Computation of the Expectation Value of the Electron – Phonon and Coulomb Interaction Hamiltonian using Second Quantization and Many Body Techniques

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ABSTRACT

The problem of the strong electron coupling in the theory of superconductivity has been discussed in many studies on the basis of electron and phonon spectral functions. For the rationale of investigating the effect of electron – phonon and Coulomb interactions in cuprate superconductors, this study has considered a Hamiltonian (H_{epc}) which includes both Coulomb interactions and electron-phonon interactions. The expectation value of this Hamiltonian was evaluated using second quantization and many body techniques. The equation for the energy of the system at ground state was obtained from the product of the expectation value and the thermal activation factor, exp ($-E_1/kT$). The equation relating specific heat and absolute temperature was obtained from the first derivative of the energy of the system at ground state with respect to absolute temperature. The equation relating entropy and absolute temperature was obtained from the specific heat equation. Values of specific heat and entropy against absolute temperature were calculated. In these calculations, the onsite energy of oxygen (E_p) was fixed at 2.0 x 10^{-6} eV. The onsite energy of copper (E_d), hybridization energy of oxygen and copper bands (t_{pd}), the electron – phonon interaction energy, (g_{ep}) and energy due to repulsion of copper holes occupying the same orbital (u_d), were varied. From the results, it was found out that increase in the parameters E_d, t_{pd}, g_{ep} and u_d leads to increase in the transition temperature. It was further found that entropy and specific heat decrease with increase in the parameters. It can therefore be concluded that long range electron – phonon and local Coulomb interactions increase the transition temperature of superconducting cuprates.

Keywords: Cuprate Superconductors, Expectation value, Coulomb interactions, Electron-Phonon interactions

INTRODUCTION

Superconductivity is a phenomenon observed in several metals and ceramic materials whereby when these materials are cooled to temperatures ranging from near absolute zero (0 K) to liquid nitrogen temperatures (-196^{0}C), their electrical resistance drops with a jump down to zero [1]. It was discovered by the Dutch physicist Heike Kamerlingh Onnes [2]. Electrical resistance in metals arises because electrons moving through the metal are scattered due to deviations from translational symmetry [3]. These are produced either by impurities, giving rise to a temperature independent contribution to the resistance, or by the vibrations of the lattice in the metal. However, in a superconductor below its critical temperature, there is no electrical resistance because these scattering mechanisms are unable to impede the motion of the current carriers [4]. As a negatively-charged electron moves through the space between two rows of positively-charged atoms, it pulls inward on the atoms of the lattice. This distortion attracts a second electron to move in behind it. The two electrons form a weak attraction, travel together in a pair and encounter less resistance overall. In a superconductor, electron pairs are constantly forming, breaking and reforming, but the overall effect is that electrons flow with little or no resistance. The current is carried then by electrons moving in pairs called Cooper pairs [1]. The second electron encounters less resistance, much like a passenger car following a truck on the motorway encounters less air resistance. Below the critical temperature these superconducting materials have no electrical resistance and so they can carry large amounts of electrical current for long periods of time without losing energy as Ohmic heat [5].

Nearly all superconductors exhibit a phenomenon called the Meissner effect [6]. This involves the expulsion of a magnetic field from a superconductor during its transition to the superconducting state [7]. A superconductor with little or no magnetic field within it is said to be in the Meissner state. The Meissner state breaks down when the applied magnetic field is too large [8]. Superconductors can be divided into two classes according to how this breakdown occurs. In Type I superconductors, superconductivity is abruptly destroyed when the strength of the applied field rises above a critical value H_c [9]. Depending on the geometry of the sample, one may obtain an intermediate state consisting of a baroque pattern of regions of normal material carrying a magnetic field mixed with regions of superconducting material containing no field [10]. In Type II superconductors, raising the applied field past a critical value H_{c1} leads to a mixed state (also known as the vortex state) in which an increasing amount of magnetic flux penetrates the material, but there remains no resistance to the flow of electric current as long as the current is not too large [9]. At second critical field strength *Hc2*, superconductivity is destroyed. The mixed state is actually caused by vortices in the electronic superfluid, sometimes called fluxons because the flux carried by these vortices is quantized. Most pure elemental superconductors, except niobium and carbon nanotubes, are Type I, while almost all impure and compound superconductors are Type II.

The transition of a metal from the normal to the superconducting state has the nature of a condensation of the electrons into a state which leaves a band gap above them. This kind of condensation is seen with superfluid helium, but helium is made up of bosons -- multiple electrons can't collect into a single state because of the Pauli Exclusion Principle [11]. Froehlich was first to suggest that the electrons act as pairs coupled by lattice vibrations in the material. This coupling is viewed as an exchange of phonons, phonons being the quanta of lattice vibration energy. Experimental corroboration of an interaction with the lattice was provided by the isotope effect on the superconducting transition temperature [12]. The boson-like behavior of such electron pairs was further investigated by Cooper and they are called "Cooper pairs". The condensation of Cooper pairs is the foundation of the BCS theory of superconductivity [1]. A key conceptual element in the BCS theory is the pairing of electrons close to the Fermi level into Cooper pairs through interaction with the crystal lattice. This pairing results from a slight attraction between the electrons related to lattice vibrations; the coupling to the lattice is called a phonon interaction [13].

Pairs of electrons can behave very differently from single electrons which are fermions and must obey the Pauli Exclusion Principle. The pairs of electrons act more like bosons which can condense into the same energy level. The electron pairs have a slightly lower energy and leave an energy gap above them on the order of 0.001 eV which inhibits the kind of collision interactions which lead to ordinary resistivity. For temperatures such that the thermal energy is less than the band gap, the material exhibits zero resistivity.

Since the discovery of cuprates, many theories have been proposed to explain both normal and superconducting properties of these materials. However, there is no clear agreement on the appropriate theoretical description of these materials even in their normal states. It is generally believed that characterizing the cuprates above T_c is a necessary first step in unraveling the superconducting mechanism. Experimental and theoretical observations point towards unusual electron – phonon and Coulomb interactions in cuprates, which remain to be quantitatively addressed. In this endeavor, this study aims to calculate the expectation value of the electron – phonon and Coulomb Interaction Hamiltonian using second quantization and many body techniques.

THEORETICAL DERIVATIONS AND CALCULATIONS

The electron – phonon and Coulomb interaction Hamiltonian, H_{epc} is expressed as:

$$H_{ep} = g_{ep}\sum_{k,\sigma}(a^{+}_{k,\sigma}\,a_{k+X,\sigma} + a^{+}_{k+X,\sigma}a_{k,\sigma}) + E_p\sum_i a^{+}_{ip}a_{ip} + E_d\sum_j a^{+}_{jd}\,a_{jd} + t_{pd} + \sum_{ij}(a^{+}_{ip}\,a_{jd} + a^{+}_{jd}a_{ip}) + u_d\sum_{ji} a^{+}_{jd}\,a^{+}_{jd}a_{ip}a_{ip} \quad (1)$$

where g_{ep} is the energy for electron – phonon interaction [14].

The expectation value of H_{epc} given in Eq. (1) was calculated by writing the trial wave function for such a system. The trial wave function was written as,

$$\Psi = (a_i a_i + a_j^{+}a_j^{+})(u + v a_i^{+}a_i^{+})\left|n,0\right\rangle \quad (2)$$

and its conjugate was

$$\Psi = \left\langle n,0\right|\left(u + v a_i a_i\right)\left(a_j a_j + a_i^{+}a_i^{+}\right) \quad (3)$$

Using the trial wave function and its conjugate, the expectation value of the H_{epc} was written as;

$$E_n = \left\langle \Psi \right| H \left| \Psi \right\rangle \quad (4)$$

Eqs. (1), (2) and (3) were substituted in eq. (4) to obtain

$$E_n = \langle n,0 | \left(u + v a_i a_i\right)\left(a_j a_j + a_i^+ a_i^+\right) \begin{bmatrix} E_p a_{ip}^+ a_{ip} \\ +E_d a_{jd}^+ a_{jd} \\ +t_{pd}(a_{ip}^+ a_{jd} + a_{jd}^+ a_{ip}) \\ +u_d a_{jd}^+ a_{jd}^+ a_{ip} a_{ip} \\ +g_x(a_{k\sigma}^+ a_{k+X,\sigma} + a_{k+X,\sigma}^+ a_{k\sigma}) \end{bmatrix} (a_i a_i + a_j^+ a_j^+)(u + v a_i^+ a_i^+ | n,0\rangle$$

(5)

After lengthy calculations using second quantization and many body techniques, the following results were obtained from eq. (5),

$$\begin{aligned} E_n = & \begin{Bmatrix} u^2(n+1)(n+2)^2 + u^2 n(n-1)(n-2) \\ +v^2(n+1)(n+2)(n+3)(n+4)^2 + v^2 n(n+1)(n+2) \end{Bmatrix} E_p \\ & + \begin{Bmatrix} u^2(n+1)(n+2)^2 + u^2 n(n-1)(n-2) + v^2(n+1)(n+2)(n+3)(n+4)^2 \\ +v^2(n+1)(n+2)(n+3)(n+4)^{\frac{5}{2}} + v^2(n-1)n(n+1)^{\frac{5}{2}}(n+2) \end{Bmatrix} E_d \\ & + \begin{Bmatrix} u^2 t_{pd} n(n-1)(n-2) + u^2 t_{pd} n(n-1)(n-2) \\ +u^2(n+1)(n+2)^2 + u^2(n+1)(n+2)^2 \\ +uvn(n+1)^2(n+2)^2 + v^2 n(n+1)^{\frac{5}{2}}(n+2)^2 \\ +v^{\frac{1}{2}}(n+1)(n+2)(n+3)(n+4)^2 \\ +v^2(n+1)(n+2)(n+3)(n+4)^2 \end{Bmatrix} t_{pd} \\ & + \begin{Bmatrix} u^{\frac{1}{2}} n(n-1)(n-2)(n-3) + u^2(n+1)^2(n+2)^2 \\ +v^2(n-2)(n-1)n(n+1)^{\frac{5}{2}}(n+2)^{\frac{3}{2}} + v^2(n+1)(n+2)(n+3)^2(n+4)^2 \end{Bmatrix} u_d \\ & + \begin{Bmatrix} u^2 n(n-1)(n-2) + u^2 n(n-1)(n-2) + u^2(n+1)(n+2)^2 \\ +u^2(n+1)(n+2)^2 + v^2 n(n+1)^{\frac{3}{2}}(n+2)^2 + v^2 n(n+1)^2(n+2)^2 \\ +v^2(n+1)(n+2)(n+3)(n+4)^2 + v^2(n+1)(n+2)(n+3)(n+4)^2 \end{Bmatrix} g_{ep} \end{aligned}$$

(6)

For n =1, when the system is in its lowest energy state (superconducting state) and substituting $u = v = 1/\sqrt{2}$ (from second quantization formalism) in eq. (6) one gets;

$$E_1 = \left\{\frac{1}{2}(2)(3)(4)(5)^2 + \frac{1}{2}(2)(3)\right\}E_p$$
$$+\left\{\frac{1}{2}(2)(3)^2 + \frac{1}{2}(2)(3)(4)(5)^2 + \frac{1}{2}(2)(3)(4)(5)^{\frac{5}{2}}\right\}E_d$$
$$+\left\{\begin{array}{l}\frac{1}{2}(2)(3)^2 + \frac{1}{2}(2)(3)^2 + \frac{1}{2}(2)^2(3)^2 + \frac{1}{2}(2)^{\frac{5}{2}}(3)^2 \\ +\frac{1}{2}(2)(3)(4)(5)^2 + \frac{1}{2}(2)(3)(4)(5)^2\end{array}\right\}t_{pd}$$
$$+\left\{\frac{1}{2}(2)(3)(4)^2(5)^2\right\}u_d$$
$$+\left\{\begin{array}{l}\frac{1}{2}(2)(3)^2 + \frac{1}{2}(2)(3)^2 + \frac{1}{2}(2)^{\frac{3}{2}}(3)^2 + \frac{1}{2}(2)^2(3)^2 \\ +\frac{1}{2}(2)(3)(4)(5)^2 + \frac{1}{2}(2)(3)(4)(5)^2\end{array}\right\}g_{ep} \quad (7)$$

Eq. (7) simplifies to

$$E_1 = 303E_p + 980E_d + 888t_{pd} + 800u_d + 720g_{ep} \quad (8)$$

Equation (8) is the expectation value of the electron – phonon and Coulomb interaction Hamiltonian.

At the temperature of interest, it is necessary to consider the difference between the states in which the hopping electron is on one site and then when it is on another site of similar symmetry or different symmetry. This difference in energy of the two sites gives the probability amplitude Green's function which according to quantum treatment of lattice vibrations [15], is equivalent to the thermal activation factor exp ($-E_1/kT$). Thus, the expectation values electron – phonon and Coulomb interaction Hamiltonian is multiplied by the thermal activation factor to obtain

$$E = E_1 e^{-\frac{E_1}{kT}} \quad (9)$$

The specific heat, C_v, of the system is obtained from the first derivative of eq. (7) with respect to absolute temperature and is written as,

$$C_v = \frac{\partial E}{\partial T} = E_1 \frac{\partial}{\partial T}\left(e^{-\frac{E_1}{kT}}\right) = \frac{E_1}{kT^2} e^{-\frac{E_1}{kT}} \quad (10)$$

To obtain the equation relating entropy, *S*, and absolute temperature *T*, one may start with the equation

$$dS = \frac{dQ}{T} = \frac{C_V dT}{T} \quad (11)$$

Taking integrals on both sides of eq. (9), one obtains,

$$\int dS = \int \frac{C_v dT}{T} \quad (12)$$

Substituting for C_v from eq. (8) in eq. (10), one obtains,

$$\int dS = \int \frac{E_1}{kT^2} e^{-\frac{E_1}{kT}} \frac{dT}{T} \quad (13)$$

From eq. (11), one obtains,

$$S = \frac{E_1}{k}\int \frac{1}{T^2} e^{-\frac{E_1}{kT}} \frac{dT}{T} = \frac{E_1}{k}\int \frac{1}{T^3} e^{-\frac{E_1}{kT}} dT \quad (14)$$

To obtain an exact calculation of the integral in eq. (12), we let

$$u = -\frac{E_1}{kT} \tag{15}$$

From eq. (13), one obtains,

$$du = \frac{E_1}{kT^2}\,dT \tag{16}$$

From eq. (14), one obtains,

$$dT = \frac{kT^2}{E_1}\,du \tag{17}$$

Substituting value of *u* and *dT* from eqs. (13) and (15) respectively in eq. (12), one obtains,

$$S = \frac{E_1}{k}\int \frac{1}{T^3} e^u \frac{kT^2}{E_1} du = \int \frac{e^u}{T} du \tag{18}$$

Substituting for $T = -\frac{E_1}{ku}$ in eq. (16), one obtains,

$$S = \int \frac{-e^u}{E_1 / ku} du = -\frac{k}{E_1}\int u e^u du \tag{19}$$

Applying integration by parts to eq. (17), one obtains,

$$S = \frac{e^{-\frac{E_1}{kT}}}{T} + \frac{k}{E} e^{-\frac{E_1}{kT}} + C \tag{20}$$

where C is a constant of integration.

As T tends to zero, S = 0 and hence, C = 0. Therefore eq. (18) becomes.

$$S = \frac{e^{-\frac{E_1}{kT}}}{T} + \frac{k}{E} e^{-\frac{E_1}{kT}} = e^{-\frac{E_1}{kT}}\left(\frac{1}{T} + \frac{k}{E}\right) \tag{21}$$

RESULTS AND DISCUSSION

For different superconductors, the values of E_p, E_d, t_{pd}, u_d and g_{ep} can be chosen to calculate E_1. For instance, for a superconductor YBaCuO, the sample values for E_p, E_d, t_{pd}, u_d and g_{ep} are 3.5 x 10^{-6} ev, 2.0 x 10^{-6} ev, 1.6 x 10^{-6} ev, 2.5 x 10^{-6} ev and 2.0 x 10^{-6} ev respectively. The values of specific heat can be calculated from eq. (10) and that of entropy from eq. (21). By drawing graphs of Cv and S against temperature T, the effects of E_p, E_d, t_{pd}, u_d and g_{ep} on the transition temperature T_c are determined. It is found that he role of long range electron phonon and Coulomb interactions is to increase the transition temperature of the cuprate superconductors. There is a recent study [16] according to which the critical temperature Tc is determined by the superfluid density of the Cooper pairs and it defies the standard BCS theory. Another such study is 'New cuprate superconductivity' may challenge classical wisdom [17]. Hence, new experimental discoveries will keep challenging the old ideas and wisdom that have been used to explain the phenomena of superconductivity. Consequently, framing a theory of superconductivity that can explain the properties of all superconductors is still a challenge for the Physicists.

REFERENCES

[1] Tinkham, M. (2012). Introduction to Superconductivity. Courier Corporation.

[2] Kamerlingh Onnes, H. (1911). The superconductivity of mercury. *Comm. Phys. Lab. Univ. Leiden*, *122*, 122-124.

[3] Rose-Innes, A. C., & Rhoderick, E. H. (1970). Introduction to superconductivity. *American Journal of Physics*, *38*(8), 1048-1049.

[4] Burmistrov, I. S., Gornyi, I. V., & Mirlin, A. D. (2012). Enhancement of the critical temperature of superconductors by Anderson localization. *Physical review letters*, *108*(1), 017002.

[5] Welp, U., Kadowaki, K., & Kleiner, R. (2013). Superconducting emitters of THz radiation. *Nature Photonics*, *7*(9), 702-710.

[6] Essén, H., & Fiolhais, M. C. (2012). Meissner effect, diamagnetism, and classical physics—a review. *American Journal of Physics*, *80*(2), 164-169.

[7] Yokoyama, T., Tanaka, Y., & Nagaosa, N. (2014). Anomalous Meissner Effect in Superconducting Junction with Spin-active Interface. *Physics Procedia*, *58*, 187-190.

[8] Huebener, R. (2013). *Magnetic flux structures in superconductors: extended reprint of a classic text* (Vol. 6). Springer Science & Business Media.

[9] Sharma, R. G. (2015). Type II Superconductors. In *Superconductivity* (pp. 49-69). Springer International Publishing.

[10] Wolchover, N. (2013). A Jewel at the Heart of Quantum Physics. *Quanta Magazine*, *17*.

[11] Zhu, G., Combescot, M., & Betbeder-Matibet, O. (2012). BCS ansatz for superconductivity in the canonical ensemble and the Pauli exclusion principle. *Physica C: Superconductivity*, *480*, 43-48.

[12] Schaeffer, A. M., Temple, S. R., Bishop, J. K., & Deemyad, S. (2015). High-pressure superconducting phase diagram of 6Li: Isotope effects in dense lithium. *Proceedings of the National Academy of Sciences*, *112*(1), 60-64.

[13] Ciudad, D. (2015). Superconductivity: Raising the temperature. *Nature Materials*, *14*(10), 962-962.

[14] Gulácsi, M., & Chan, R. (2001). High-temperature superconductivity: The attractive Up regime. *Journal of superconductivity*, *14*(6), 651-658.

[15] Alling, B., Körmann, F., Grabowski, B., Glensk, A., Abrikosov, I. A., & Neugebauer, J. (2016). Strong impact of lattice vibrations on electronic and magnetic properties of paramagnetic Fe revealed by disordered local moments molecular dynamics. *Physical Review B*, *93*(22), 224411.

[16] Božović, I., Wu, J., He, X., & Bollinger, A. T. (2019). What is really extraordinary in cuprate superconductors?. *Physica C: Superconductivity and its Applications*, *558*, 30-37.

[17] Li, W. M., Zhao, J. F., Cao, L. P., Hu, Z., Huang, Q. Z., Wang, X. C., ... & Yu, R. Z. (2019). Superconductivity in a unique type of copper oxide. *Proceedings of the National Academy of Sciences*, *116*(25), 12156-12160.