IOSR Journal Of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 13, Issue 3 Ser. II (May – June. 2021), PP 10-14
www.Iosrjournals.Org

Spin-Mediated Energy of Cuprate Superconductors.

[1]Simon Mwatulo Lusamamba [*], [1]Micheal Waswa Nakitare, and [2]Thomas Welikhe Sakwa

[1] Kibabii University, P.O BOX 1699-50200, Bungoma, Kenya
[2] Masinde Muliro University of Science and Technology, P.O BOX 190-50100, Kakamega, Kenya.

Abstract
Spin fluctuation in strong correlated systems give rise to superconductivity in cuprate superconductors. The correlation effects in copper oxide (CuO_2) layers give rise to collective excitations in high-T_C cuprates. Here, the energy of 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) within the Heisenberg-Hubbard-Holstein model by means of the Bogoliubov-Valatin Transformation (BVT) approach. The energy of the system is seen to be very low for $T < 185K$ and an exponential increase in the energy of the system at $T > 185K$ for the four cuprates. At $T = T_C$, there is transition of state from normal material to superconducting state and the energy at this particular point was determined to be, $E{\sim}0.013\ for\ NCCO, E{\sim}0.023\ for\ PCCO, E{\sim}0.013\ for\ LSCO\ , E{\sim}0.011\ for\ YBCO$).

Keywords: *Spin Fluctuation, Superconductivity, Correlation effects*

Date of Submission: 17-06-2021 Date of Acceptance: 02-07-2021

I. Introduction

Despite of immense efforts in the field of theoretical physics, spin fluctuations and electron-phonon interaction seem to be not well understood (1). This is because of the competing phenomena's like superconductivity, the presence of strong charge and spin fluctuations (2). Spin fluctuations normally manifests itself in the antiferromagnetism (AFM) phase at low temperatures and is one of the main properties of cuprates. Cuprates exhibit strong superconductivity. Furthermore, spin fluctuations provides an avenue for electron pairing, playing the role of the phonons; lattice distortions, electron-phonon coupling (3). Discoveries in superconductivity of high-T_C cuprate superconductors have shown that magnetism which arises due to spin fluctuation is an important factor in spin fluctuation-mediated superconductivity (4). One of the model that can be used to study spin-fluctuation superconductivity is the Heisenberg model which was discovered in 1928 and it gives a description of the physical properties of ferromagnets; the second order phase transition between ferromagnetic and paramagnetic states at the Curie Temperature T_C and the Curie-Weiss magnetic susceptibility; $\aleph = \frac{C}{(T-T_C)}$ above T_C (5). This model was further extended to include the exchange interactions of a wide spatial range so that properties such as antiferromagnetism, ferrimagnetism and their temperature dependencies can be best described using extended Heisenberg spin Hamiltonians (6).

Theoretical studies on the extensions of the Heisenberg model has been done including those based on the Hubbard (7), the t-J (8) and the Heisenberg spin-fermion models (9). All this methods does not fully describe the properties of the cuprates (10). The non-perturbative techniques such as the quantum field theoretical approaches (11), Bethe ansatz (12), Dynamical mean field theories (13), Renormalization group (14), slave-boson approach (15) have also been developed. Numerical techniques such as the exact diagonalization (16) and Monte Carlo (17) have used to study the properties of the cuprates. These approaches mentioned above have given insights on the properties of high-T_C cuprate superconductors.

Angle Resolved Photoemission Spectroscopy (ARPES) have revealed a wide energy range and "kinks" in cuprate superconductors (18). In cuprate superconductors, spin fluctuations give rise to normal and anomalous self-energies where the peak-dip-hump in the phase diagram arises as a result of the normal self-energy whereas the sharp peak is due to the anomalous self-energy and is an important contribution to the superconducting gap (19). The spin energy has shown a damped and well-defined dispersive spin excitations in the phase diagram (20). From the theoretical perspective, a simplified Hamiltonian that can capture the interplay between antiferromagnetism (AFM), charge density wave CDW, and superconductivity (SC) is the single-band Hubbard-Holstein model (HHM). It exhibits Coulomb repulsion between electrons, leading to spin fluctuations; and also electron-ion interactions, which enhance charge/pairing correlations (21). This model has been extensively studied in one-dimensional systems to show the competitions between spin-density wave, bond-order-wave, CDW, and phase separation behavior in phase diagrams (22). By contrast, the properties such as the energy of the HHM in two-dimensional systems are entirely not clear, even for simple geometry like the square lattice.

In view of the above open issues, and the understanding of the role of electron-phonon interactions in strongly interacting cuprate superconductors, we investigate in this article we develop another extension of the Heisenberg model; the Heisenberg-Hubbard-Holstein model use to study the energy of cuprate superconductors: NCCO, PCCO, LSCO and YBCO. This model is so unique such that it considers spin-fluctuations as well as the strong electron-phonon interactions at the same time.

II. FORMALISM

a) A Model Hamiltonian of Heisenberg-Hubbard-Holstein in Cuprate Superconductors

A cuprate superconductor consisting of electrons interacting with a long-range order is given by (23)

$$H_{Heisen} = \sum_{ij} J\left(S_i S_j - \frac{1}{4} n_i n_j\right) \qquad (1)$$

Where H_{Heisen} is the Heisenberg 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. The Hubbard- Holstein (H-H) Hamiltonian is the sum of an electronic part, a phononic part and an electron-phonon part

$$H_{HH} = H_{electron} + H_{Phonon} + H_{electron-phonon} \qquad (2)$$

According to (24), the Hubbard-Holstein model is given by

$$H_{HH} = -t\sum_{k,-k}(C_k^+ C_k + H.c) + \omega_0 \sum_k b_k^+ b_k + g\omega_0 \sum_{ij\sigma} n_k (b_k + b_k^+) + U\sum_k n_{k\uparrow} + n_{k\downarrow} \qquad (3)$$

Where $C_k^+$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 $n_k \equiv C_k^+ C_k$, a_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.

Combing equation (1) and (3) gives the model Hamiltonian of the Heisenberg-Hubbard-Holstein (H-H-H) as;

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

Equation (4) was then expressed in terms of the number operators, fermion operators, creation and annihilation operators and then diagonalized to obtain the elements of the Hamiltonian that correspond to stationary states where the system is in equilibrium. BVT formalism was used to transform equation (4).This was achieved by defining two new operators that are related to the fermion creation and annihilation operators as follows;

The number operators n_i and n_j are given by;

$$n_i = (1 - b_i^+ b_i) \qquad (5a)$$

and

$$n_j = \left(1 - b_j^+ b_j\right) \qquad (5b)$$

The product of the number operators is;

$$n_i n_j = (1 - b_i^+ b_i)\left(1 - b_j^+ b_j\right) \qquad (5c)$$

The Heisenberg exchange term interms of fermion operators was written as,

$$S_i . S_j = -\frac{1}{4} f_{i\sigma}^+ f_{j\sigma} f_{i\beta}^+ f_{j\beta} - \frac{1}{4}\left(f_{i\uparrow}^+ f_{j\downarrow}^+ - f_{i\downarrow}^+ f_{j\uparrow}^+\right)\left(f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow}\right) + \frac{1}{4}\left(f_{i\sigma}^+ f_{i\sigma}\right) \qquad (5d)$$

The fermionic creation and annihilation operators are defined as follows;

$\gamma_{i\sigma} = U_{i\sigma} f_{i\sigma} - V_{i\sigma} f_{i\sigma'}^+$ and $\gamma_{i\sigma'} = U_{i\sigma} f_{i\sigma'} + V_{i\sigma} f_{i\sigma}^+$ (6a)

$\gamma_{j\sigma} = U_{j\sigma} f_{j\sigma} - V_{j\sigma} f_{j\sigma'}^+$ and $\gamma_{j\sigma'} = U_{j\sigma} f_{j\sigma'} + f_{j\sigma}^+$ (6b)

The bosonic creation and annihilation operators are

$$\ell_k = U_k b_k - V_k b_k^+ \qquad (6c)$$

The inverse fermionic and bosonic operators are;

$$f_{i\sigma} = U_{i\sigma}\gamma_{i\sigma} + V_{i\sigma}\gamma_{i\sigma'}^+ \qquad (7a)$$

$$b_k = U_k \ell_k + V_k \ell_k^+ \qquad (7b)$$

Substituting equation (6) and its complex conjugate, equation (5) and equation (7) in equation (4), we obtain the Hamiltonian of the Heisenberg-Hubbard-Holstein model as,

$H_{H-H-H} = \left\{\sum_{k,-k} J \left\{\left[-\frac{1}{4}\left(V_k^3 U_k \gamma_k^+ \gamma_{-k'}^+ + V_k^3 U_k \gamma_{k'} \gamma_{-k} - V_k^3 U_k \gamma_{k'} \gamma_{-k} - V_k^3 U_k \gamma_k^+ \gamma_{-k'}^+ + 2U_k V_k^3 \gamma_{-k}^+ \gamma_{-k'}^+ -\right.\right.\right.\right.$
Uk2Vk2γk′+γ−k++Uk2Vk2γk+γ−k+−2UkVk3γkγ−k′+2Uk2Vk2+Vk4+14Vk2−14+14Vk2+14Vk2−14Vk4+14UkVkγk′+γk′++14UkVkγ−k′γk+−14UkVk+14UkVk3−14UkVk+14UkVk3𝒷k+𝒷k++𝒷k𝒷k +−tk,−k(Uk2−Vk2)mk+Vk2−UkVkγ−k+γk++γkγ−kUk2+Vk2−UkVk𝒷−k𝒷k+𝒷k+𝒷−k+−UkVk𝒷−k+𝒷k++𝒷k𝒷−k+Uk2mk−Vk2mk+Vk2−UkVkγ−k+γk++γkγ−k+ωok,−kUk2−Uk2−Vk2nk−UkVk𝒷 −k+𝒷k++𝒷k𝒷−k+gωok,−k2Uk3nk+2UkVk2−UkVk2n−k+nk−Uk2Vk𝒷−k+𝒷k+𝒷k+𝒷−k𝒷k𝒷k+2 Uk2Vknk+2Vk3−2Vk3nk−UkVk2𝒷−k+𝒷k+𝒷−k++𝒷−k𝒷k𝒷−k++2Uk,−k1−Uk2+Uk2nk+Vk2n−k −UkVk(𝒷−k+𝒷k++𝒷k𝒷−k) (8)

On rearranging terms in equation (8) and neglecting the higher order terms, number operators and off-diagonal terms, the diagonalized form of the H-H-H Hamiltonian becomes;

$$H_{diag} = \sum_{k,-k} J \left\{\frac{3}{4} V_k^2 - \frac{1}{4} - \frac{1}{2} V_k^4 - \frac{1}{2} U_k^2 V_k^2\right\} + 2U_k^2 V_k^2 - U_k V_k - U_k^3 V_k^2 - U_k^2 V_k^3 \quad (9)$$

On solving equation (9), we obtain;

$U_k = \sqrt{2}$ and $V_k = \sqrt{1}$

(b). The superconducting energy of the modified Hubbard-Holstein model.

Inorder to obtain the magnitude of ground state energy of the system, equation (10) was substituted in equation (9) to obtain;

$$E_o = J + 2t - 2\omega_0 - 2g\omega_o + 2U \quad (11)$$

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

$$E = (J + 2t - 2\omega_0 - 2g\omega_o + 2U).e^{-\left(\frac{J+2t-2\omega_0-2g\omega_o+2U}{100kT}\right)} \quad (12)$$

III. Results And Discussion

Table 1. Numerical values of pre-factors used in data analysis.

Constants	*NCCO*	*PCCO*	*YBCO*	*LSCO*
J(eV)	0.168	0.152	0.176	0.152
t(eV)	0.42	0.38	0.44	0.38
U(eV)	5.04	4.56	5.28	5.16
G	0.030	0.027	0.54	0.037
ω_o(K)	0.12	0.10	0.2	0.14

Equation (12) was used to show how the energy (E) varies with temperature (T) using the parameters listed in Table 1. The results obtained for electron-doped cuprates PCCO and NCCO, holed-doped cuprates LSCO and YBCO are shown in figures (1.1) and (1.2) respectively.

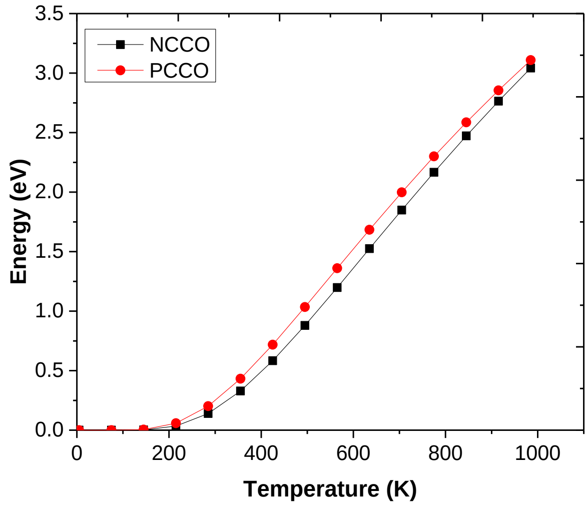

Figure 1.1: Variation of System's Energy with Temperature for NCCO and PCCO for Heisenberg-Hubbard-Holstein model

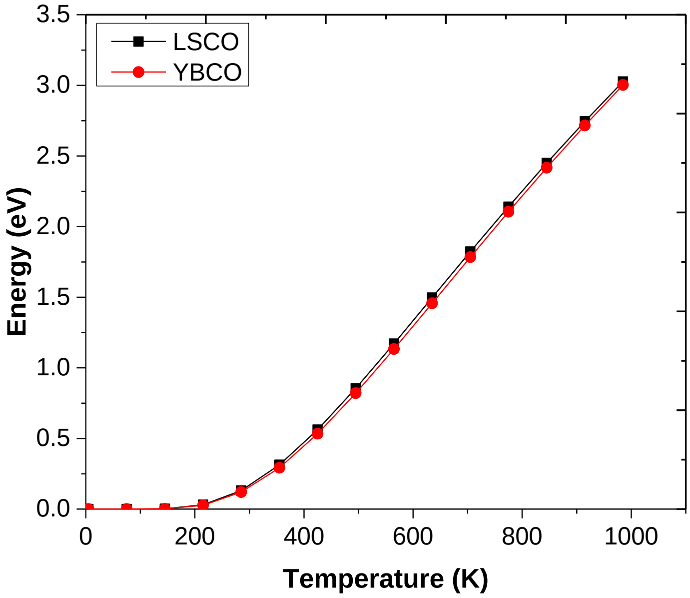

Figure 1.2: Variation of System's Energy with Temperature for LSCO and YBCO for Heisenberg-Hubbard-Holstein model

It can be seen that the shapes of the curves for both electron-doped and hole-doped cuprates are nearly the same. At temperature very close to absolute zero, the energy of the four cuprates is at its lowest value ($E_k = 0$) meaning that most of the electrons in a superconductor are paired and therefore do not participate in conduction mechanism and therefore the state below the superconducting gap is filled whereas the space above the superconducting gap is empty. From figure 1.1, PCCO has a higher energy as compared to NCCO. At 285 K, NCCO and PCCO have energies 0.14 eV and 0.202 eV respectively. The two cuprates have the same energy at higher temperatures of 3.109 eV at T=985 K. On the contrary, the YBCO and LSCO cuprates gave an energy of 0.314 eV and 0.12 eV at T= 285 K and registers higher energies thereafter. Both the hole doped and electron doped cuprates have comparable energies at 285 K. This transition temperature is in close proximity with (18) who used ARPES data to calculate the critical temperature of the energy of the *d*-wave superconducting state arising from the exchange of spin fluctuations within the Hubbard model and found it to be T_c=174 K. However, NCCO and YBCO are thought to have the least energy at room temperature and would be an ideal material for room temperature superconductivity. Of the four cuprates, the energy is seen to be very low for $T < 185K$. There exists an exponential increase in the energy of the system at $T > 185K$ for the four cuprates. At about 185K, both LSCO and YBCO have nearly a common value of 0.011 eV an indication of a transition from the superconducting state to the normal state. Beyond this point, the graphs begin to broaden. Similar findings were obtained by (25,26,27).

IV. Conclusions

In this work, Heisenberg-Hubbard-Holstein model Hamiltonian was diagonalized using Bogoliubov-Valatin transformation and the quasi- particle ground state energy obtained. From the ground state energy, the spin-mediated energy of the high-Tc cuprate superconductors was determined. The results obtained for the energy of the cuprate superconductors are in tandem with the Finite Temperature- Variation After Projection (FT-VAP) study of thermodynamic properties of small superconductors. The H-H-H model predicts higher transition temperature in both electron-doped and hole-doped superconducting cuprates. The H-H-H model which captures spin fluctuations and strong electron-phonon correlations in cuprate superconductors can be used to predict the transition temperature of cuprates.

Acknowledgement

Our sincere gratitude to Kibabii University of Science for giving us an enabling environment under which this research was done.

References

[1]. Evgeny A.S, Lars P and Rubtsov N.A (2018).Quantum spin fluctuations and evolution of electronic structure in cuprates.*npj Quantum Materials* **3,** Article Number 54.

[2]. Scalapino, D.J (2012),A Common thread: the pairing interactions for unconventional superconductors. *Rev.Mod.Phys.* **84** , 1383-1417.

[3]. Brommer P.E (2005), Spin Fluctuations, *Encyclopedia of Materials; Science and Technology*.

[4]. Sara A. Lopez-Paz, Sari D.P, Hillier A.D and Aliaro-Franco M.A (2021), Coexistence of magnetism and superconductivity in the Iron containing $FeSr_2YCu_2O_{7.57}$ cuprate as studies by µSR, *AIP Advances* **11**, 015011.

[5]. Lei Z, Jiyu F, Li L (2010), Critical properties of the 3D- Heisenberg ferromagnet $CdCr_2Se_4$, *Europhysics Letters*, **91** (5).

[6]. Moriya Toru (2006), Development of the theory of spin fluctuations and spin fluctuation-induced superconductivity, *Proceedings of the Japan Academy, Series B Physical and Biological Sciences*, **82** (1), 1-16.

[7]. Kung Y.F, Nowadnick A, Jia C.J, Johnston S, Moritz B, Scalletar T and Devereaux T.P(2015), Doping evolution of Spin and charge excitations in the Hubbard model, *Physical Review B*, **92**, 195108.

[8]. Nakitare M.W, Ayodo Y.K, Sakwa T.W, Ndinya B and Kibe E. H. (2017). Doped Mott Insulators within the Strong Coupling Regime. *International Journal of Recent Engineering Research and Development (IJRERD), 2*(7), 102-108.

[9]. Chubukov A.V , Schmalian J, and Pines D. (2008). A Spin Fluctuation Model for d-wave Superconductivity. doi:10.1007/978-3-540-73253-2 22

[10]. Yucel Yildirim (2007), Numerical Study of spin-fermion models Diluted magnetism semiconductor and High-Tc cuprates, College of Arts and Sciences, Florida State University.

[11]. Goswami Partha. (2013). A Theoretical Approach to Pseudogap and Superconducting transitions in hole-doped cuprates. Retrieved January 18, 2020, from https://dx.doi.org/10.1155/2013/210384

[12]. Mona Berciu and Sajeev John (2000), A Microscopic model for d-wave pairing in cuprates, *Physica B*, **296**, 143. doi:10.1016/s0921-4526(00)00792-4.

[13]. Lin Nan (2012), Cluster dynamical Dynamical Mean field theory: Applications to High-Tc Cuprates and to Quantum Chemistry, Ph.D Thesis, Colombia University.

[14]. Rice M.T, Yang Kai-Yu and Zhang C.F (2011), A Phenological Theory of the Anomolous Pseudogap Phase in underdoped cuprates, www.arXiv.1109.0632v1.

[15]. Maksimov G.E , Kulic L.M and Dolgov V.O (2010), Bosonic Spectral Function and the electron-phonon interaction in HTSC cuprates, https://doi.org/10.1155/2010/423725.

[16]. Harland M, Berberich T, Katonelson M and Lichtenstein A (2018), Plaquette Valence band theory of cuprate High-Temperature superconductivity, *Universal Journal of Physics and Applications*, **12** (4), 76-81.

[17]. Yanigasawa, T. (2019). Mechanism of High temperature superconductivity in orrelated-Electron Systems. Retrieved June 8, 2020, from https://doi.org/10.3390/condmat4020057

[18]. Dahm. T, Hinkov V, Borisenko. S.V, Kordyuk A.A, Buchner B, Scalapino D.J, Hanke W and Keimer B. (2009). Strength of the Spin-Fluctuation-mediated pairing interaction in a high-temperature superconductor. *Nature Physics*, 5, 217-221.

[19]. Liu Y, Lan Y and Feng S (2021), Peak structure in the self-energy of cuprate superconductors, *Physical Review B*, **103**, 024525.

[20]. Kuang L, Lan Y, Zhao H and Feng S (2015), High energy magnetic excitations in the cuprate superconductors, *International Journal of Modern Physics B*, **29**, Number 25 and 26, 1542001.

[21]. Natanel C.C , Kazuro S, Seiji Y and Sandro S. (2020). Phase Diagram of the two-dimensional Hubbard-Holstein model. *Communication Physics, 3*, Article number 80.

[22]. Lavanya C.U, Sankar I.V and Chatterjee A . (2017). Metallicity in a Holstein-Hubbard Chain at Half Filling with Gaussian Anharmonicity. *Scientific Reports, 7*, 3774.

[23]. Lee Patrick and Nagaosa Naomoto. (2003). Collective modes in the Superconducting ground states in the theory discription of the Cuprates. Physical Review B, 68, 024516.

[24]. Sahinur R and Satoshi N. (2018). Phase diagram of Hubbard model on 4-leg tube system at quarter filling. Retrieved May 15, 2018, from http://www.avXiv.1809.07282.

[25]. Lusamamba M. Simon. . (2019). The Energy, Entropy and Critical Temperature of a Square Lattice YBCO and LSCO Cuprates. *Journal of Multidisciplinary Engineering Science and Technology (JMEST), 6*(10), 10864-10866.

[26]. Nakitare M.W, Ayodo Y.K, Sakwa T.W, Ndinya B and Kibe E. H. (2017). Doped Mott Insulators within the Strong Coupling Regime. *International Journal of Recent Engineering Research and Development (IJRERD), 2*(7), 102-108.

[27]. Rapando B. W., Khanna K. M., Tonui J. K., Sakwa T. W., Muguro K. M., Kibe H., Ayodo Y. K., and Sarai A. (n.d.). The dipole mediated t-J model for high-Tc superconductivity. *International Journal of Physics and Mathematical Sciences, 5*(3), 32-37.

Simon Mwatulo Lusamamba, et. al. “Spin-Mediated Energy of Cuprate Superconductors.” *IOSR Journal of Applied Physics (IOSR-JAP)*, 13(3), 2021, pp. 10-14.