ be defined in terms of the old operators, $\not{f}_{i\sigma}$ as follows;

i. $\gamma_{i\sigma} = U_{i\sigma}\not{f}_{i\sigma} - V_{i\sigma}\not{f}_{i\sigma'}^{+}$ and $\gamma_{i\sigma'} = U_{i\sigma}\not{f}_{i\sigma'} + V_{i\sigma}\not{f}_{i\sigma}^{+}$ (5)

ii. $\gamma_{j\sigma} = U_{j\sigma}\not{f}_{j\sigma} - V_{j\sigma}\not{f}_{j\sigma'}^{+}$ and $\gamma_{j\sigma'} = U_{j\sigma}\not{f}_{j\sigma'} + V_{j\sigma}\not{f}_{j\sigma}^{+}$ (6)

The complex conjugates of the operators in equations (5) and (6) are;

$\gamma_{i\sigma}^{+} = U_{i\sigma}\not{f}_{i\sigma}^{+} - V_{i\sigma}\not{f}_{i\sigma'}$ and $\gamma_{i\sigma'}^{+} = U_{i\sigma}\not{f}_{i\sigma'}^{+} + V_{i\sigma}\not{f}_{i\sigma}$ (7)

$\gamma_{j\sigma}^{+} = U_{j\sigma}\not{f}_{j\sigma}^{+} - V_{j\sigma}\not{f}_{j\sigma'}$ and $\gamma_{j\sigma'}^{+} = U_{i\sigma}\not{f}_{j\sigma'}^{+} + V_{j\sigma}\not{f}_{j\sigma}$ (8)

The constants $U_{(i,j)}$ and $V_{(i,j)}$ are screened Coulomb repulsion term and the electron interaction term respectively [10] and ought to satisfy the condition $U_{k(i,j)}^2 + V_{k(i,j)}^2 = 1$ for fermions.

Using equations (5),(6),(7) and (8) into equation (4) gives

$$H_{Heinsberg} = \sum_{ij} J\left\{-\frac{1}{4}\left[(U_{i\sigma}\gamma_{i\sigma}^{+} + V_{i\sigma}\gamma_{i\sigma'})\left(U_{j\sigma}\gamma_{j\sigma} + V_{j\sigma}\gamma_{j\sigma'}^{+}\right)\left(U_{j\sigma}\gamma_{j\sigma'}^{+} - V_{j\sigma}\gamma_{j\sigma}\right)(U_{i\sigma}\gamma_{i\sigma'} - V_{i\sigma}\gamma_{i\sigma}^{+})\right] - \frac{1}{4}\left[(U_{i\sigma}\gamma_{i\sigma}^{+} + V_{i\sigma}\gamma_{i\sigma'})\ \left(U_{j\sigma}\gamma_{j\sigma'}^{+} - V_{j\sigma}\gamma_{j\sigma}\right) - (U_{i\sigma}\gamma_{i\sigma'}^{+} - V_{i\sigma}\gamma_{i\sigma})\left(U_{j\sigma}\gamma_{j\sigma} + V_{j\sigma}\gamma_{j\sigma'}^{+}\right)\right]\left[\left(U_{j\sigma}\gamma_{j\sigma'} - V_{j\sigma}\gamma_{j\sigma}^{+}\right)\left(U_{j\sigma}\gamma_{j\sigma} + V_{j\sigma}\gamma_{j\sigma'}^{+}\right) - \left(U_{j\sigma}\gamma_{j\sigma} + V_{j\sigma}\gamma_{j\sigma'}^{+}\right)\left(U_{j\sigma}\gamma_{j\sigma'} - V_{j\sigma}\gamma_{j\sigma}^{+}\right)\right] + \frac{1}{4}\left[(U_{i\sigma}\gamma_{i\sigma}^{+} + V_{i\sigma}\gamma_{i\sigma'})(U_{i\sigma}\gamma_{i\sigma} + V_{i\sigma}\gamma_{i\sigma'}^{+})\right]\right\} \quad (9)$$

If we the particle spin up state as k and spin down as $-k$, then the scattered particle spin states will be represented by k' and $-k'$ for spin up and spin down, respectively. Rearranging terms in equation (9) and neglecting the higher order terms, number operators and off-diagonal terms, the diagonalized form of the Heinsberg Hamiltonian becomes;

$$H_{diag} = \sum_{k,-k} J\left\{-\frac{1}{4} + \frac{3}{4}V_k^2 - \frac{1}{2}V_k^4 - \frac{1}{2}U_K^2V_k^2\right\} \quad (10)$$

On diagonalization,we obtain the values of U_K and V_k as;

$$U_k = \sqrt{2} \text{ and } V_k = 1 \quad (11)$$

RESULTS AND DISCUSSIONS

a. Energy of the Heinsberg system

Substituting equation (11) back to equation (10) gives the ground state energy of the system as;

$$E_0 = (J) \quad (12)$$

The energy of the system at any temperature, E as a function of temperature is obtained by multiplying the ground-state energy, E_0 by the thermal activation factor, $e^{-\frac{\Delta\epsilon}{kT}}$ [11], where k is Boltzmann's constant and $\Delta\epsilon$ is the energy gap. The energy gap for superconductors is a very small quantity and it is generally 1% of the minimum energy of the system [11]. Thus $\Delta\epsilon = 0.01E_0$. So at any temperature T, the energy of the system is given as;

$$E = E_0 e^{-\frac{0.01E_0}{kT}} = E_0 e^{-\frac{E_0}{100kT}} \quad (13)$$

Substituting equation (12) in equation (13), we obtain the energy of the system at any given temperature as;

$$E = (J).e^{-\left(\frac{J}{100kT}\right)} \quad (14)$$

b) Specific Heat capacity of the system

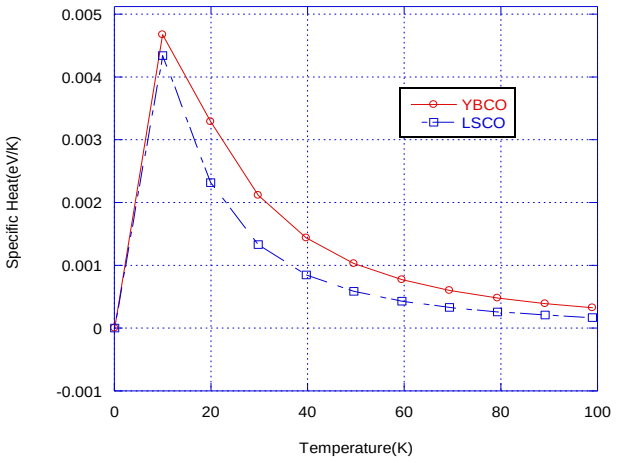
The specific heat capacity at constant volume c_v of the system was obtained by determining the first derivative of the energy of the system with respect to the temperature [3,10,11] . Hence, using equation [14], we obtain the expression of c_v as;

$$C_v = \frac{(J)^2}{100kT^2}.e^{-\left(\frac{J}{100kT}\right)} \quad (15)$$

Numerical values of specific Heat

One of the characteristics quantities in the thermodynamic properties of cuprates is the specific heat, which can be obtained by evaluating the temperature-derivative of the internal energy .Fig. 2, we plot the specific heat Cv as a function of temperature for hole doped cuprates (YBCO and LSCO). The parameters used are J = 0.17eV for YBCO and J=0.13eV for LSCO. The curves obtained for the Fermi hybrid model assumes a dome-shaped nature. Similar curves were obtained by [1]; [12] while investigating specific heat as a function of temperature for triangular-lattice superconductors under different conditions. Apparently, the main feature of the specific-heat observed experimentally on the cuprate superconductors is qualitatively reproduced. At the peaks, superconducting phase transition occurs and we can estimate T_C at this point. Peak specific heat occurs at critical temperature [3]. As expected the transition temperature corresponding to this phase transition is lower for LSCO compared to YBCO. The step-like transition occurs at T_C≈50 K and T_C≈30 K for YBCO and LSCO respectively. The values of specific heats corresponding to this jump are; C_V=1.33 ×10^{-3}eV/K for YBCO and 1.031 ×10^{-3}eV/K for LSCO. It is worth noting that our model predicts comparable value of specific heat although at different transitional temperatures. However, both cuprates registered very high T_C values compared to their experimental values. The experimental value for YBCO is 24.5 K while that of LSCO is 14 K [13].

Figure 2. Varriation of Specific Heat with Temperature for YBCO and LSCO



The large and sharp peak we observe is therefore due to electronic effects beyond the band structure [12].

CONCLUSIONS

The Bogoliubov-Valatin transformation was used to diagonalize the Heinsberg Hamiltonian of a square lattice to obtain the ground state energy. From the ground state energy, the specific heat of high-T_C superconductors was determined. The results obtained for specific heat predicted a higher transition temperature for both in the electron-doped YBCO and LSCO superconducting cuprates.

ACKNOWLEDGEMENT

The author would like to appreciate Kibabii University for the enabling environment under which this research was carried on.

REFERENCES

1. M. Xixiao, Q. Ling, Z. Huaisong, L. Yu and F. Shiping (2016), Thermodynamic properties in triangular-lattice superconductors, website: https//:www.arXiv:1511.00842v2.
2. J. L. Tallon, C. Bernhard, H. Shaked, R. L. Hitterman,and J. D. Jorgensen(1995), Electronic Transport and Specific heat anomaly at Tc of Ca-doped YBa_2 Cu_3 O_x *Phys. Rev. B* vol. 51, 12911.
3. M.W. Nakitare ,T.W Sakwa, Y.K. Ayodo, and B. Ndinya (2017), Specific Heat Of Doped High-TC Cuprate Superconductors Within The Bose-Fermi-Hubbard Model, *Journal of Multidisciplinary Engineering Science and Technology (JMEST)*, Vol.4, issue 4,Pp 7020-7025.
4. J. Mesot,1,2 M. R. Norman,1 H. Ding,3 M. Randeria,4 J. C.Campuzano,1,2 A. Paramekanti,4 H. M. Fretwell,2 A. Kaminski,2T. Takeuchi,5 T. Yokoya,6 T. Sato,6 T. Takahashi,6 T. Mochiku,7and K. Kadowaki (1999), BSCCO Superconductors: Hole-Like Fermi Surface and Doping Dependence of the Gap Function, *Journal of Low Temperature Physics,*Vol. 117*, Nos. 314.*
5. S. P. Brown, J. Chang, C.J. Bowell, M. Laver, A. Holmes, L. Maechler,R. Gilardi (2012), Spin density wave induced disordering of the vortex lattice in superconducting $La_{2-x}Sr_xCuO_4$, *Phys. Rev. B* **85(13)**.
6. D.E. Pavel and F.V Boris (2018), Pseudogap and Fermi surface in the presence of spin-vortex checkerboard for 1/8-doped lanthanum cuprates, website: www. arXiv:1705.08542v2.
7. A. Allais, D. Chowdhury, and S. Sachdev (2014), Nat. Commun.**5**, 5771 .
8. G. W. Bennett, B. Bousquet, H. N. Brown, G. Bunce, R. M. Carey, P. Cushman, G. T. Danby, P. T. Debevec, M. Deile, H. Deng, W. Deninger, S. K. Dhawan, V. P. Druzhinin, L. Duong, E. Efstathiadis, F. J. M. Farley, G. V. Fedotovich, S. Giron, F. E. Gray, D. Grigoriev, M. Grosse-Perdekamp, A. Grossmann, M. F. Hare, D. W. Hertzog, X. Huang (2002), Measurement of the Positive Muon Anomalous Magnetic Moment to 0.7 ppm, *Phys. Rev. Lett.* 89, 101804.
9. R. Gilardi, J. Mesot, A.J. Drew, U. Divakar, S.L. Lee, N.H. Andersen, J. Kohlbrecher, N. Momono, M. Oda (2002), Field-induced hexagonal to square transition of the vortex lattice in overdoped La1.8Sr0.2CuO4, *Phys. Rev. Lett.* **88**, 217003.

10. B.W. Rapando, J.K. Tonui, K.M. Khanna, and P.A. Mang'are, (2015), The diagonalized t-J Hamiltonian and the thermodynamic properties of High-Tc superconductors, *American Research Journal of Physics (ARJP)* , Vol.2016**,**Pp 1-11.
11. T.W. Sakwa, Y.K. Ayodo, P.O. Saisi, A. Sarai, B.W. Rapando and C.A.Omondi (2013), A Non-Degenerate Binary System of Helium Isotopes, *East African Journal of Engineering, Science & Technology,*Vol.1,issue 2,Pp 66-70.
12. B. Michon, C. Girod, S. Badoux, J. Kačmarčík, Q. Ma, M. Dragomir,H. A. Dabkowska, B. D. Gaulin, J.-S. Zhou, S. Pyon, T. Takayama, H. Takagi,S. Verret, N. Doiron-Leyraud, C. Marcenat, L. Taillefer, T. Klein (2019),Thermodynamic signatures of quantum Critically in cuprates, *Nature,***567**(7747).
13. K. A Saxena (2010). *High Temperature Superconductors.* Berlin: Springer-Verlag.