



The Diagonalized t-J Hamiltonian and the Thermodynamic Properties of High- T_c Superconductors

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Abstract: The Bogliubov transformation was used in this study to diagonalize the t-J model Hamiltonian yielding the quasi-particle Hamiltonian and the thermodynamic properties of high temperature superconductors. Formulae for ground state Energy E_0 , specific heat, c_v , and entropy, s of high temperature superconductors have been derived in the framework of the t-J model. Transition temperature for Lanthanum Strontium Copper Oxide (LSCO) in the t-J formalism is obtained $T_c = 102.5K$. Transition temperature for Yttrium Barium Copper Oxide (YBCO) in the t-J formalism is obtained $T_c = 111.8K$. Calculated T_c that is higher than the experimental value has been obtained for the LSCO and YBCO Cuprates. Highest heat capacity of the superconducting state in the t-J model is found to be $4.7 \times 10^{-3} eV/K$ while the highest entropy value is $3.15 \times 10^{-3} eV/K$ for high- T_c superconductors. The total energy of the system increases exponentially with the temperature.

Keywords: Bogliubov Transformation, t-J model Hamiltonian, Transition temperature, Superconducting State, Ground State Energy.

List of Symbols and Abbreviations Used

Abbreviation/ symbol	Name
\hbar	Reduced Planck's constant
BCS	Berdeen-Cooper-Schrieffer Theory
Bi2201	Bismuth-Strontium-Copper-Oxide
FT-PAV	Finite Temperature Projection After Variation
FT-VAP	Finite Temperature Variation After Projection
H_c	Critical magnetic field
Hg1223	Mercury-Barium-Calcium-Copper-Oxide
HTS	High temperature superconductors
J	Spin exchange energy
LSCO	Lanthanum-Strontium-Copper-Oxide
NCCO	Niodium-Cellenium- Copper Oxide
t	Electron hopping energy
T_c	Transition/Critical temperatu

t-J model	Model based on electron hopping and exchange energy
Tl2212	Thallium-Barium-Calcium-Copper-Oxide
U	On-site Coulomb energy
U_k, V_k	Transformation constants
YBCO	Yttrium-Barium-Copper-Oxide

INTRODUCTION

The problem of the nature of interactions between charge carriers and the elementary excitations which lead to superconductivity in the doped copper oxides can be studied in the two-dimensional Hubbard model, and its strong coupling limit, the t-J model [3, 13]. This model is generally assumed to be the simplest model possibly able to describe some essential features of these materials, an important feature being the metal-insulator transition on doping. The Hubbard model, based on the electron-electron interaction could explain superconductivity on a two-dimensional square lattice of copper oxide. It considered strong repulsive Coulombic interaction energy, U , on lattice sites and gave the Hamiltonian of the interacting electrons in terms of hopping energy matrix, t and electron creation and annihilation operators on neighbor sites, (i and j), $C_{i\sigma}^+$ and $C_{j\sigma}C_{j\sigma}$ respectively, and electron occupation number operators, n_i [9]. The Hamiltonian H_{Hub} , is given in equation 1;

$$H_{Hub} = -t \sum_{(i,j)} (C_{i\sigma}^+ C_{j\sigma} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

The purpose of the two-dimensional Hubbard model was to investigate whether the stripe states exist in the electron doped cuprate, Niodium Celenium Copper Oxide (NCCO) or the bilayer system such as $YBa_2Cu_3O_{6+y}$. Using the variational Monte Carlo method for the two dimensional $t-t'-t''$ Hubbard model, it was established that although the stripe states with the periodicity which were consistent with experiments for $La_{2-x}Sr_xCuO_4$ are stabilized in the case of $t'/t < 0$, the positive t'/t makes the stripe state unstable with the lowest energy state being the commensurate AF state [8]. This state is consistent with experiments on the electron doping system such as $Nd_{2-x}Ce_xCuO_4$. In this model, it was also shown that the stripe state was sensitive to the value of t'/t and the results indicated that the nesting condition was a critical factor to the stripe instability. However, this model does not give the nature of pairing mechanism that leads to the phenomenon of superconductivity. The physical properties of the superconducting state such as specific heat, thermal energy and entropy were not discussed. In this paper the physical properties of the superconducting state are discussed.

While working on the Hubbard model, Heisenberg found that when copper oxide is doped to half-filling level and the onsite Coulomb energy is increased to large values, the cuprate system becomes anti-ferromagnetic with neighboring electrons acquiring opposite spins; hence an electron would gain energy in hopping 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.

From Hubbard model, the Heisenberg model was developed. The Heisenberg Hamiltonian was expressed in terms of spin exchange integral, J, the electron spin operators in the neighboring sites, S_i and S_j , and the number operators, n_i and n_j as:

$$H_{Heisenberg} = J \sum_{(i,j)} (S_i S_j - \frac{n_i n_j}{4}) \quad (2)$$

Combining the Hubbard model and the Heisenberg model in the strong Coulomb repulsion or in the limit of large U resulted into the t - J model whose Hamiltonian is expressed in both the hopping integral t and spin transfer integral, J . The t - J model therefore, describes an anti-ferromagnetic system in which if in the initial and final states, alignment of electrons is such that they have like spins for closest neighbor electrons, both t and J will be zero, while opposite spin pairing will give rise to energy gain in the magnitude of $\pm \frac{J}{2}$ or $\pm(2t^2)/U$ [9].

The spin fluctuation of superconductivity was first proposed as an explanation of superconductivity in heavy fermions [7]. This model is based on short range Coulomb interaction leading to an exchange coupling $J \times S_i S_j$ between near- neighbor copper spins and strong spin fluctuations. The super-exchange constant is denoted by J . In cuprates it has an extremely high magnitude, $J \approx 125 \text{ meV}$. The underlying microscopic physics can be described by the t - J model. In this paper, we proceed to diagonalize the t - J model Hamiltonian in order to obtain the ground state energy of the quasi- particles and hence, the thermodynamic properties of the superconducting state.

Objectives

1. To determine the quasi-particle Hamiltonian.
2. To investigate and determine the thermodynamic properties of high temperature superconductors.

METHODOLOGY

Theoretical Derivations

The t - J Hamiltonian is given as in equation 2 [6];

$$H_{t-J} = \sum_{ij} J (S_i S_j - \frac{1}{4} n_i n_j) - \sum_{ij, \sigma} t_{ij} (C_{i\sigma}^+ C_{j\sigma} + H. C) \quad (3)$$

Here, transfer energy, $t_{ij} = t, t', t''$ for the nearest, second nearest, and third-nearest-neighbour pairs, respectively, and it is the electron transfer energy from i th location to the j th location, S_i and S_j are the electron spin operators in the i th and j th locations respectively, n_i and n_j are electron occupation number operators, J is the spin exchange energy while $H. C$ stands for the Hermitian conjugate of the electron creation operator, $C_{i\sigma}^+$ and annihilation operator, $C_{j\sigma}$. The effect of the strong Coulomb repulsion is represented by the fact that the electron operators $C_{i\sigma}^+$ and $C_{j\sigma}$ are the projected ones in which double occupation is forbidden. Thus the constraint for the operators is written as an inequality, given in equation 4;

$$\sum_{\sigma} C_{i\sigma}^+ C_{i\sigma} \leq 1 \quad (4)$$

This constraint can only be handled by the slave-boson method [2] by representing the electron operator as in equation 5;

$$C_{i\sigma}^+ = f_{i\sigma}^+ b_i + \epsilon_{\sigma\sigma'} f_{i\sigma'} d_i^+ \quad (5)$$

where $\epsilon_{\uparrow\downarrow} = -\epsilon_{\downarrow\uparrow} = 1$ is the anti-symmetric tensor and $f_{i\sigma}^+$ and $f_{i\sigma}$ are the fermion operators, b_i and d_i^+ , are the slave- boson operators. To produce all the algebra of the fermion operators, we impose another constraint such that;

$$f_{i\uparrow}^+ f_{i\uparrow} + f_{i\downarrow}^+ f_{i\downarrow} + b_i^+ b_i + d_i^+ d_i = 1 \quad (6)$$

The results in equation 6 show that there are four states per site such that b_i^+ , b_i correspond to the vacant state and d_i^+ , d_i correspond to double occupancy. Excluding the double occupancy by applying the Pauli Exclusion Principle Equation 5 simplifies to equation 7 given as;

$$c_{i\sigma}^+ = \not{f}_{i\sigma}^+ b_i \tag{7}$$

The Heisenberg exchange term written in terms of fermion operators is given in equation 8 [3];

$$S_i \cdot S_j = -\frac{1}{4} \not{f}_{i\sigma}^+ \not{f}_{j\sigma} \not{f}_{j\beta}^+ \not{f}_{i\beta} - \frac{1}{4} (\not{f}_{i\uparrow}^+ \not{f}_{j\downarrow}^+ - \not{f}_{i\downarrow}^+ \not{f}_{j\uparrow}^+) (\not{f}_{j\downarrow} \not{f}_{i\uparrow} - \not{f}_{j\uparrow} \not{f}_{i\downarrow}) + \frac{1}{4} (\not{f}_{i\sigma}^+ \not{f}_{i\sigma}) \tag{8}$$

The number operators n_i and n_j are given by equation 9 and 10;

$$n_i = (1 - b_i^+ b_i) \tag{9}$$

and

$$n_j = (1 - b_j^+ b_j) \tag{10}$$

Thus, the product of n_i and n_j yields to equation 11;

$$n_i n_j = (1 - b_i^+ b_i) (1 - b_j^+ b_j) \tag{11}$$

Substituting equation 7 and its Hermitian conjugate, equation 8 and 11 in equation 3, yields the t-J Hamiltonian given in equation 12;

$$H_{t-J} = \sum_{ij} J \left\{ -\frac{1}{4} \not{f}_{i\sigma}^+ \not{f}_{j\sigma} \not{f}_{j\beta}^+ \not{f}_{i\beta} - \frac{1}{4} (\not{f}_{i\uparrow}^+ \not{f}_{j\downarrow}^+ - \not{f}_{i\downarrow}^+ \not{f}_{j\uparrow}^+) (\not{f}_{j\downarrow} \not{f}_{i\uparrow} - \not{f}_{j\uparrow} \not{f}_{i\downarrow}) + \frac{1}{4} (\not{f}_{i\sigma}^+ \not{f}_{i\sigma}) - \frac{1}{4} (1 - b_i^+ b_i) (1 - b_j^+ b_j) \right\} - \sum_{ij,\sigma} t_{ij} (\not{f}_{i\sigma}^+ b_i \not{f}_{j\sigma} b_j^+ + \not{f}_{i\sigma} b_i^+ \not{f}_{j\sigma} b_j) \tag{12}$$

The Canonical Transformation

In order to obtain the quasi particles of the Hamiltonian given in equation 12, the Hamiltonian is diagonalized by performing a canonical transformation that will convert the old operators into new operators that obey the same commutation laws. The most convenient way to do this is by use of the Bogoliubov- Volatin transformation [5]. In the canonical transformation, new operators are defined as given in equation 13 -16;

(a) Electron Operators

Let the new operators, be defined in terms of the old operators, as;

$$i \quad \gamma_{i\sigma} = U_{i\sigma} \not{f}_{i\sigma} - V_{i\sigma} \not{f}_{i\sigma}^+, \text{ and } \gamma_{i\sigma}^+ = U_{i\sigma} \not{f}_{i\sigma}^+ + V_{i\sigma} \not{f}_{i\sigma} \tag{13}$$

The complex conjugates of the operators in equation 13 are;

$$\gamma_{i\sigma}^+ = U_{i\sigma} \mathfrak{f}_{i\sigma}^+ - V_{i\sigma} \mathfrak{f}_{i\sigma}' \quad \text{and} \quad \gamma_{i\sigma}' = U_{i\sigma} \mathfrak{f}_{i\sigma}' + V_{i\sigma} \mathfrak{f}_{i\sigma}^+ \quad (14)$$

$$\text{ii} \quad \gamma_{j\sigma} = U_{j\sigma} \mathfrak{f}_{j\sigma} - V_{j\sigma} \mathfrak{f}_{j\sigma}' \quad \text{and} \quad \gamma_{j\sigma}' = U_{j\sigma} \mathfrak{f}_{j\sigma}' + V_{j\sigma} \mathfrak{f}_{j\sigma}^+ \quad (15)$$

Their complex conjugates are;

$$\gamma_{j\sigma}^+ = U_{j\sigma} \mathfrak{f}_{j\sigma}^+ - V_{j\sigma} \mathfrak{f}_{j\sigma}' \quad \text{and} \quad \gamma_{j\sigma}'^+ = U_{j\sigma} \mathfrak{f}_{j\sigma}' + V_{j\sigma} \mathfrak{f}_{j\sigma}^+ \quad (16)$$

The constants $U_{(i,j\sigma)}$ and $V_{(i,j\sigma)}$ are the conversion constants [5]. A suitable choice of these constants facilitates the elimination the off-diagonal terms of the Hamiltonian. They are chosen to be real and positive constants and for fermions, they obey the condition in equation 17;

$$U_{(i,j\sigma)}^2 + V_{(i,j\sigma)}^2 = 1 \quad (17)$$

With this condition, the new and old operators obey the same fermion anti-commutation relations as given in equation 18 and 19.

$$\{\gamma_{(i,j\sigma)}, \gamma_{(i,j\sigma)'}\} = \{\gamma_{(i,j\sigma)}, \gamma_{-(i,j\sigma)}\} = \{\gamma_{(i,j\sigma)}^+, \gamma_{-(i,j\sigma)}^+\} = 0 \quad (18)$$

and

$$\{\gamma_{(i,j\sigma)}^+, \gamma_{(i,j\sigma)}\} = \{\gamma_{-(i,j\sigma)}^+, \gamma_{-(i,j\sigma)}\} = \delta_{(i,j\sigma)(i,j\sigma)'} = \begin{cases} 1, & (i,j\sigma) = (i,j\sigma)' \\ 0, & (i,j\sigma) \neq (i,j\sigma)' \end{cases} \quad (19)$$

(b) Boson operators

Let the new boson operators be defined in terms of the old operators as in equation 20

$$\mathfrak{b}_i = U_i b_i - V_i b_i^+ \quad (20)$$

The complex conjugate of the boson operator in equation 20 is now expressed as in equation 21;

$$\mathfrak{b}_i^+ = U_i b_i^+ - V_i b_i \quad (21)$$

Also, a new boson operator is defined in terms of the old operators as given in equation 22 and whose complex conjugate is given as complex conjugate 23.

$$\mathfrak{b}_j = U_j b_j - V_j b_j^+ \quad (22)$$

$$\mathfrak{b}_j^+ = U_j b_j^+ - V_j b_j \quad (23)$$

For this canonical transformation, the new and old boson operators obey the same commutation relations such that;

$$[\mathcal{b}_{(i,j)}^+, \mathcal{b}_{(i,j)}^+] = [\mathcal{b}_{(i,j)}, \mathcal{b}_{-(i,j)}] = [\mathcal{b}_{(i,j)}, \mathcal{b}_{(i,j)}] = 0 \quad (24)$$

and

$$[\mathcal{b}_{(i,j)}, \mathcal{b}_{(i,j)}^+] = [\mathcal{b}_{(i,j)}, \mathcal{b}_{-(i,j)}^+] = \delta_{(i,j)(i,j)} = \begin{cases} 0, & (i,j) \neq (i,j)' \\ 1, & (i,j) = (i,j)' \end{cases} \quad (25)$$

The constants U_k and V_k are real and for bosons, they obey the condition that;

$$U_{(i,j)}^2 - V_{(i,j)}^2 = 1 \quad (26)$$

On substituting the inverse transformation of the operators in equation 12, the t-J model Hamiltonian becomes;

$$\begin{aligned} H_{t-J} &= \sum_{ij} J \left\{ -\frac{1}{4} [(U_{i\sigma} \gamma_{i\sigma}^+ + V_{i\sigma} \gamma_{i\sigma}') (U_{j\sigma} \gamma_{j\sigma} + V_{j\sigma} \gamma_{j\sigma}') (U_{j\sigma} \gamma_{j\sigma}^+ - V_{j\sigma} \gamma_{j\sigma}') (U_{i\sigma} \gamma_{i\sigma}' - V_{i\sigma} \gamma_{i\sigma}^+)] \right. \\ &\quad - \frac{1}{4} [(U_{i\sigma} \gamma_{i\sigma}^+ + V_{i\sigma} \gamma_{i\sigma}') (U_{j\sigma} \gamma_{j\sigma}^+ - V_{j\sigma} \gamma_{j\sigma}') \\ &\quad - (U_{i\sigma} \gamma_{i\sigma}' - V_{i\sigma} \gamma_{i\sigma}) (U_{j\sigma} \gamma_{j\sigma} + V_{j\sigma} \gamma_{j\sigma}')] [(U_{j\sigma} \gamma_{j\sigma}' - V_{j\sigma} \gamma_{j\sigma}^+) (U_{j\sigma} \gamma_{j\sigma} + V_{j\sigma} \gamma_{j\sigma}') \\ &\quad - (U_{j\sigma} \gamma_{j\sigma} + V_{j\sigma} \gamma_{j\sigma}') (U_{j\sigma} \gamma_{j\sigma}' - V_{j\sigma} \gamma_{j\sigma}^+)] + \frac{1}{4} [(U_{i\sigma} \gamma_{i\sigma}^+ + V_{i\sigma} \gamma_{i\sigma}') (U_{i\sigma} \gamma_{i\sigma} + V_{i\sigma} \gamma_{i\sigma}') \\ &\quad - \frac{1}{4} [1 - (U_i \mathcal{b}_i^+ + V_i \mathcal{b}_i) (U_i \mathcal{b}_i + V_i \mathcal{b}_i^+)] [1 - (U_j \mathcal{b}_j^+ + V_j \mathcal{b}_j) (U_j \mathcal{b}_j + V_j \mathcal{b}_j^+)] \left. \right\} \\ &\quad - \sum_{ij,\sigma} t_{ij} \left\{ (U_{i\sigma} \gamma_{i\sigma}^+ + V_{i\sigma} \gamma_{i\sigma}') (U_i \mathcal{b}_i + V_i \mathcal{b}_i^+) (U_{j\sigma} \gamma_{j\sigma} + V_{j\sigma} \gamma_{j\sigma}') (U_j \mathcal{b}_j^+ + V_j \mathcal{b}_j) \right. \\ &\quad + (U_{i\sigma} \gamma_{i\sigma} + V_{i\sigma} \gamma_{i\sigma}') (U_i \mathcal{b}_i^+ + V_i \mathcal{b}_i) (U_{j\sigma} \gamma_{j\sigma}^+ + V_{j\sigma} \gamma_{j\sigma}') (U_j \mathcal{b}_j \\ &\quad \left. + V_j \mathcal{b}_j^+) \right\} \end{aligned} \quad (27)$$

By considering the particle spin up state as \mathbf{k} and spin down as $-\mathbf{k}$, then the scattered particle spin states will be represented by \mathbf{k}' and $-\mathbf{k}'$ for spin up and spin down, respectively. Rearranging terms in equation 27 and neglecting the higher order terms, number operators and off-diagonal terms, the diagonalized form of the t-J Hamiltonian becomes;

$$H_{diag} = \sum_{k,-k} J \left\{ -\frac{1}{4} + \frac{3}{4} V_k^2 - \frac{1}{2} V_k^4 - \frac{1}{2} U_k^2 V_k^2 \right\} - \sum_{kk'} t_{kk'} \left\{ U_k^2 V_k^2 \right\} \quad (28)$$

On diagonalization, we find that;

$$U_k = \sqrt{2} \quad \text{and} \quad V_k = 1 \quad (29)$$

RESULTS AND DISCUSSION

Numerical Calculations and Discussion

i. Superconducting energy for the t-J system

Substituting equation 29 in equation 28, the magnitude of the ground state energy of the system, becomes;

$$E_0 = (J + 4t) \tag{30}$$

The energy, E, of the system can be expressed as a function of temperature, T by multiplying the ground-state energy, E_0 , by the thermal activation factor, $e^{-\frac{\Delta E}{kT}}$ where k is Boltzmann's constant and ΔE is the energy gap [5]. The energy gap for high temperature superconductors is a very small quantity and it is generally 1% of the minimum energy of the system [5, 11]. Thus at any temperature T, the energy of the system is given as;

$$E = E_0 e^{-\frac{0.01E_0}{kT}} = E_0 e^{-\frac{E_0}{100kT}} \tag{31}$$

Substituting equation 30 in equation 31, the magnitude of energy of the system at any given temperature can be determined as;

$$E = (J + 4t) \cdot e^{-\left(\frac{J+4t}{100kT}\right)} \tag{32}$$

ii. The specific heat capacity for the t-J system

The specific heat capacity at constant volume of the system is obtained by determining the first derivative of the energy of the system with respect to temperature [5]. Hence, using equation 32, the magnitude of C_v can be calculated as in equation 33;

$$c_v = \frac{(J + 4t)^2}{100kT^2} \cdot e^{-\left(\frac{J+4t}{100kT}\right)} \tag{33}$$

iii. Entropy of the t-J system

Entropy s of the system is obtained by evaluating the integral given in equation 34 [4];

$$s = \int \frac{c_v dT}{T} \tag{34}$$

Where C_v is specific heat capacity at constant volume and T is the temperature of the system.

Thus the superconducting entropy by this model is given as;

$$s = \frac{(J + 4t)}{T} e^{-\left(\frac{J+4t}{100kT}\right)} - k \cdot e^{-\left(\frac{J+4t}{100kT}\right)} \tag{35}$$

iv. Transition temperature for the t-J system

Transition temperature of the superconducting state, T_c is calculated based on the condition given in equation 36 [4];

$$\left[\frac{\partial c}{\partial T} \right]_{T=T_c} = 0 \tag{36}$$

Evaluating the partial derivative in equation 36 yields;

$$T_c = \frac{(J + 4t)}{200k} \tag{37}$$

Numerical Evaluation of the Transition Temperature in the T-J Model

Substituting the values $J=0.13$ eV and $t=0.41$ eV for LSCO and $k= 8.63 \times 10^{-5}$ eV/K in equation 35, the numerical value of T_c for LSCO gives 102.5 K However, the experimental value of for LSCO is 38 K [1]. The t-J model thus predicts a critical temperature value for LSCO that is 2.7 times higher than the present experimental value. Substituting $J=0.17$ eV, $t=0.44$ eV for YBCO [12] in equation 35, the numerical value of $T_c=111.8$ K, which is higher than the current experimental value of 90 K [10] by 21.8 K. By applying the same calculations, then the room temperature superconductivity ($T_c=300$ K) in LSCO is possible if the transfer energy is 1.262 eV and 1.252 eV in YBCO.

Since the lowest ever achieved experimental exchange energy for high- T_c superconductors is $J=0.13$ eV, it is held constant and used together with experimental T_c values for various high- T_c superconductors to calculate the appropriate transfer energies of the t-J system. The results are summarized in the Table 1.0.

Table 1.0: A summary of transfer energy values of the t-J system for various high- T_c superconducting cuprates

Cuprate	Symbol	T_c (K)	Transfer energy, t (eV)
$Bi_2Sr_2CuO_6$	Bi2201	~12	0.0193
$Nd_{2-x}Ce_xCuO_4$	NCCO	24	0.0711
$YBa_2Cu_3O_{6+x}$	YBCO	93	0.3688
$Bi_2Sr_2CaCu_2O_8$	Bi2212	95	0.3774
$Tl_2Ba_2CuO_6$	Tl2201	95	0.3774
$HgBa_2CuO_4$	Hg1201	98	0.3904
$Tl_2Ba_2CaCu_2O_8$	Tl2212	105	0.4206
$Bi_2Sr_2Ca_2Cu_3O_{10}$	Bi2223	110	0.4422
$Tl_2Ba_2Ca_2Cu_3O_{10}$	Tl2223	125	0.5069
$HgBa_2CaCu_2O_8$	Hg1212	128	0.5241
$TlBa_2Ca_2Cu_4O_{11}$	Tl1224	128	0.5198
$HgBa_2Ca_2Cu_3O_{10}$	Hg1223	135	0.5500

Two very important observations can be made from Table 1.0. First, it is observed that using the t-J model, the current critical temperature values of the various high- T_c superconducting cuprates can be achieved at transfer energy lower than the current experimental values. A good example is YBCO whose experimental transfer energy of 0.44 eV has been lowered to 0.3688 eV. This is a 19.3 % decrease. Secondly, the critical temperature increases with increase in transfer energy for high- T_c superconductors. It is, therefore, possible

to achieve higher T_c by increasing the value for t . This Transfer energy, t can be increased by increasing onsite Coulombic repulsion energy U since $J = \frac{2t^2}{U}$ [9]. The challenge experienced in this approach is that for a given superconductor, U is increased by increasing charge carriers on a centre and these charges can only be increased to a certain maximum value beyond which stability will not be sustained. The second challenge is that for t-J system, the experimental ratio $\frac{J}{t}$ should be equal to a third. However, this can be overcome by increasing J proportionately.

Numerical Values of C_v

Using the experimental values $J=0.13\text{eV}$, $t=0.41\text{eV}$ for LSCO, $J=0.17\text{eV}$, $t=0.44\text{eV}$ for YBCO, the calculated value of c_v is $6.65 \times 10^{-3} \text{eV/K}$ for LSCO using $T=T_c=102.5$. Similarly, for YBCO, $c_v = 5.28 \times 10^{-3} \text{eV/K}$ at $T=T_c=111.8$ K. In the derivation of ground state energy formula, all terms in the Hamiltonian were allowed to vanish and remained with the quasi particle excitation creation terms so that only pairs of quasi particles could be excited. The minimum energy required to create such excitations is the exponential 2Δ [5]. Thus, the heat capacity drops with increase in the energy which leads to the creation of quasi particles. The variation of specific heat with temperature is shown in Figure 1.

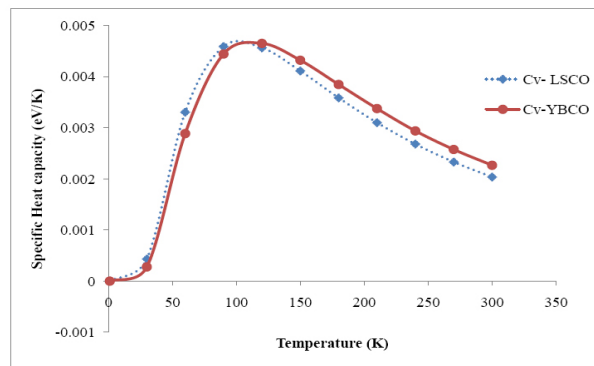


Fig1. Variation of specific heat with temperature

Numerical Entropy of the t-J

The t-J model value of entropy at $T=T_c=102.5$ K for LSCO was calculated as $3.308 \times 10^{-3} \text{eV/K}$ and $2.58 \times 10^{-3} \text{eV/K}$ for YBCO at $T=T_c=111.8$ K. It was established that Entropy varied with temperature as shown in Figure 2.

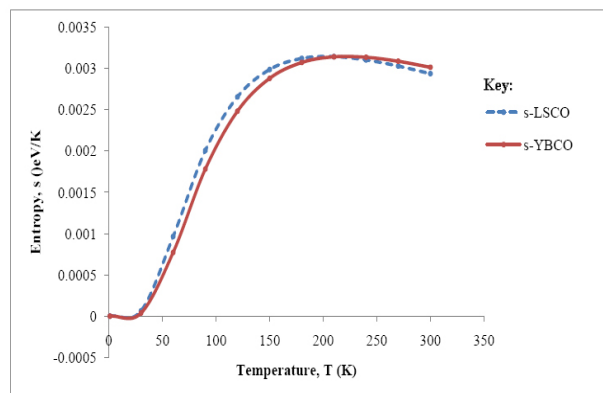


Fig2. Variation of entropy with temperature for the t-J model.

The results shown in Figure 2 illustrate an exponential growth of entropy with temperature for both LSCO and YBCO. With small variation, the maximum entropy for LSCO and YBCO is approximately 3.13×10^{-3} eV/K. At maximum entropy, critical temperature of LSCO is $T_c = 200$ K and that of YBCO is $T_c = 220$ K. It was also noted that the rate of increase of entropy with temperature of the system for LSCO was higher than that of YBCO. High- T_c superconductivity requires low entropy hence YBCO is better in building superconductors that can work at room temperature.

Thermodynamic properties of small superconductors involving application of the Finite Temperature Variation-After-Projection (FT-VAP) technique in minimizing free energy of superconducting state established that the entropy of the system is given as $s = -k_B \sum_i D_i^N \ln D_i^N$, where k_B is Boltzmann constant and D_i^N are the eigenvalues of the statistical operator in the Fock space composed by all the many body configurations with N particles. The variation of entropy with temperature graph was a smooth curve showing an exponential decrease of entropy with temperature from a maximum value of 0.125 eV/K. The trend of the graph is in agreement with t-J. The maximum value of entropy in the FT-VAP theory is lower than the corresponding value of the t-J system as expected since the FT-VAP theory is dealing with very low temperatures (0 K-5 K).

CONCLUSION

In this work, t-J model Hamiltonian was diagonalized using Bogliubov-Volatin transformation and the quasi-particle ground state energy obtained. From the ground state energy, thermodynamic properties of high- T_c superconductors, namely, energy, heat capacity, entropy and critical temperature have been determined. It is revealed that the current experimental T_c values can be achieved at lower transfer energy, t . Additionally, T_c as a function of transfer energy, t , can be raised by raising t . The results obtained for C_v and S are in fine agreement with the Finite Temperature- Variation After Projection (FT-VAP) study of thermodynamic properties of small superconductors. The t-J model predicts higher transition temperature in both electron-doped and hole-doped superconducting cuprates. The t-J model, being a model that captures strong electronic correlations in HTS predicts the possibility of achieving more than double the experimental value of T_c for the electron-doped LSCO.

ACKNOWLEDGMENT

Our sincere gratitude goes to Masinde Muliro University of Science and Technology and the University of Eldoret for granting us conducive environment under which this research was conducted.

REFERENCES

- [1] Andrei, M. (2004). Room-Temperature superconductivity, Cambridge International Sciences Publishing, 7 Meadow Walk, Great Abington, Cambridge, U.K
- [2] Barnes, S. E. and Maekawa, S. (1976). A Jordan- Wigner transformation for the t-J and Hubbard models with holes. J. Phys.F: Met.Phys. 6. P1375.
- [3] Baskaran, G., Zou, Z. and Anderson, P. W. (1987). The resonating valence bond state and high- T_c superconductivity- A mean field theory. Solid State Comm. 63. Pp 973-976.
- [4] Khanna, K. M and Kirui, M. S. K. (2002). Anharmonic apical oxygen vibration in high- T_c superconductors. Indian Journal of Pure & Applied Physics. 40, 887-895.
- [5] Khanna, K. M. (2008). Superconductivity, ISBN: 9966-854-48-7, Moi University Press, Moi University Eldoret, Kenya page. Pp 26-37.

- [6] Lee, P. A. and Nagaosa, N. (2003). Collective modes in the superconducting ground states in the gauge theory description of the cuprates, *Physical Review B*. 68. Pp 1 -19.
- [7] Miyake, K., Schmitz-Rink, S. and Varma, C.M. (1986). Spin fluctuation mediated even parity pairing in heavy fermion superconductors *Physical Review B*. 34(9). Pp 6554-6556.
- [8] Mitake, M. (2005). Effects of Higher Hopping. *Journal of Superconductivity*. 18. Pp 727-730.
- [9] Park, K. (2005). Quantum Anti-ferromagnetism and High TC Superconductivity; A close connection between the t-J model and the projected BCS Hamiltonian. *Physical Review Letters*. 95. 027001.
- [10] Puri, R. K. and Baabar, V. K. (2001). *Solid State Physics*. S Chard & Company Limited, Ramnagar New Delhi 1100s.
- [11] Rapando, B.W., Ayodo, Y. K., Sakwa, T.W., Khanna, K. M. and Sarai, A. (2013). Transition Temperature of Hybridized Cuprate Systems. *International Journal of Physics and Mathematical Sciences*. 3(2). Pp104-109.
- [12] Tsendin, K.D. and Denisov, D. V. (2001). Theoretical possibility of increasing of superconducting transition temperature in High Temperature superconductors by replacing Oxygen with Chalcogens. *Journal of Optoelectronics and Advanced Materials*. 3. Pp 549-552.
- [13] Zhang, F.C., Gros, C., Rice, T. M. and Shiba, H. (1988). A renormalized Hamiltonian approach to resonant valence bond wave function. *Superconductivity ScienceTechnology*.1. Pp 36-37.

Citation: Rapando B. W., Tonui J. K Khanna K. M, Mang'are P. A, *The Diagonalized T-J Hamiltonian and the Thermodynamic Properties of High-Tc Superconductors*, *American Research Journal of Physics*, Volume 2016; pp:1-11

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