Superconducting Transition Temperature within the Modified Bose-Fermi-Hubbard Model

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Abstract: - Determining the conduction mechanism that would raise the T_C of cuprate high temperature superconductors remains a puzzle. Here, we modify the existing Bose-Fermi-Hubbard model, diagonalize it using Bogoliubov-Valatin Transformation in order to determine the Transitional temperature, T_C of hole doped-($YBa_2Cu_3O_7$ and $La_{2-x}Sr_xCuO_4$ & electron-doped-($Nd_{2-x}Ce_xCuO_4$and $Pr_{2-x}Ce_xCuO_4$) cuprates. Our model predicts enhanced T_C values and hence it lays a very good platform in the study of high-T_C superconductivity.

Key Words: — ***Bose-Fermi-Hubbard model, Transitional temperature.***

I. INTRODUCTION

A sudden loss of electrical resistance to the flow of DC current in mercury near 4.2 K [1] marked the discovery of superconductivity. Zero resistivity and perfect diamagnetism are the main fundamentals to superconductivity [2]. The two properties i.e zero resistance and Meissner effect account for various applications of superconductors ranging from loss-less transmission lines, more efficient energy production, computers with reduced size and power consumption, very strong magnets, levitating trains to medical diagnostics etc. However, for a very long time after the discovery [1], the practical applications could not be realized mainly because superconductivity appeared to be a very low temperature phenomenon and the materials had to be cooled to below liquid Helium temperature, which is expensive as well as difficult to handle [3]. The BCS theory envisages an attractive interaction between electrons mediated by phonons resulting in the formation of the so called Cooper pairs [4,5]. The electrons in these pair states are no longer required to obey the Fermi-Dirac Statistics but instead the cooper pairs undergo a form of Bose-Einstein condensation, which is associated with superfluidity. The formation of the electron pair condensate gives rise to the rigidity of the superconducting wave function [6]. The theory was very successful, making many predictions that were quickly confirmed by experiment [7].

The BCS theory was further validated by the flux quantization measurement and Josephson Effect both of which suggested that super-currents involve pair of electrons. However, the superconductors that fit in the BCS theory have low TC which greatly limits their practical applications. The discovery of superconductivity in the cuprate oxides [8] challenged the BCS theory on many fronts such as isotope shift, short coherence length, high transition temperatures, electric and magnetic anisotropies etc., which were notably different from conventional superconductors.

One of the central issues about the cuprates is what determines the enhancement of TC of a specific system. The answer to this question lies in the pairing mechanisms. Finding a suitable mechanism that would enhance the TC is apparently a key step in solving high-TC superconductivity. Understanding the mechanisms that drive Cooper pair formation and condensation of high-temperature superconductivity from electron matter remains a challenge [9]. Spin fluctuation mechanism (where pairs are bound because of magnetic interactions between the electrons' spins) has been tried with little success. Superconducting currents in cuprates are carried by pairs of holes or electrons similar to that of BCS superconductors. However, a viable description of the pairing interaction is yet to be found [10]. The nature of the electron-boson interaction in high-TC cuprate superconductors remains unresolved issue [11] due to incomplete comprehension of the electronic correlation that leads to the pseudogap formation ([12]. The Bose-Hubbard and Fermi-Hubbard models are an improvement on the original Hubbard model in that they contain the chemical potential term which controls the filling of the band or regulates the system density. Consequently, while the Bose-Hubbard

Manuscript revised June 25, 2021; accepted June 26, 2021.
Date of publication June 27, 2021.
This paper available online at www.ijprse.com
ISSN (Online): 2582-7898

model [13] takes care of the repulsive on-site interaction energy, Fermi-Hubbard model [14] contains attractive interaction energy, U in addition to their respective hopping terms. Thus, neither the Bose-Hubbard model nor the Fermi-Hubbard model can singularly and conclusively describe interacting particles in a doped high-TC cuprate system (containing free electrons or fermions and Cooper pairs or bosons) and hence in this paper we propose a modified Bose-Fermi-Hubbard (B-F-H) model that can effectively describe the dynamics of cuprates. In this paper, we report transitional temperatures, TC of selected high-TC superconductors within the confines of modified Bose-Fermi-Hubbard (B-F-H) model.

II. Model And Approach

The effective Hamiltonian, in the context of modified Bose-Fermi-Hubbard model system in a strong coupling regime and considering all forms of interactions among the particles is given by [15];

$$H = J\sum_{k,-k}\left(b_k^\dagger b_k + b_{-k}^\dagger b_{-k}\right) - \mu\sum_k b_k^\dagger b_k + \frac{U}{2}\sum_k b_k^\dagger b_k\left(b_k^\dagger b_k - 1\right) + t\sum_k c_k^\dagger c_k + U\sum_{k,k'} c_k^\dagger c_{-k}^\dagger c_{-k'} c_{k'} - \mu\sum_k c_k^\dagger c_k + U\sum_k c_k^\dagger c_k\, b_k^\dagger b_k \qquad (1.1)$$

This Hamiltonian (1.1) is a modified form of Bose-Fermi-Hubbard model and can be diagonalized by a canonical transformation of both bosonic and fermionic nature. This generates the final form of the diagonalized Hamiltonian which corresponds to ground state energy, E_0 of the system;

$$E_0 = tv_k^2 + \triangle\, u_k v_k - 2\mu v_k^2 + 2Jv_k^2 + \frac{U}{2}\left(v_k^4 - v_k^2\right) + Uv_k^4 \qquad (1.2)$$

Introducing the thermal activation term (1.2) becomes;

$$E_T = (t + 1.4\Delta - 2\mu + 2J + U)e^{-\frac{(t+1.4\Delta-2\mu+2J+U)}{100kT}} \qquad (1.3)$$

The temperature derivative of (1.3) yields;

$$C_v = \frac{(t+1.4\Delta-2\mu+2J+U)^2}{100kT^2} e^{-\frac{(t+1.4\Delta-2\mu+2J+U)}{100kT}} \qquad (1.4)$$

The transitional temperature, T_C is obtained from specific heat capacity using the relation,

$$\left(\frac{\partial C_v}{\partial T}\right)_{T=T_C} = 0 \qquad (1.5)$$

Equation (1.4) is substituted in equation (1.5) to obtain;

$$\frac{\partial}{\partial T}\left(\frac{(t+1.4\Delta-2\mu+2J+U)^2}{100kT^2}.e^{-\left(\frac{(t+1.4\Delta-2\mu+2J+U)}{100kT}\right)}\right)_{T=T_C} = 0 \qquad (1.6)$$

The partial derivative in equation (1.6) works out to become;

$$\frac{(t+1.4\Delta-2\mu+2J+U)^2}{100k}.e^{-\left(\frac{(t+1.4\Delta-2\mu+2J+U)}{100kT}\right)}.\left\{-\frac{2}{T_C^3} + \frac{(t+1.4\Delta-2\mu+2J+U)}{100kT_C^4}\right\} = 0 \qquad (1.7)$$

Solving for T_C in (1.7) yields;

$$T_C = \frac{(t+1.4\Delta-2\mu+2J+U)}{200k} \qquad (1.8)$$

III. Results And Discussion

Using equation (1.8), the transition temperature for YBCO, LSCO, NCCO and PCCO were determined. By substituting the values of pre-factors and constants in equation (1.8), we obtain for: YBCO; T_C = 182.6 K, LSCO; T_C = 165.9 K, NCCO; T_C = 141.1 K and PCCO; T_C = 114.9 K as detailed in Table 1.1. Thus our model predicts higher T_C values compared to other theoretical values and hence is a better tool to study cuprates. This is attributed to the fact that, in our system, there is stronger correlations [16] hence higher T_C values. For the four cuprates, the theoretically determined T_C values and those from the graph of specific heat against temperature are with minimum variations in agreement.

Table 1.1: T_C, values for the Modified B-F-H Model.

Cuprate Formula	Cuprate Symbol	Theoretical Tc (K)
$Nd_{2-x}Ce_xCuO_4$	NCCO	52.1
$Pr_{2-x}Ce_xCuO_4$	PCCO	40.9
$YBa_2Cu_3O_7$	YBCO	99.6
$La_{2-x}Sr_xCuO_4$	LSCO	65.9

Hole-doped superconductors characterize much higher values of the critical temperature (T_C) than the electron-doped compounds [17]. In the family of the electron-doped superconductors, the highest critical temperature is equal to ~ 30 K, and it has been obtained for $La_{2-x}Ce_xCuO_4$ (LCCO). However, $Sr_{0.9}La_{0.1}CuO_2$ possesses T_C ~ 40 K, but the synthesis of this compound is extremely difficult. Our model confirms these findings by predicting equally high T_C values for hole-doped cuprates which could be attributed to the higher transfer energies and stoichiometry of oxygen content.

IV. CONCLUSION

Our results directly demonstrate the emergence of high transition temperatures to the tune of over 40 % in the framework of the modified Bose-Fermi-Hubbard model. Our model predicts significantly very high-TC values and hence it lays a very good platform in the study of high-TC superconductivity.

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