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The Energy, Entropy and Critical Temperature Of A Square Lattice YBCO and LSCO Cuprates

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***Abstract*— The thermodynamics of the quantum Heisenberg antiferromagnet on a square lattice of hole doped Yttrium Barium Copper Oxide YBa_2CuO_7 (YBCO) and Lanthanum Strontium Copper Oxide $La_{2-x}Sr_xCuO_4$ (LSCO) is revisited through a linearized spin- theory which is well defined at any temperature. We re-examine in details the temperature dependence of the internal energy, the entropy and the critical temperature. Most conclusions of the thermodynamics in previous studies can be reproduced in our linearized spin- theory. It was seen that the maximum entropy for YBCO and LSCO was approximately 0.003139 eV/K and 0.003153 eV/K respectively.**

Keywords—Entropy, spin, antiferromagnetic

I. Introduction

The spin-1/2 Heisenberg antiferromagnet on the square lattice is associated with high-temperature superconductivity [1].The undoped parent compounds of high-$_{Tc}$ cuprate superconductors are antiferromagnetic Mott insulators. With carrier doping the antiferromagnetism disappears and a superconducting state with a high transition temperature is realized. Antiferromagnetic (AF) correlations however remain even in the superconducting state and the understanding of magnetic properties has been widely recognized as a major issue in the theory of high-*Tc* cuprates [2]. The study of cuprates has received enormous advances in theories of strongly correlated electron systems, and in experimental techniques, particularly angle-resolved photoemission (ARPES) and scanning tunneling microscopy (STM) [3].This area is however with contradictions as there is no accepted theory that explains superconductivity in cuprates [4]. The lanthanum family of high-T_c's was the first family of materials to be discovered, by Bednorz and Muller in 1986 [5]. The discovery of YBCO followed that of LSCO within a year. YBCO was the first material to break the 77 K (liquid nitrogen) temperature boundary. The optimal T_c is now 93 K. YBCO has been the most highly studied because it is the cleanest and most ordered crystal. Studies of YBCO is quite interesting because there are two CuO planes: the square plane and the chain plane. By analogy with the other HTSC families, it is thought that the superconductivity originates in the square plane, but it is hard to isolate the behaviors of the planes [6].

One of the challenge of BCS theory is that it could not explain superconductivity above 34*K*. Properties such as the isotope effect, coherence length, high transition temperatures, electric and magnetic anisotropies could not be explained by the BCS theory. On the theoretical perspective, different models have been advanced to study high temperature superconductivity in cuprates; the Hubbard model which is solvable in one dimension under any repulsive non-zero interaction has been extensively used [7].

Cuprate based high temperature superconductors have a wide applications in the field of Bio-magnetism, electronics and even commercial power. With this in mind, a variety of numerical techniques have been spawned to study this regime, including exact Diagonalization (limited to small clusters), quantum Monte Carlo and its derivatives (variational and fixed node approximations to get around the issue of negative probabilities in fermion simulations), dynamical mean field theory(DMFT) [8].

A study of superconducting instabilities of the fermions in the presence of weak electron-electron interactions at zero chemical potential has been done, this study did not consider the energy of interaction, entropy as well as specific heat capacity. The research is shifting to the nature of unconventional symmetry of the superconducting order parameter [9] because the microscopic mechanism for phase transition has not been determined in HTS, yet light to unearth superconductivity points at electronic and physical structure of pseudogap [10].

In this research work , the internal energy, E, entropy, S and the Critical Temperature of a hole doped square lattice cuprates are determined. The cuprates YBa_2CuO_7 (Y123) and La_{2-x} Sr_xCuO4 (LSCO) are studied using Bogoliubov-Valatin transformation technique.

MODEL AND APPROACH

In Mott insulators, magnetic interactions arise from virtual charge hopping back and forth between two neighboring sites. The charge transfer processes are spin independent, which means that the total spin on a given bond is conserved. The effective spin Hamiltonian can thus be written as an inner product of the two spins; i.e. the interaction is isotropic.

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

where J spin exchange integral, S_i and S_j are the electron spin operators in the neighboring sites.

Equation (1) is now written in fermion operators as [11],

$$H_{Heinsberg} = J\sum_{ij} -\frac{1}{4} f^{+}_{i\sigma} f_{j\sigma} f^{+}_{j\beta} f_{i\beta} - \frac{1}{4}\left(f^{+}_{i\uparrow}\ f^{+}_{j\downarrow} - f^{+}_{i\downarrow} f^{+}_{j\uparrow}\right)\left(f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow}\right) + \frac{1}{4}\left(f^{+}_{i\sigma} f_{i\sigma}\right) \quad (2)$$

This Hamiltonian is then diagonalized by fermionic canonical transformations resulting into ground state energy of the system as,

$$E_0 = (J) \quad (3)$$

It ought to be that at high temperatures most of the electrons are thermally excited to higher energy states and thus, all the occupation numbers are equal to zero and the coefficients of the off diagonal terms gives

$$U_k = \sqrt{2} \quad \text{and } V_k = 1 \quad (4)$$

Inorder to introduce temperature dependence and the system's properties, the ground-state energy, E_0 is multiplied by the thermal activation factor, $e^{-\frac{\Delta\epsilon}{kT}}$, where k is Boltzmann's constant and $\Delta\epsilon$ is the energy gap. The energy gap is normally too small hence $\Delta\epsilon = 0.01E_0$. So at any temperature T, the energy of the system is given as [7][11];

$$E = E_0 e^{-\frac{0.01E_0}{kT}} = E_0 e^{-\frac{E_0}{100kT}} \quad (5)$$

The entropy of the system was found to be

$$S = \left(\frac{J}{T}\right) e^{-\left(\frac{J}{100kT}\right)} \quad (6)$$

By finding the second derivative and equating the result to zero the expression of the energy of the system, we obtain the transition temperature as;

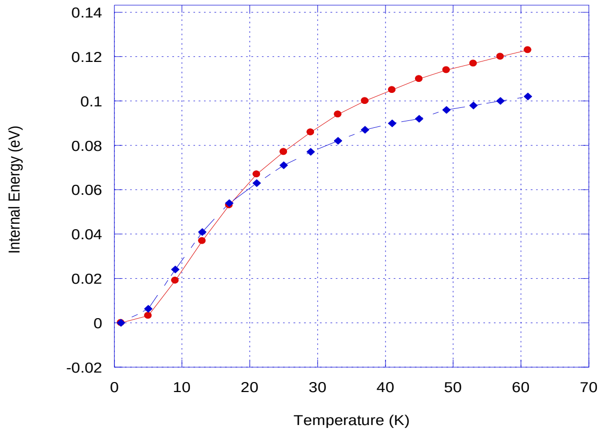
$$T_C = \frac{J}{200k} \quad (7)$$

RESULTS AND DISCUSSIONS

I. Evaluation of Internal energy

The results for hole-doped cuprates are shown in figure 1. The curves for YBCO (Red in colour) and LSCO (blue in colour), show a similar behavior which is in agreement with other theoretical findings [7] [12]. Quantitatively however, LSCO has higher energy than YBCO up to a temperature of ≈18K where both have same energy (0.055 eV). Perhaps, this energy could be an indication of the transition point from the superconducting state to the normal state. However, at temperatures approaching room temperature (T>18 K), the trend is reversed with YBCO showing a lower rate of change of system energy. The spin exchange integral (J) corresponding to YBCO and LSCO are 0.17 eV and 0.13 eV respectively. Hence the displayed results are a manifestation that superconductors with higher spin exchange integral undergo a high temperature rate of change of energy and the converse is true for those with lower spin exchange integral. Based on these findings, one can argue that YBCO would be a better candidate for the construction of a room-temperature superconductor compared to LSCO since high- T_C superconductivity is a low-energy process which demands that the system energy should be kept as low as possible

Figure 1:Varriation of internal Energy with Temperature



II. Evaluation of Entropy

The qualitative features of the observed cuprate entropy are reproduced using our model for hole doped cuprate [11], [12], and [13]. An exponential growth of entropy for both cases is noted at lower temperatures as in figure 2. The entropy curves concurs with the ones obtained by [14] while studying low temperature statistical thermodynamics of binary Bose-Fermi system. The maximum entropy for YBCO (Red curve) and LSCO (Blue Curve) is approximately 0.003139 eV/K and 0.003153 eV/K respectively. It has been shown clearly from Figure 2 that the rate of increase of entropy with temperature of the system is higher for LSCO compared to that of YBCO and hence YBCO is a better candidate material for High- TC superconductivity due to its lower entropy value. The transition temperature corresponding to the peak entropy for YBCO is T_C = 23 K and that of LSCO is T_C = 14K. From a thermodynamic point of view, the superconducting (SC) phase appears below the T_C because the free energy of the SC phase becomes less than the free energy of the normal phase for all temperatures below T_C [14]. Our value for entropy is in faithful conformity with other theoretical studies as reported by [7], [11] and [13].

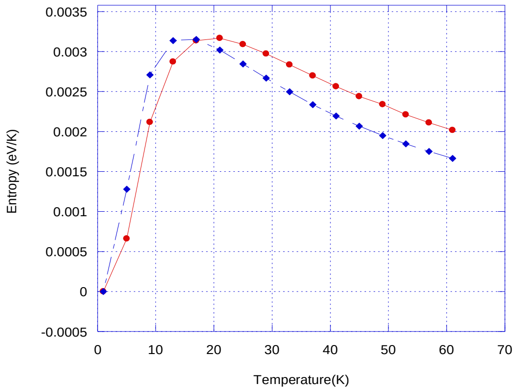


Figure 2:Varriation of Entropy with Temperature

CONCLUSIONS

The Heinsberg square lattice model was modified and diagonalized using BVT. The internal energy , entropy and the transition temperature from the diagonalized Hamiltonian were studied. Therefore, superconductivity is a low energy process and hence, YBCO is projected to be the likely suitable material for the construction of room temperature superconductors

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