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Internal Energy Of Hybrid S-Wave And D-Wave Pairing In Bismuth Cuprates

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***Abstract*—Bogoliubov-Valatin Transformation was used to diagonalize a Hybrid Hamiltonian for electron-electron and electron-cooper pair interaction. From the diagonalized Hamiltonian, an expression for ground state energy was obtained and used to determine internal energy of the system of Bismuth cuprates. It was noted that the internal energy of Bi-2201 is higher than of Bi-2212 and Bi-2223. At experimental transition temperature (Tc) (20 K, 95 K and 110 K), internal energies were recorded as 0.4843 eV, 0.010 eV and 0.0058 eV. While at room temperature (300 K), internal energy was found to be 0.9528 eV, 0.2323 eV and 0.1514 eV respectively for Bi-2201, Bi-2212 and Bi-2223. The observations are discussed with a view of explaining the cause for high temperature superconductivity which can help in achieving room temperature superconductivity. Considering this model, high Tc superconductors can be identified and used to model room temperature superconductors.**

Keywords—Ground state energy, superconductivity, Transition temperature.

I. INTRODUCTION

The theory of high temperature superconductivity has not been fully explained to date [1]. This is because of the many pairing mechanisms, superconducting states and correlations involved between electrons. Pairing mechanisms between electrons determine thermodynamic properties of superconductors. Different researchers have used different pairing mechanisms and formalism to explain the phenomena in different materials and in determining thermodynamic properties. However, the mechanism of high energy pairing is yet to be fully explained. It is not clear whether a single theory of superconductivity can be used or various mechanisms are involved [2]. As a result, this area remains to be of great interest because of new behavior of materials to be explored beside the conventional superconductivity [3]. The interaction between electrons and cooper pairs in cuprates is important in explaining high energy pairing. High-Tc superconductivity and Mott insulator behavior in strongly correlated electron systems can also be explained by pairing mechanisms [4]. Many experiments on high-Tc superconductors show simultaneous existence of electron-phonon and electron-electron interactions [5]. This model is advanced to explain thermodynamics based on these phenomena.

Development of Anti-Ferromagnetic fluctuations in a superconductor produces magnetic pseudo gap called the superconducting gap. If phonons dominate during gap formation, it leads to s-superconducting gap. And when Anti-Ferromagnetic fluctuations are strong enough, a d-gap is formed [6]. The gap leads to density of states at the Fermi level as electrons pair up around the Fermi surface creating a range of energies which have no single electron excitations [7]. It is therefore possible to calculate internal energies at different temperatures. The total energy of a system results from the interaction between the particles of the system [8]. As a result, a decrease in temperature towards critical temperature (Tc) reduces the total energy of the system. This is because some electrons condense into cooper pairs which have low energy than normal electrons reducing the interactions within the system. The energy of the system at any temperature is found by multiplying the diagonal Hamiltonian H_D by the thermal activation factor. By varying temperature, there exists an exponential increase in the energy of the system as the temperature increase [2]. This is attributed to increased thermal fluctuations which enhances the population of conduction electrons [1]. At T=0K all the electrons are superconducting, while for T≥Tc they are all normal. For temperatures in between, the system is a mixture of superconducting and normal electrons [9]. In view of this, considering s-wave (electron-electron) or d-wave (electron-cooper pair) pairing independently limits the energy of the system both at temperature below Tc and above Tc. The Hybrid model is therefore a better tool for determining internal energy as it considers both condensed electrons and normal electrons as they interact within the system.

1.1: s-Wave Pairing

s-wave superconductors have a superconducting gap which is isotropic in all directions. An s-wave corresponds to $s = 0$ and $l = 0$. The two electrons of a pair have equal and opposite momentum k and -k, so that the centre-of-mass momentum of a Cooper pair is zero [10]. For an attractive electron-electron interaction, the bound state is symmetric upon exchange of electron positions, so it must be an ant symmetric singlet upon exchange of electron spins to satisfy the Pauli Exclusion Principle. Thus, at any instant of time, electrons in a Cooper pair are in a state (k↑, k ↓) and the wave function describing the pair consists of all states ``i'' occupied by the pair during its lifetime [9]. An attractive interaction between two electrons results in a potential energy contribution which is negative, and thus lowers the total energy of the electron system. The negative potential energy associated with a cooper pair is the binding energy of that pair.

1.2: d-Wave Pairing

The presence of nodes in cuprates implies d-pairing mechanism that gives an angular momentum greater than zero. It is induced in superconducting cuprates by electron phonon interactions [11]. d-wave superconductors have a superconducting gap which is anisotropic and it is identically zero at four-line nodes located at diagonals of Brillouin zone [12]. The gap breaks rotational symmetry such that different regions of the order parameter differ by 180-degrees [13]. A d-wave state is stable to coulomb perturbation because of a longer distance of separation between electrons. Strong coulomb repulsion also leads to anti-ferromagnetism at half-filling in cuprates. The magnetic fluctuations suppress phonon mediated superconducting order [11].

1.3: Singlet, Doublet and Triplet States

The spin component of interacting electrons can be in a cooper pair of opposite spin, $(s = 0)$or in cooper pairs of the same spin, $(s = 1)$. These leads to four pairing possibilities ↑↑, ↑↓, ↓↑ and ↓↓. This is readily generalized to k and spin dependent pairing states. The BCS state pairs an up spin at k with a down spin at –k. This gives a spin singlet combination with zero centre of mass momentum [14]. In singlet state, all electrons are paired$\uparrow\downarrow \; or \; \downarrow\uparrow$. A singlet is therefore a linked set of particles whose net angular momentum is zero, or whose overall spin quantum number $s = 0$. In this case, the spin part of the wave function is ant-symmetric and orbital part is even, $(l = 0, 2, 4 \ldots.)$,[1]. The angular momentum $l = 0$ results to s-wave pairing and $l = 2$ is for d-wave pairing. Due to ant-symmetric exchange property, switching two electrons corresponds to change of sign in the Hamiltonian [15]. Comparatively, a doublet state contains one unpaired electron and a triplet state has two unpaired electrons$\uparrow\uparrow \; or \; \downarrow\downarrow$. If the spin part of the wave function is symmetric and the orbital part is odd $(s = 1, 3)$triplet cooper pairs are formed [16]. As temperature reduces in a superconductor, the pairing response that diverges first determines the type of superconductivity present [17]. This implies that at Tc, the response is linear but below Tc, it is non-linear and can allow hybridization if they respond at the same time.

2.0: Methodology

2.1: Derivations

In s-wave interaction, free electrons interact with each other and the lattice of the material with Coulomb force. With the Fermi level $\in_f = 0$, The Hamiltonian according to Froehlich equation is given by [2];

$$H_s = \sum_k \mathcal{E}_k a_k^\dagger a_k - \sum_{kk'} V_q \, a_{k'+q}^\dagger a_{k-q}^\dagger a_{k'} a_k \quad 1$$

Where $a_k^\dagger$ and a_k are creation and annihilation operators in state k and state q for opposite direction. For a d-wave, an electron interacts with a cooper pair. A Cooper pair in momentum state k, comprises of two electron creation operators in state k, spin up $a_k^\dagger$, and spin down$a_{-k}^\dagger$. The independent electron in an excited state q is created by $a_q^\dagger$ in a vacuum $|0\rangle$ [20]. With the Fermi level $\in_f = 0$, the Hamiltonian is given as;

$$H_d = \sum_q \mathcal{E}_q a_q^\dagger a_q + \sum_k \mathcal{E}_k b_k^\dagger b_k + \sum_{kq} V_{Kq} a_q^\dagger a_q \left(b_k^\dagger - b_k\right) - \sum_{kq} U_{kq} a_q^\dagger a_q \, b_k^\dagger b_k \quad 2$$

By combining equation 1 and equation 2 the model Hamiltonian is written in terms of creation and annihilation operators as:

$$H_H = \sum_k \mathcal{E}_k a_k^\dagger a_k - \sum_{kk'} V_q \, a_{k'+q}^\dagger a_{k-q}^\dagger a_{k'} a_k + \sum_q \mathcal{E}_q a_q^\dagger a_q + \sum_k \mathcal{E}_k b_k^\dagger b_k + \sum_{kq} V_{Kq} a_q^\dagger a_q \left(b_k^\dagger - b_k\right) - \sum_{kq} U_{kq} a_q^\dagger a_q \, b_k^\dagger \quad 3$$

This is the Hybrid Hamiltonian where ε_k is kinetic energy of free electrons, ε_q is kinetic energy of a cooper pair, V_k is positive coulomb potential between free electrons, V_{kq} is positive interaction potential between an electron and a cooper pair and U_{kq} is the negative coulomb interaction between an electron and a cooper pair. All these constants have known experimental values. The electrons in s-wave singlet states have opposite spins leading to attractive interaction hence the negative sign [5].

By writing equation 3 in terms of Valatin operators γ using the relationships

$a_k = u_k \gamma_k + v_k \gamma_{-k}^\dagger$, $a_k^\dagger = u_k \gamma_k^\dagger + v_k \gamma_{-k}$, $a_{-k} = u_k \gamma_{-k} - v_k \gamma_k^\dagger$ and $a_{-k}^\dagger = u_k \gamma_{-k}^\dagger - v_k \gamma_k$; the expanded Hybrid Hamiltonian in Valatin operators is obtained. By substituting particle number operators for particles created from commutation and anti-commutation rules, the Hybrid Hamiltonian with diagonal and off diagonal terms is obtained.

The off diagonal terms are without number operators and when solved by equating to zero; both values of $u_k^2 and \; v_k^2$ are found to be$\mp \frac{3}{2}$. If $\upsilon > 0$, the pairing lowers the energy of the molecular structure which supports superconductivity and if $\upsilon < 0$, the pairing of electrons increases the energy of the molecular structure which suppresses superconductivity [21]. In this work we will consider the model with the external pair potential only where $\upsilon > 0$.

The diagonal terms of the Hybrid Hamiltonian represent the Hamiltonian of quasi-particles responsible for high temperature superconductivity. This is represented as shown below;

$$H_D = \sum_k \varepsilon_k [u_k^2 m_k + v_k^2 (1 - m_{-k})] - \sum_{kk'} V_{kk'} [u_k^2 v_k^2 m_k m_k - u_k^2 v_k^2 m_k (1 - m_{-k}) + u_k^2 v_k^2 (1 - m_{-k})(1 - m_{-k}) - u_k^2 v_k^2 m_k (1 - m_{-k})] + \sum_q \varepsilon_q \left[u_q^2 m_q + v_q^2 \left(1 - m_{-q}\right)\right] +$$

$\sum_k \varepsilon_k[u_k^2 m_k + v_k^2(1-m_{-k})] - \sum_{kq} U_{kq}\left[u_q^2 u_k^2 m_q m_k + u_q^2 u_k^2 m_q(1-m_{-k}) + v_q^2 u_k^2 m_k(1-m_{-q}) + v_q^2 u_k^2(1-m_{-q})(1-m_{-k})\right]$ 4

Considering the condition for high temperature superconductivity, the occupancy numbers are assumed to be zero [2]. Therefore, $m_q = m_{-q} = m_k = m_{-k} = 0$ and equation 4 is written as;

$H_D = \sum_k \varepsilon_k v_k^2 - \sum_{kk'} V_{kk'} u_k^2 v_k^2 + \sum_q \varepsilon_q v_q^2 + \sum_k \varepsilon_k v_k^2 - \sum_{kq} U_{kq} v_q^2 u_k^2$ 5

Equation 5 simplifies to;

$H_D = \varepsilon_k v_k^2 - V_{kk'} u_k^2 v_k^2 + \varepsilon_q v_q^2 + \varepsilon_k v_k^2 - U_{kq} v_q^2 u_k^2$ 6

For electrons to interact with cooper pairs, they must be in the same state [2]. We therefore ignore all other states and consider state k.

$H_D = 2\varepsilon_k v_k^2 + \varepsilon_q v_q^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk})$ 7

This is the diagonalized Hybrid Hamiltonian which corresponds to the equilibrium state of the system.

2.2: Expression for Internal Energy

Diagonalized Hamiltonian corresponds to the ground state energy of the system E_0 and it is equal to the Hamiltonian of the system when particles are in equilibrium.

$E_0 = H_D$ 8

Ground state energy is therefore given by;

$E_0 = 2\varepsilon_k v_k^2 + \varepsilon_q v_q^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk})$ 9

Multiplying E_0 with $e^{\frac{-E_k}{K_B T}}$ where K_B is Boltzmann constant ($8.63\text{x}10^{-5}$eV/K) and E_k is the energy of quasi particles gives internal energy of the system as;

$E_T = E_O e^{\frac{-E_k}{K_B T}}$ 10

E_k is 1% of the internal energy of the system E_o; Then;

$E_k = \frac{E_O}{100}$ 11

For a given temperature T, the internal energy of the system becomes;

$E_T = E_o e^{\frac{-E_O}{100 K_B T}}$ 12

Replacing equation (9) in equation (12) we get;

$E_T = (2\varepsilon_k v_k^2 + \varepsilon_q v_q^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk})) e^{\frac{-(2\varepsilon_k v_k^2 + \varepsilon_q v_q^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk}))}{100 K_B T}}$ 13

3.0: Results and Discussion

The graph of total internal energy against temperature (Figure 1) is a half stretched sigmoid curve for Bi-2212 and Bi-2223 cuprates. Below 20 K, very low energy is recorded for Bi-2201 while for Bi-2212 and Bi-2223 very low energy is recorded up to about 90 K (where 1, 2 and 3 are copper oxide planes for Bismuth cuprates). This implies that there is maximum formation of cooper pairs below Tc. For Bi-2201, very low energy is recorded below 10 K with a sharp rise in energy from 10 K to 30 K. This is attributed to a small energy gap that causes low binding energy between the particles of Bi-2201. An increase in temperature leads to an increase in internal energy of the Bi-cuprates where more conduction electrons gain kinetic energy and get liberated from the super fluid condensate to move freely within the system. The cooper pairs break up above Tc and the system reverts to a pure s-wave state. This observation concurs with figure 1 where low energy is observed below Tc and high energy observed above Tc. This kind of graph was also observed by [1], [19], [22] and [23].

At experimental Tc; 20 K, 95 K and 110 K; internal energies were recorded as 0.4843 eV, 0.010 eV and 0.0058 eV for Bi-2201, Bi-2212 and Bi-2223 respectively. At room temperature, 300 K; the internal energy was recorded as 0.9528 eV, 0.2323 eV and 0.1514 eV in the same order. Internal energy of Bi2201 is higher than that of Bi-2212 and Bi-2223 in both cases. The superconductor is therefore likely to have more normal electrons than cooper pairs which reduce superconductivity. Bi-2223 has low internal energy and cooper pairs are likely to stay coupled for long as well as the superconducting state because low energy favors formation of cooper pairs. The graph of Bi-2201 is higher than Bi-2212 and Bi-2223 showing that internal energy increase with decrease in the number of copper oxide layers. This may be because the increase in planes increases the binding energy of particles (increases the energy gap) reducing the kinetic energy of the system. Energy at Tc converted to Joules gives $7.759\text{x}10^{-20}$ J, $1.602\text{x}10^{-21}$ J, $9.293\text{x}10^{-21}$ J. Comparatively, [24] while studying Thermodynamic Properties of an Interaction between cooper pairs and electrons in Bismuth based Cuprate Superconductivity finds energy of Bi-2201, Bi-2212 and Bi-2223 as $0.747\text{x}10^{-22}$ J, $3.548\text{ x}10^{-22}$ J, and $4.109\text{ x}10^{-22}$ J respectively at the experimental Tc; The difference may be resulting from the nature of interactions considered. Compared with the experimental values of 0.60 eV ($9.613\text{x}10^{-20}$J), 0.075 eV ($1.202\text{x}10^{-20}$J) and 0.0063 eV ($1.009\text{x}10^{-21}$ J) respectively at experimental Tc [3],[18]and [25]. The calculated values are lower but in close conformity with experimental energy. The differences may be resulting from doping effects in the experimental samples investigated and vibrations of the machine used.

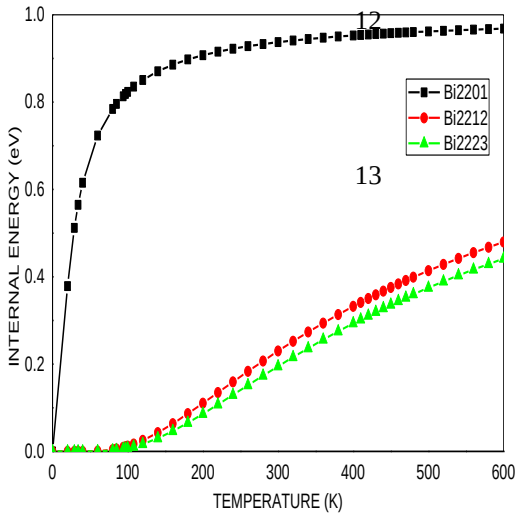

Figure 1: Graph of internal energy against temperature

4.0: Conclusion

For the first time, a hybrid s-wavez and d-wave Hamiltonian has been developed for the Bi-cuprates diagonalized using BVT formalism. From the diagonalized

Hybrid Hamiltonian, the total internal energy for the Bi-cuprates were determined at Tc and found to be $7.759x10^{-20}$ J, $1.602x10^{-21}$ J, $9.293x10^{-21}$ J which are in close agreement with those in other research findings. We have looked at the variation of system energy with temperature and we notice that the energy of Bi-cuprates increases exponentially with temperature due to thermal excitation of electrons. Bi-2223 has a lower internal energy and hence projected as a better material for the construction of room temperature superconductors compared to the other Bi-cuprates under study. From this, we note that room temperature superconductivity can be achieved by increasing the copper oxide planes which lowers internal energy in cuprates.

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Conflict of Interest
The authors declare no conflict of interest regarding publication of this paper.

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