Effect of Internal Energy on Specific Heat of Cuprates using s-Wave and d-Wave Hybrid Model

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Abstract- **The observation of an exponential decay of the specific heat at low temperatures shows that specific heat (Cv) of cuprates depend on the energy spectrum of a superconductor. This means that devising ways of varying internal energy of a system without necessarily varying temperature can help achieve room temperature superconductivity. In this paper, the relationship between internal energy and specific heat is investigated using a Hamiltonian generated from a Hybrid of s-wave and d-wave. The Hamiltonian was diagonalized by Bogoliubov-Valatin (BVT) formalism and used to analyze specific heat of Bismuth cuprates. The graph of Cv versus temperature was a skewed Gaussian shaped curve. Maximum Cv was observed at Tc (32 K, 94 K and 108 K) respectively as 2750 eV/K, for Bi-2201, Bi-2212 and Bi-2223. Increasing the number of copper oxide layers can therefore help increase binding energy and increase the temperature at which maximum Cv of the system is attained, a prerequisite for attaining high transition temperature (Tc). As a consequence, room temperature superconductivity can be achieved by varying the binding energy (increasing copper oxide planes) in a lattice of a cuprate superconductor.**

Key words- **Specific heat, Transition temperature, Binding energy, superconductivity, energy gap.**

I. INTRODUCTION

Superconductivity arises when electronic quasi particles bind together into Cooper pairs which condense into a macroscopic quantum state. The interaction which drives the pairing could be charge or spin polarized [1]. Spin normally determines the character, rate of collision and subsequently the properties of ultra cold systems [2].The pairing interaction could involve high energy virtual transitions across the Mott gap with energy set by the Hubbard U which is a large energy [3]. The basic low-energy excitations are charge-carrier quasi particles, the spin excitations, and the electron quasi particles. In this case, the charge transport is mainly governed by the scattering of charge carriers due to spin fluctuations, and the scattering of spins due to charge-carrier fluctuations dominates the spin dynamics. As a result of the charge-spin recombination, the electron quasi particles are responsible for the electronic properties [4]. The effective attractive interaction between charge carriers originates in their coupling to spin excitation and therefore the spin excitation has been suggested as the pairing glue [5]. Furthermore, recent numerical work based on the t-J model, has shown that the main contribution to the pairing glue is provided by the spin fluctuations with characteristic energies of at most a few hundred meV [6]. Coupling and particle interactions have significantly strong influence on the physical properties of the system. For instance the anomalously high superconducting transition temperature (Tc) is considered to be related to the anomalous features near the Mott transition in a 2D system [7]. However a proper description of the superconducting condensate in the cuprates is possible only when the pairing mechanism would inseparably link together the strong electron correlations and the crystal lattice vibrations. Unfortunately, the pairing mechanism for the planar problem remains highly controversial and many different hypotheses are suggested [8]

Coulomb energy is a major factor in the total energy balance stabilizing the superconducting state. Cuprates contains a strong Coulombic contribution due to the restriction of no doubly occupancy of a given site [9]. Experiments demonstrate that it impossible to determine the changes of Coulomb correlation energy associated with a superconducting phase transition, and they constitute a promising first step in the experimental exploration of the Coulomb correlation energy as a function of momentum and energy [10].When the interaction energy is much larger than the kinetic energy, Coulomb energy is very high and electrons try to be as further away from each other as possible. This means, they would all move to the lattice boundaries. However, this creates an enormous uncompensated positive charge of ions which makes them arrange into an electron lattice of spacing comparable to the average inter-electron distance in the liquid phase [11].Phonons in a solid do not interact only in the harmonic approximation because in-harmonism results in the phonon-phonon interaction. However, the interaction is weak at low energies not because the coupling constant is weak but because the scattering rate of phonons on each other is proportional to temperature [12]. As a result, at small energy transfer, phonons and fermions are almost free quasi-particles and the interaction may as well be strong. On the other hand, because of the Pauli principle, weakly excited states interact weakly [13].

The main point of the BCS theory is that the attractive electron-electron interaction mediated by the phonons gives rise to cooper pairs, (bound states formed by two electrons of opposite spins and momenta). These Cooper pairs form a coherent macroscopic ground state. Key to the formation of cooper pairs is the existence of a well-defined Fermi surface. There will be a bound state only if the attractive interaction is strong enough where charge carriers are held together in d-wave pairs at low temperatures by the attractive interaction in the particle-particle interaction. Interactions originate directly from kinetic energy by the exchange of spin excitation and then these charge-carrier pairs condense to the d-wave SC-state [14]. On the other hand, the same charge-carrier interaction mediated by spin excitations that induces the SC-state in the particle-particle channel also generates the normal-state pseudo gap state in the particle-hole channel [15]. As a consequence, the SC gap and normal-state pseudo gap coexist but compete in the whole SC dome [16]. The normal-state SC gap corresponds to s-wave superconductivity. The s-wave energy gap at the vicinity of the superconducting state existence weakly depends on temperature and it vanishes below Tc [17]. In the actual many-body system, only the electrons near the Fermi level will be affected by the attractive interaction. Two electrons near the Fermi level are unstable towards the formation of a Cooper pair for an arbitrarily small attractive interaction. Thus, we expect that the many-body electronic system will be unstable towards the formation of a new ground state, where these Cooper pairs proliferate [18]. This observation favors the Hybrid approach in the study of thermodynamic properties due to existence of both super-fluid and normal fluid within the superconducting lattice. In a Fermi liquid, the quasi particles at the Fermi momentum,(zero temperature) have an infinite lifetime with zero excitation energy (Fermi energy)and their lifetime decreases with excitation energy. Despite the existence of a Fermi surface in momentum space, there are no quasi particles in the normal state of cuprates near the (π, 0) point of the Brillouin zone [19]. Below Tc, the superconducting gap is maximum and sharp quasi particle peaks are observed. This is because the energy dispersion of the electronic states in this region of the zone is very weak, [20]. The non-existence of quasi particles in the normal state appears to be a general property of cuprate superconductors. Therefore, the formation of quasi particles must be related to the presence of a superconducting state. However, the normal-state pseudo gap crossover temperature is much larger than *T*c disappearing together with superconductivity at the end of the SC dome. This energy driven SC mechanism therefore provides an explanation of both state pairing mechanism for superconductivity and the origin of the normal-state pseudo gap.

In strongly correlated electron systems like cuprates, pair breaking is highly suppressed by electronic correlations. Quasi-particles only exist if thermal energy overcomes the gap energy Δo because of strong on-site Coulomb repulsion between the electrons [21]. In a conventional BCS superconductor, screening and retardation effects work to minimize the role of Coulomb interaction. However, owing to the effect of strong on-site Coulomb repulsion between electrons, the role of the coulomb interactions is crucial in cuprates where the charge degrees of freedom are partially frozen. In this case the SC-state in cuprates is determined by the need to reduce kinetic energy of the system. High kinetic energy in the normal-state is partially reduced upon entering the SC-state, indicating that reducing kinetic energy causes superconductivity [22]. Superconductivity in cuprate superconductors arises from lowering of the kinetic energy and raising the potential energy which favors cooper pairing. More importantly, the recent experimental results [23] from the ARPES measurements on cuprate superconductors indicate that *T*c is correlated with the charge-carrier kinetic energy, which supports the notion of the energy driven superconductivity.

By constructing an effective Hybrid Hamiltonian for spin polarons forming in cuprates, it has been demonstrated that the driving mechanism which gives rise to superconductivity in such system is the suppression of the kinetic energy [24].

II. FORMALISM

The Hybrid Hamiltonian developed from electron-electron (s-wave) and electron-cooper pair (d-wave) interaction in terms of creation and annihilation operators is given as;

$$H_H = \sum_k \varepsilon_k a_k^\dagger a_k - \sum_{kk'} V_q\, a_{k'+q}^\dagger a_{k-q}^\dagger a_{k'} a_k + \sum_q \mathcal{E}_q a_q^\dagger a_q + \sum_k \mathcal{E}_k b_k^\dagger b_k + \sum_{kq} V_{Kq} a_q^\dagger a_q \left(b_k^\dagger - b_k\right) - \sum_{kq} U_k a_q^\dagger a_q\, b_k^\dagger b_k \quad 1$$

Where ε_q is kinetic energy of free electrons, ε_k is kinetic energy of a cooper pair, V_q is positive coulomb potential between free electrons, V_{kq} is positive interaction potential between an electron and a cooper pair and U_k is the negative coulomb interaction between an electron and a cooper pair. Diagonalized by Bogoliubov-Valatin transformation (BVT) formalism, the Hamiltonian is given as;

$$H_D = 2\mathcal{E}_k v_k^2 + \mathcal{E}_q v_k^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk'}) = E_o \quad 2$$

Where E_o is equal to ground state energyof quasi particles at equilibrium. Multiplying E_o with $e^{\frac{-E_k}{K_B T}}$ where K_B is Boltzmann constant (8.63x10⁻⁵eV/K) and E_k is the energy of quasi particles which is 1% of the ground state energy of the systemE_o;

$$E_k = \frac{E_0}{100} \quad 3$$

For a given temperature T, the internal energy equation becomes

$$E_T = \left(2\mathcal{E}_k v_k^2 + \mathcal{E}_q v_k^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk'})\right) e^{\frac{-\left(2\mathcal{E}_k v_k^2 + \mathcal{E}_q v_k^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk'})\right)}{100 K_B T}} \quad 4$$

Specific Heat is the amount of heat required to raise the temperature of a unit mass of substance by a unit degree. It is the first derivative of internal energy with respect to temperature of the system. This is given by;

$$C_v = \frac{\partial}{\partial T}\left(E_0 \mathrm{e}^{\frac{-E_K}{K_B T}}\right) \quad 5$$

Simplified to;

$$C_v = \frac{E_0^2}{K_B T^2}\, \mathrm{e}^{\left(\frac{-E_0}{100\, K_B T}\right)} \quad 6$$

Replacing equation (2) in equation (6) gives

$$C_v = \frac{\left(2\varepsilon_k v_k^2 + \varepsilon_q v_k^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk'})\right)^2}{K_B T^2}$$

$$\mathrm{e}^{\left(\frac{-\left(2\varepsilon_k v_k^2 + \varepsilon_q v_k^2 - u_k^2 v_k^2 (V_{kk'} + U_{kk'})\right)}{100 K_B T}\right)} \quad 7$$

III. RESULTS AND DISCUSSION

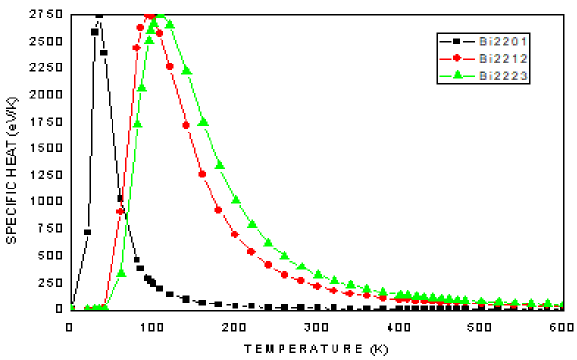

Fig I: Graph of specific heat capacity against temperature

The graph of specific heat versus temperature is a skewed Gaussian shaped curve as seen in fig 1. Below the critical temperature (the peak), specific heat increases with increase in temperature since particles have very low internal energy (high potential energy). Below the peak, the graphs decrease to very low values as temperature decreases because lattice vibrations are eliminated and there is a quick formation of the super fluid condensate reaching maximum. The maximum specific heat was observed at 32 K, 94 K and 108 K respectively as 2750 eV/K, for Bi-2201, Bi-2212 and Bi-2223. Where 1, 2, and 3 are copper oxide planes in Bismuth cuprates. This could be attributed to maximum cooper pair formation in the system as $T \rightarrow Tc$. Above Tc, the graph slowly reduce to low values as the normal state sets in leading to maximum electron-electron interaction and maximum lattice vibrations due to increase in kinetic energy. Similar findings were observed by [2],[25], [26], [27] and [28]. The graph of Bi-2201 peaks and falls faster than Bi-2212 and Bi-2223 because Bi-2201 has low binding energy and cooper pairs easily break up reverting the system to s-wave state. Bi-2223 which has a higher binding energy requires high energy and hence high temperature for the cooper pairs to break up. The binding energy can therefore be increased by increasing copper oxide planes of cuprates. This raises the Tc and room temperature superconductivity can be achieved. At temperatures above Tc, Cv increases with increase in copper oxide planes and increases with decrease in internal energy. This means that Bi-2223 has high coulomb interactions after pair breaking because of the many free electrons liberated from the super fluid condensate. At room temperature (300K), Bi-2223 has higher specific heat (316 eV/K) compared to 16 eV/K and 215 eV/K for Bi-2201 and Bi-2212. At this temperature, the internal energies are 0.95 eV, 0.23 eV and 0.15 eV respectively for Bi-2201, Bi-2212 and Bi-2223. This indicates that a decrease in internal energy raises the specific heat. High specific heat on the other hand raises the transition temperature this can be achieved by increasing Coulomb force.

IV. CONCLUSION

Specific heat for the Bi-cuprates was also derived from the diagonalized Hamiltonian. The graph for temperature dependence of specific heat was a Gaussian curve with maximum specific heat at a lower temperature in Bi-2201 and at highest temperature in Bi-2223. From this observation, as the number of CuO_2 planes increase, the specific heat increases. In general, the specific heat decreases with increase in temperature above Tc, and increases with increase in temperature below Tc.

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