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Research Article

THE DIPOLE MEDIATED t-J MODEL FOR HIGH-Tc SUPERCONDUCTIVITY

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ABSTRACT
The t-J model has been modified for a dipole mediated t-J Hamiltonian and used to study the thermodynamic properties of high-T_c superconductivity. In point of fact, we looked at the system energy, specific heat capacity, and entropy and transition temperature. The effective Hamiltonian of this model is obtained from the sum of the separately diagonalized t-J model and the electronic dipole interaction Hamiltonian. The contribution of dipole vibration energy to the t-J model energy in the superconducting state has been considered. We clearly envisage higher transition temperatures for enhanced onsite Coulomb repulsion energy within the operating limits of the system.

Keywords: *Dipole Mediated t-J Hamiltonian*

INTRODUCTION
The t-J model which describes strongly correlated electron systems may be used in the study of high temperature superconductivity in doped anti-ferromagnets (Park, 2005). The Hubbard model, as the beginning point of the t-J model, exclusively relied on the electron-electron interaction to explain superconductivity on a two-dimensional square lattice of copper oxide in view of the fact that the phonon mediation fell short of explaining the occurrence of superconductivity in high-T_c superconducting systems with large electron correlations. 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 gains energy on 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 (Andrei, 2004).
The Heisenberg Hamiltonian is 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:

$$H_{Heisenberg} = J\sum_{(i,j)}(S_i S_j - \frac{n_i n_j}{4}) \quad (1)$$

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 hoping integral t and spin exchange integral, J, and electron creation and annihilation operators in the neighboring sites (i,j) $C_{i\sigma}^{+}$ and $C_{j\sigma}$ respectively as:

$$H = \sum_{ij} J\left(S_i S_j - \frac{1}{4}n_i n_j\right) - \sum_{ij,\sigma} t_{ij}\left(C_{i\sigma}^{+} C_{j\sigma} + H.C\right) \quad (2)$$

The t-J model therefore, describes an anti-ferromagnetic system in which alignment of electrons in the initial and final states have like spins for closest neighbor electrons, thus 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 $\pm\frac{2t^2}{U}$. It is well known that the electron correlation is strong enough to produce a Mott insulation at half-filling. Furthermore, the one-band t-J model captures the essence of the low-energy electronic excitations of the cuprates.

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Coulomb interactions play an important role in superconducting process in the cuprates. A frequently used model for describing this is the three-band model. The model includes the Cu-O hopping integrals and the Coulomb interaction between two electrons on the Cu orbital. From this model, the t-J model can be written such that each site corresponds to a copper atom in the copper-oxide plane. In the undoped system, corresponding to all copper atoms being in the d^9 configurations, each site is occupied by one hole. In a hole-doped system the holes go primarily on to the O sites. Such an O hole forms a Zhang-Rise singlet with a Cu hole.

A Zhang-Rise singlet is described by an empty site in the t-J model.

As an essential generalization of the t-J model, the t-J_p-U model (Alexandrov, 2012) was introduced. The model discussed electron-electron and electron-phonon correlations providing a microscopic explanation of the high-Tc superconductivity phenomenon.

It showed that the inclusion of the residual on-site interaction $\widetilde{U}$ which was neglected in the t-J model drives the system to a Bose-Einstein Condensation / Berdeen-Cooper-Schrieffer cross over that reconciles the polaron-bipolaron theory of superconductivity with the observation of large Fermi surface in overdoped cuprate conductors.

The energy of the system, the specific heat C, the entropy S and the transition temperature T_C were calculated resulting to a comparative data.

Theoretical Formulation

The interaction Hamiltonian of a dipole moment P(R, t) at the location R interacting with an electron at position r is given by (Heebok and Sharma, 1995);

$$H_{eq} = \sum_{k\sigma k'\sigma' q' q\lambda} h_{k\sigma k'\sigma' q' q\lambda}\left(b_{q\lambda}^{+} + b_{q\lambda}\right)C_{k'\sigma'}^{+}C_{k\sigma'} \quad (3)$$

where $C_{k'\sigma'}^{+}$ and $C_{k\sigma'}$ are the creation and annihilation operators for an electron with wave vector k and spin σ while $b_{q\lambda}^{+}$ and $b_{q\lambda}$ are the creation and annihilation operators for a collective dipole quantum with wave vector q and polarization λ. The constant $h_{k\sigma k'\sigma' q' q\lambda}$ is defined as;

$$h_{k\sigma k'\sigma' q' q\lambda} = r|P_x(0)|\left[\frac{\hbar}{2I_k N\omega_\lambda(q)}\right]^{\frac{1}{2}}\left(\xi_{q\lambda}(k-k')\right)D_d^{kk'}\delta_{k-k',q+G} \quad (4)$$

where G is a reciprocal vector, $\omega_\lambda(q)$ is the frequency of vibration of a dipole with polarization index λ at a generalized location q, I_k is the moment of inertia of the oscillating dipole, $\xi_{q\lambda}$ is the λ^{th} component of the unit polarization vector ξ_q of the collective wave, N is the number of the oscillating dipoles in the crystal. $P(0)_x$ is the dipole moment in the x-direction at time t=0, i.e static state and $P = \propto E$ where $\propto$ is polarazability and E is the electric field. The dynamic matrix $D_d^{kk'}$ is defined as;

$$D_d^{kk'} = \int d^3r\, U_{k'\sigma'}(r)e^{-ik'r}\frac{e}{\epsilon|r-R|}U_{k\sigma}(r)e^{ikr} \quad (5)$$

where e is the electronic charge unit, ϵ is energy of an electron and $U_{k\sigma}(r)e^{ikr}$ is the Bloch state of the electron in the system. By considering equation (3), we diagonalized the t-j model and dipole Hamiltonians distinctively to get to get their sum as

$$H_d = \sum_{k,-k} J\left\{-\frac{1}{4}+\frac{3}{4}V_k^2 - \frac{1}{2}V_k^4 - \frac{1}{2}U_K^2V_k^2\right\} - \sum_{kk'} t_{kk'}\left\{2U_k^2V_k^2\right\} - \sum_{kk} h_{kk'}\left\{\mathrm{U_k^2V_k^2}\left(\mathrm{U_k^4 - V_k^4}\right)\right\} \quad (6)$$

Thermal Properties

Equation (6) is now used to study the thermodynamic properties of the material in question. The rigorous calculations let to the ground state energy of the t-J-d system as;

$$E_0 = \left(J + 4t_{kk'} + 6h_{kk'}\right) \quad (7)$$

To enable us look at how the energy of the system, E, is affected by temperature the thermal activation factor, $e^{-\frac{\Delta\in}{kT}}$, is introduced to the ground-state energy, E_0. On the thermal activation term, $\Delta\in$ corresponds to the energy gap which is approximated to $\Delta\in = \frac{E_0}{100}$. Thus;

$$E = \left(J + 4t_{kk'} + 6h_{kk'}\right).e^{-\left(\frac{\left(J+4t_{kk'}+6h_{kk'}\right)}{100kT}\right)} \quad (8)$$

The specific heat capacity at constant volume c_v and entropy of the system s were then determined in the conventional manner to give us respectively,

$$c_v = \frac{\left(J+4t_{kk'}+6h_{kk'}\right)^2}{100kT^2}.e^{-\left(\frac{\left(J+4t_{kk'}+6h_{kk'}\right)}{100kT}\right)} \quad (9)$$

$$s = \left[\frac{\left(J + 4t_{kk'} + 6h_{kk'}\right)}{T} - k\right].e^{-\left(\frac{\left(J+4t_{kk'}+6h_{kk'}\right)}{100kT}\right)} \quad (10)$$

At the transition temperature, it is expected that

$$\left(\frac{\partial C}{\partial T}\right)_{T_C} = 0 \quad (11)$$

The transition temperature of the system was then computed as;

$$T_c = \frac{\left(J + 4t_{kk'} + 6h_{kk'}\right)}{200k} \quad (12)$$

Equations (8) – (12) are basically inherent of the thermodynamics of the system/ materials under study.

RESULTS AND DISCUSSION

Using the values *J=0.13eV, t=0.41eV* for LSCO, *J=0.17eV, t=0.44eV* for YBCO in Eq. (33), the energy is found to vary with the temperature of the system as shown in the graph in figure 1.

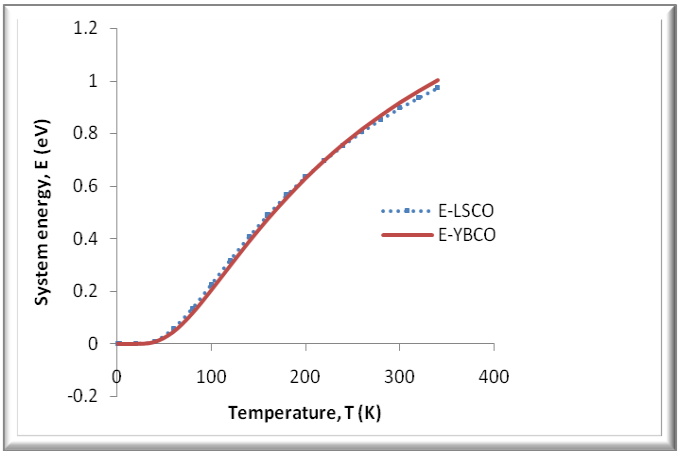

Figure 1: Variation of energy with temperature

For both LSCO and YBCO, the t-J-d system exhibits an exponential increase in the energy of the system as the temperature increases approaching a certain constant value dependent on type of the superconductor. The rate of increase of energy with temperature for LSCO is lower than that of YBCO in the temperature range of 0 K-220 K. However, at high temperatures approaching room temperature (T>220 K), the trend is reversed with YBCO showing a lower rate of change of system energy. High-T_c superconductivity, being a low-energy process requires that the system's energy should be kept as low as possible. Thus YBCO would be a better candidate for the exploration of a room-temperature superconductor. Danilo and Denis (2012) used variational theory applied to low temperature small systems of particles and had quite similar elucidation only that our case can be biased to large systems.

The known T_c values (Andrei, 2004) for various high-temperature superconducting cuprates was used to generate the corresponding transfer energies as shown in the table 1.0.

Table 1.0: Transfer energy values of the t-J-d system for various high-T_c superconducting cuprates

Cuprate	Abbreviation	T_c (K)	Transfer energy, t (eV)
$Bi_2Sr_2CuO_6$	Bi2201	~12	0.0131
$Nd_{2-x}Ce_xCuO_4$	NCCO	24	0.0649
$YBa_2Cu_3O_{6+x}$	YBCO	93	0.3626
$Bi_2Sr_2CaCu_2O_8$	Bi2212	95	0.3712
$Tl_2Ba_2CuO_6$	Tl2201	95	0.3713
$HgBa_2CuO_4$	Hg1201	98	0.3842
$Tl_2Ba_2CaCu_2O_8$	Tl2212	105	0.4144
$Bi_2Sr_2Ca_2Cu_3O_{10}$	Bi2223	110	0.4360
$Tl_2Ba_2Ca_2Cu_3O_{10}$	Tl2223	125	0.5001
$HgBa_2CaCu_2O_8$	Hg1212	128	0.5136
$TlBa_2Ca_2Cu_4O_{11}$	Tl1224	128	0.5136
$HgBa_2Ca_2Cu_3O_{10}$	Hg1223	135	0.5439

The variation of critical temperature of the superconducting cuprates with transfer energy is clearly a linear relationship as shown in figure 2. We clearly envisage higher transition temperatures for enhanced onsite Coulomb repulsion energy within the operating limits of the system (Jakub, 2011).

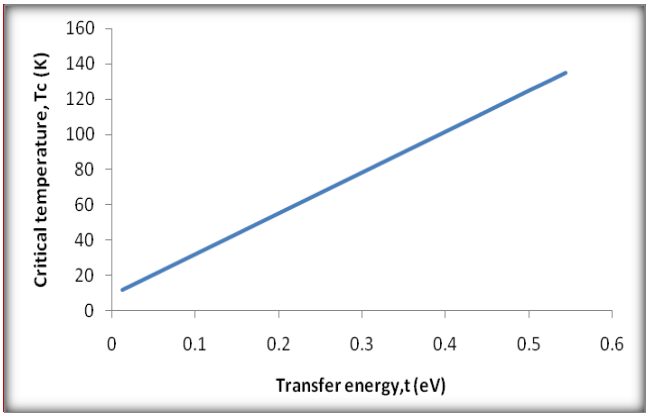

Figure 2: Variation of critical temperature with transfer energy.

For both LSCO and YBCO, the heat capacity is observed to drop exponentially with temperature from a given peak value which is the same for both LSCO and YBCO (regardless of the value of t) as shown in figure 3.

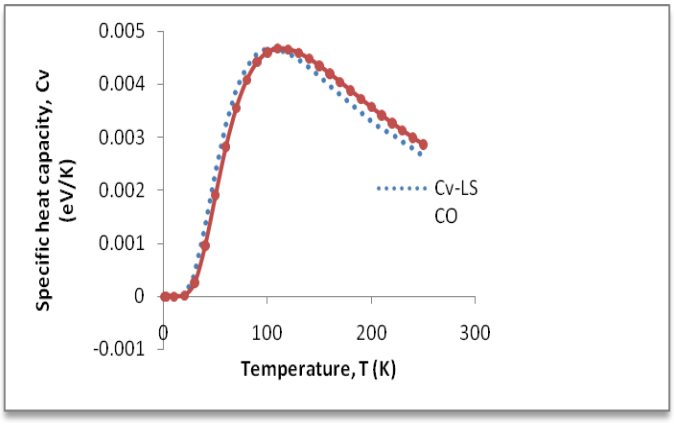

Figure 3: Variation of specific heat capacity with temperature

The peak, which is at $4.7\times10^{-3}eV/K$, is reminiscent if at transition point. Using the J and t values of LSCO and the calculated $h_{kk'}=0.0041139$ our T_c value for LSCO is projected at 103.98 K which is higher than a similar projection done on a t-J system (102.5 K) while the experimental value is at 38 K (Andrei, 2004). A similar projection for YBCO is 113.2 K on the basis of our work which nearly concurs with that of the t-J model (111.8 K). For $Bi_2Sr_2CuO_6$ whose first neighbor hoping energy is t=0.27 eV (Jakub, 2011), T_c for the t-J-d model is projected to be 71.5 K compared to the experimental value of 12 K implying that our model seem to assume a lower transfer/ hoping energy for cuprates as a prerequisite for higher critical temperatures.

Clearly, T_c for LSCO is approximately 100 K which is higher than the experimental value of 38 K (Andrei, 2004). This value is approximately equal to the calculated value of 102.5 K. The graph of YBCO gives T_c= 110 K which is also approximately equal to the calculated value of 111.8 K. In principle, this work is in fine agreement with that of Khanna and Kirui (2002) for the variation of heat capacity with temperature for the cuprates $Tl_2Ba_2Ca_2Cu_3O_{10}$ and $YBa_2Cu_3O_{7-\delta}$. In both cases heat capacity drops exponentially from a peak value and vanishes at T=0 K. In their study on anharmonic apical oxygen vibration in high-T_c superconductors, the peak of the graph gives T_c= 255 K for $YBa_2Cu_3O_{7-\delta}$ which is far above the experimental value, and is a fairly big shift from our data. We harmoniously rate this findings with that of Volya *et al.*, (2001) who applied the finite temperature BCS (FT-BCS) approximations in the diagonalization of the quasi- particle pairing Hamiltonian for a small system of particles, N=10 particles.

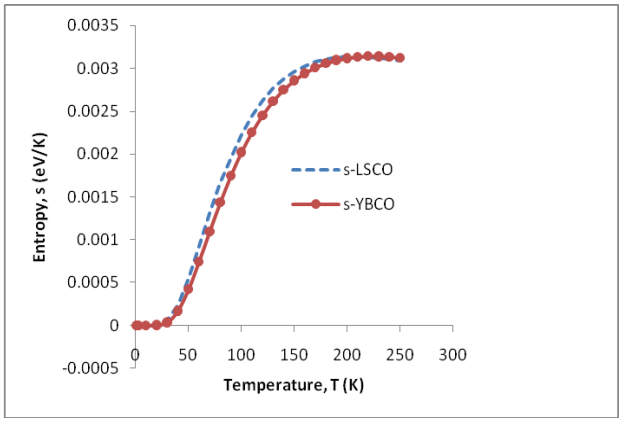

Figure 4: Variation of entropy with temperature

At maximum entropy, the critical temperature of LSCO is projected at T_c= 200 K while that of YBCO is at T_c= 220 K. We also note that the rate of increase of entropy with temperature of the system for LSCO is higher than that of YBCO. The maximum entropy of both LSCO and YBCO is found to be 3.15×10^{-3} eV/K. It is clear from our model that the entropy at the plateau, is common for both systems and is unyielding to the variation of the exchange energy.

Conclusion

In this study, we have basically modified the t-J model and used to study the thermodynamic properties of both LSCO and YBCO materials. The effective Hamiltonian of was obtained from the sum of the separately diagonalized t-J model and the electronic dipole interaction Hamiltonian resulting to what we are referring to as the t-J-d model. The contribution of dipole vibration energy to the t-J model in the superconducting state was been considered. Calculations done in this perspective gave the ground state energy of LSCO as 1.794eV, which is higher than both the t-J system (E_o =1.774eV). The ground state energy of YBCO was obtained as 1.9547eV. It is also higher than the t-J energy of 1.89 eV. Notably, the transfer energy in the t-J-d model is found to be lower than that of the t-J model. The analysis of heat capacity and entropy variation with temperature reveals exponential drop of both quantities with rise in temperature. This is a conventional observation. It would be interesting for one to look at the effect of the on-site Coulomb energy U, which may give more insight in the study of strong coupling when U>>t in

the Heisenberg model and weak coupling when U=0 eV. This on-site Coulomb energy may effectively reduce the transfer energy.

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