THEORETICAL STUDY OF HIGH TEMPERATURE SUPERCONDUCTIVITY: THE CASE OF CUPRATE ($YBA_2CU_3O_{6.93}$)

Mequanint Assefa*

P.Singh*

Abstract

In this work, we determine the superconducting transition temperature and the superconducting order parameter for high temperature superconductor, particularly, for optimally doped $Y\,Ba_2Cu_3O_{6:93}$ analytically. In order to compute these, we have used retarded Green function method, equation of motion and Hamiltonian model. Furthermore, we obtain appropriate result which is very close to the experimental result. High temperature superconductor is very important phenomenon for changing the whole world of energy transport, and distribution as well as various scientific and technological applications.

Keywords:

Superconductivity, Superconducting transition temperature, order parameter, Green function, Hamiltonian model

* Department of Physics, Addis Ababa University, P.O.Box, 1176, Addis Ababa, Ethiopia

1. Introduction

Superconductivity is the ability of certain materials to conduct electricity with zero resistance below the superconducting transition temperature. This property was first discovered by Physicist Kammerling Onnes in Leiden in 1911, while cooling elemental mercury with liquid helium about 4.2K [1]. He noticed that its resistance suddenly disappeared. Superconductivity remained an empirical science for several decades. After quantum mechanics was introduced. Theorists gradually began to suspect that superconductivity was quantum phenomena.

The first widely accepted theoretical understanding of superconductivity was advanced in 1957 by American physicist John Bardeen, León Cooper and John Schrieffer [2].Their theory of superconductivity became known as the BCS theory.

In 1986 Bednorz and Muller discovered superconductivity in a lanthanum based cuprate perovskite material, transition temperature of 35K which is the high temperature superconductors [3]. In 1995,the highest temperature superconductor (at ambient pressure) is mercury barium calcium copper oxide ($HgBa_2Ca_2\,Cu_3O_x$),whose T_c is 135K at ambient pressure [4] and reaches 164K under high pressure [5] discovered. Cuprates remained a high priority due to its high T_c until the discovery of superconductivity in iron-pnictides be led by Yoichi Kamihara [6] who discovered that CuO plane is not a requirement for superconductivity.In 2008, the highest superconducting transition temperature non-cuprate superconductor is pnictide ($Ca_{1-x}Nd_xFeAsF$) with $T_c = 57K$ [7].

High temperature superconductivity could revolutionize technologies ranging from magnetically-levitated trains to electrical power transmission. however, the mechanism by which these cuprate materials become superconducting and the superconducting transition temperature had remained a mystery for the last 29 years, moreover, there are different scenarios' for proposed mechanisms for high temperature superconductivity, these are exciton ,bi-exciton, polarons, bi-polarons, and magnon [8].In this paper we tried to suggest that the possible mechanism for high temperature superconductivity magnon (spin wave fluctuation) mediated superconductivity.

The paper organized as follows:

In section2, we drive equation of motion for Heisenberg operator. In Section 3 formulation of problem. We obtain the result and discussion in section 4. Lastly, in 5 conclusion of the result is given.

2. The Green function Method

In this section, we employ the basic concept of retarded Green function method as mathematical technique which is very essential to formulate problem on high temperature superconductivity. In this technique, we have tried to derive the equation of motion of operator. Green function defined for two operators a and b which do not need to be hermitian.

The Retarded Green function is defined as

$$G_r(t,t') = \ll a(t)b(t') \gg = -i\theta(t-t') < [a(t),b(t') > ------------- (1)$$

Where <<…..>> represents the Green function, $\theta(t-t')$ is the Heaviside step function

a(t) and b(t') are annihilation and creation operators respectively

2.1 Equation of motion

Now let us derive the equation of motion, The Retarded Green function is

$$G_r(t,t') = \ll a(t)b(t') \gg = -i\theta(t-t') < [a(t),b(t') >$$

Differentiating eqn(1) with respect to t

$$\frac{dG_r(t,t')}{dt} = -i\frac{d\theta(t-t')}{dt} < [a(t),b(t') > -i\theta(t-t') < [\frac{da(t)}{dt},b(t')] >$$

Applying $\frac{da(t)}{dt} = -i[a(t),H]$

We obtain

$$\omega \ll a(t)b(t') \gg = < [a(t),b(t')] > + \ll [a(t),H]b(t') \gg ----------- (2)$$

This the equation of motion

3. Formulation of the problem

In this section, we have tried to solve and determine the superconducting transition temperature, superconducting order parameter for optimal doped $YBa_2Cu_3O_{6.93}$ using a model Hamiltonian with Green function formalism

The Hamiltonian for optimal doped $YBa_2Cu_3O_{6.93}$ is given by

$$\hat{H} = \hat{H_o} + \hat{H}_{sf} ----------------------(3)$$

Where

$$\hat{H_0} = \sum_{k\sigma} \xi_{k\sigma} a^{+}_{k\sigma} a_{k\sigma} + \sum_{k\sigma} \hbar\omega \, b^{+}{}_{k\sigma} b_{k\sigma} -----------(4)$$

Hamiltonian describes for itinerant and localized electrons

$$\hat{H}_{sf} = J \sum_{k\sigma,} S^{\alpha}{}_{k} \, . \sigma^{\alpha}_{\sigma,\sigma'} a^{+}_{k\sigma} a_{k'\sigma} -----------(5)$$

The spin-fermions interaction between two sets of electrons

Where σ represents Pauli matrix and S represents spin operator

$$\sum_{\alpha} S^{\alpha}_{k} . \sigma^{\alpha}_{\sigma,\sigma'} = S^{z}_{k} \sigma^{z} + S^{x}_{k} \sigma^{x} + S^{y}_{k} \sigma^{y}$$

This is reduced to

$$\sum_{\alpha} S^{\alpha}_{k} . \sigma^{\alpha}_{\sigma,\sigma'} = S^{z}_{k} \sigma^{z} + S^{+}_{k} \sigma^{-} + S^{-}_{k} \sigma^{+}$$

$$\hat{H}_{sf} = J \sum_{k\sigma,} [S^{z}_{k} \sigma^{z} + S^{+}_{k} \sigma^{-} + S^{-}_{k} \sigma^{+}] a^{+}_{k\sigma} a_{k'\sigma} -------(6)$$

$$\hat{S}^{z}{}_{k} = \frac{1}{2} \sum_{k,k'} [a^{+}_{k\uparrow} a_{k'\uparrow} - a^{+}_{k\downarrow} a_{k'\downarrow}]$$

$$\hat{S}^{+}{}_{k} = \sum_{k\sigma,} a^{+}_{k\uparrow} a_{k'\downarrow}$$

$$\hat{S}^{-}{}_{k} = \sum_{k\sigma,} a^{+}_{k\downarrow} a_{k'\uparrow}$$

The spin operator $\hat{S}^{+}{}_{k}$ destroyed a down spin and created an up spin, while in $\hat{S}^{-}{}_{k}$, it is the other way around. We also see that $\hat{S}^{z}{}_{k}$ counts the number of up spins minus the number of down spins

The spin-electron interaction Hamiltonian will be

$$\hat{H}_{sf} = \frac{1}{2}\sum_{k,k'} J[a^{+}_{k\uparrow}a_{k''\uparrow} - a^{+}_{k\downarrow}a_{k'\downarrow}][a^{+}_{k\uparrow}a_{k''\uparrow} - a^{+}_{k\downarrow}a_{k'\downarrow}]$$

$$+ \mathrm{J}\sum_{k\sigma,}[a^{+}_{k\uparrow}a_{k'\downarrow}\ a^{+}_{k\downarrow}a_{k'\uparrow} + a^{+}_{k\downarrow}a_{k'\uparrow}\ a^{+}_{k\uparrow}a_{k'\downarrow}] - -(7)$$

$$\hat{H}_{sf} = \frac{1}{2}J\sum_{k,k'}[a^{+}_{k\uparrow}a_{k'\uparrow}\ a^{+}_{k\uparrow}a_{k'\uparrow} - a^{+}_{k\uparrow}a_{k'\uparrow}a^{+}_{k\downarrow}a_{k'\downarrow} - \ a^{+}_{k\downarrow}a_{k'\downarrow}\ a^{+}_{k\uparrow}a_{k'\uparrow} + a^{+}_{k\downarrow}a_{k'\downarrow}\ a^{+}_{k\downarrow}a_{k'\downarrow}]$$

$$+ \quad \mathrm{J}\sum_{k\sigma,}[a^{+}_{k\uparrow}a_{k'\downarrow}\ a^{+}_{k\downarrow}a_{k'\uparrow} + a^{+}_{k\downarrow}a_{k'\uparrow}\ a^{+}_{k\uparrow}a_{k'\downarrow}] - - - - - - - - - - (8)$$

Employing mean field approximation $\hat{H}_{sf}$

$$\hat{H}_{sf} = \frac{1}{2}J\sum_{k,k'}[< a^{+}_{k\uparrow}a^{+}_{k\uparrow} > a_{k'\uparrow}a_{k'\uparrow} + < a_{k'\uparrow}a_{k'\uparrow} > a^{+}_{k\uparrow}a^{+}_{k\uparrow} - < a^{+}_{k\uparrow}a^{+}_{k\downarrow} > a_{k'\uparrow}a_{k'\downarrow} - < a_{k\uparrow}a_{k'\downarrow}$$

$$> a^{+}_{k\uparrow}a^{+}_{k\downarrow} - < a^{+}_{k\downarrow}a^{+}_{k\uparrow} > a_{k'\downarrow}a_{k'\uparrow} - < a_{k'\downarrow}a_{k'\uparrow} > a^{+}_{k\downarrow}a^{+}_{k\uparrow} +$$

$$< a^{+}_{k\downarrow}a^{+}_{k\downarrow} > a_{k'\downarrow}a_{k'\downarrow} + < a_{k'\downarrow}a_{k'\downarrow}$$

$$> a^{+}_{k\downarrow}a^{+}_{k\downarrow}]$$

$$+ \mathrm{J}\sum_{kk',}[< a^{+}_{k\uparrow}a^{+}_{k\downarrow} > a_{k'\downarrow}a_{k'\uparrow} + < a_{k'\downarrow}a_{k'\uparrow} > a^{+}_{k\uparrow}a^{+}_{k\downarrow} +$$

$$< a^{+}_{k\downarrow}a^{+}_{k\uparrow} > a_{k'\uparrow}a_{k'\downarrow} + < a_{k'\uparrow}a_{k'\downarrow} > a^{+}_{k\downarrow}a^{+}_{k\uparrow}] - - - - - - - - - - (9)$$

The superconducting order parameter is defined as

$$\Delta^{\uparrow\uparrow} = J\sum_{k\sigma,} < a_{k'\uparrow}a_{k\uparrow} >$$

$$\Delta^{\uparrow\downarrow} = J\sum_{kk',} < a_{k\uparrow}a_{k\downarrow} >$$

From equation of motion, we have

$$\omega \ll a_{k\uparrow} a_{k\uparrow}^{+} \gg = < [a_{k\uparrow}, a_{k\uparrow}^{+}] > + \ll [a_{k\uparrow}, H] a_{k\uparrow}^{+} \gg ----------- (10)$$

When we evaluate $[a_{k\uparrow}, H]$

$$[a_{k\uparrow}, H] = \xi_k \ a_{k\uparrow} + \frac{1}{2}\Delta^{\uparrow\uparrow} a_{k\uparrow}^{+} + \Delta^{\uparrow\downarrow} a_{k\downarrow}^{+} --------------- (11)$$

Plugging eqn(11) into eqn(10),we obtain

$$(\omega - \xi_k) \ll a_{k\uparrow} a_{k\uparrow}^{+} \gg = 1 + \frac{1}{2}\Delta^{\uparrow\uparrow} \ll a_{k\uparrow}^{+} a_{k\uparrow}^{+} \gg - \Delta^{\uparrow\downarrow} \ll a_{k\downarrow}^{+} a_{k\uparrow}^{+} \gg ---- (12)$$

Similarly

$$(\omega + \xi_k) \ll a_{k\uparrow}^{+} a_{k\uparrow}^{+} \gg = -\frac{1}{2}\Delta^{+\uparrow\uparrow} \ll a_{k'\uparrow} a_{k\uparrow}^{+} \gg - \Delta^{\uparrow\downarrow} \ll a_{k'\downarrow} a_{k\uparrow}^{+} \gg ---- (13)$$

$$(\omega + \xi_k) \ll a_{k\downarrow}^{+} a_{k\uparrow}^{+} \gg = -\frac{1}{2}\Delta^{+\downarrow\downarrow} \ll a_{k'\downarrow} a_{k\uparrow}^{+} \gg - \Delta^{+\uparrow\downarrow} \ll a_{k\downarrow} a_{k\uparrow}^{+} \gg ---- (14)$$

$$(\omega - \xi_k) \ll a_{k\downarrow} a_{k\uparrow}^{+} \gg = \frac{1}{2}\Delta^{\downarrow\downarrow} \ll a_{k\downarrow}^{+} a_{k\uparrow}^{+} \gg + \Delta^{\uparrow\downarrow} \ll a_{k\downarrow}^{+} a_{k\uparrow}^{+} \gg ------ (15)$$

Combining eqn(12),eqn(13),eqn(14)and eqn(15),we obtain

$$\ll a_{k\uparrow}^{+} a_{k\uparrow}^{+} \gg = \frac{-\frac{\Delta^{+\uparrow\uparrow}}{2}}{(\omega^2 - \xi_k{}^2 - \frac{1}{4}(\Delta^{+\uparrow\uparrow})^2)} --------------- (16)$$

The superconducting order parameter for $(\uparrow\uparrow)$ is given by

$$\Delta^{+\uparrow\uparrow} = \frac{1}{\beta}\sum_{n,k} J \ll a_{k\uparrow}^{+} a_{k\uparrow}^{+} \gg --------------------- (17)$$

$$\Delta^{+\uparrow\uparrow} = \frac{1}{\beta}\sum_{n,} \int_0^\infty d\xi \, D(\xi_k) J \frac{-\frac{\Delta^{+\uparrow\uparrow}}{2}}{\left(\omega^2 - \xi_k{}^2 - \frac{1}{4}(\Delta^{+\uparrow\uparrow})^2\right)} ----------- (18)$$

Applying

$\Delta(k) = \sum_{k,k'} \eta \Delta(k')$ and $D(\xi) = \eta \Delta D(0)$, For D-wave pairing $\eta = \frac{1}{2}$

$\lambda_{sf} = \sum_{k,k'} JD(0)$

Replacing $\xi^2 = \xi_k{}^2 + \frac{1}{4}(\Delta^{+\uparrow\uparrow})^2$ and $\omega_n = \frac{(2n+1)\pi}{\beta}$

$\omega = i\omega_n$ for Matsubara frequency of fermions

$$1 = \frac{\lambda_{sf}}{\beta} \sum_{n,} \int_0^{\hbar\omega} d\xi \frac{1}{((2n+1)^2\pi^2 - \beta^2\xi^2)}$$

Let $z = \beta\xi$

$$\frac{1}{\lambda_{sf}} = \frac{1}{\beta} \sum_{n,} \int_0^{\hbar\omega} d\xi \frac{1}{((2n+1)^2\pi^2 - z^2)} \text{-----------------}(19)$$

$$\frac{1}{\beta} \sum_{n,} \frac{1}{((2n+1)^2\pi^2 - z^2)} = \frac{\tanh\left(\frac{\beta z}{z}\right)}{2z}$$

$$\frac{1}{\lambda_{sf}} = \int_0^{\hbar\omega} d\xi \frac{\tanh\left({}^{\beta}/{}_{2}\sqrt{\xi^2 + (\frac{\Delta}{4})^2}\right)}{\sqrt{\xi^2 + (\frac{\Delta}{4})^2}} \text{-----------------}(20)$$

1) When $T = T_c \Rightarrow \Delta = 0$ equation()becomes

$$\frac{1}{\lambda_{sf}} = \int_0^{\hbar\omega} d\xi \frac{\tanh(\frac{\beta\xi}{2})}{\xi} \text{--------------------}(21)$$

Integration by parts

$$\frac{1}{\lambda_{sf}} = \ln\left(\frac{\beta_c\hbar\omega}{2}\right)\tanh\left(\frac{\beta_c\hbar\omega}{2}\right) - \frac{\beta}{2}\int_0^{\hbar\omega} d\xi \frac{\ln(\frac{\beta\xi}{2})}{Cosh(\frac{\beta\xi}{2})^2} \text{---------}(22)$$

$$\frac{1}{\lambda_{sf}} = \log\left(\frac{\beta_c \hbar\omega}{2}\right) + \gamma - \log\left(\frac{\pi}{4}\right) ----------------(23)$$

$$T_c = \frac{\hbar\omega_m}{k_B} e^{\frac{-1}{\lambda_{sf}}} ------------------------(24)$$

2) At finite temperature

$$\frac{1}{\lambda_{sf}} = \int_0^{\hbar\omega} d\xi \frac{\tanh\left({}^{\beta}/_{2}\sqrt{\xi^2 + (\frac{\Delta}{4})^2}\right)}{\sqrt{\xi^2 + (\frac{\Delta}{4})^2}} ---------------(25)$$

Using Taylor expansion

$$\frac{1}{\lambda_{sf}} = \int_0^{\infty} d\xi \frac{\tanh\left({}^{\beta}/_{2}\sqrt{\xi^2 + (\frac{\Delta}{4})^2}\right)}{\sqrt{\xi^2 + (\frac{\Delta}{4})^2}}$$

$$= \int_0^{\hbar\omega} d\xi \frac{\tanh(\frac{\beta\xi}{2})}{\xi} + \frac{\Delta^2}{8}\int_0^{\infty} \frac{\beta z - \sinh(\beta z)}{2z^2 Cosh^2(\frac{\beta z}{2})} --(26)$$

$$\int_0^{\infty} \frac{\beta z - \sinh(\beta z)}{2z^2 Cosh^2\left(\frac{\beta z}{2}\right)} = \frac{-14\zeta(3)}{\pi^2} -----------------(27)$$

Where ζ zeta functions

Employing this equation into eqn(26),we obtain

$$\frac{1}{\lambda_{sf}} = \int_0^{\infty} d\xi \frac{\tanh(\frac{\beta\xi}{2})}{\xi} + \frac{\Delta^2}{8}\left[\frac{\beta_c^2}{8}\right]\frac{-14\zeta(3)}{\pi^2} ------------(28)$$

$$\ln\left(\frac{2\beta_c \omega e^{\gamma}}{\pi}\right) = \ln\left(\frac{2\beta\omega e^{\gamma}}{\pi}\right) - \frac{14\Delta^2\zeta(3)}{64\pi^2 k_B^2 T_c^2}$$

$$\ln\left(\frac{T}{T_c}\right) = -\frac{14\Delta^2\zeta(3)}{64\pi^2 k_B^2 T_c^2} ----------------------(29)$$

We use approximation $e^x \approx 1 + x$, Where $x = -\frac{14\Delta^2 \zeta(3)}{64\pi^2 k_B^2 T_c^2}$ and $\zeta(3) = 1.2025$

Employing this equation into

$$\Delta = 6.12 k_B T_c \sqrt{\left[1 - \frac{T}{T_c}\right]} \quad (30)$$

This is the superconducting order parameter as a function of temperature

4. Result and Discussion

This section concerned with theoretical results of high temperature superconductivity which are obtained using the equations derived in section 3.The main focus is on the superconductive transition temperature, the superconducting order parameter and coupling strength. The expression of superconducting transition temperature from eqn (24) is

$$T_c = \frac{\hbar\omega_m}{k_B} e^{\frac{-1}{\lambda_{sf}}} = 8.67X10^{-12}\omega_m \ e^{-\frac{1}{\lambda_{sf}}}$$

Now taking $\frac{\hbar\omega_m}{k_B} = 158.7K, \lambda_{sf} = 1.5$

$$\Rightarrow T_c \approx 92.4K$$

Moreover, the results of our work are best described by figures depicted below

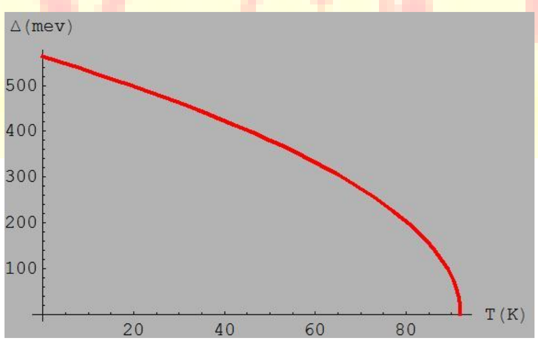

Fig1 superconducting order parameter versus temperature

From Fig .1, we can observe that the superconducting order parameter decreases monotonically as the temperature increases and vanishes at $T_c = 92.4K$. Below T_c , it is the region of superconducting state whereas above T_c ,it is normal state.

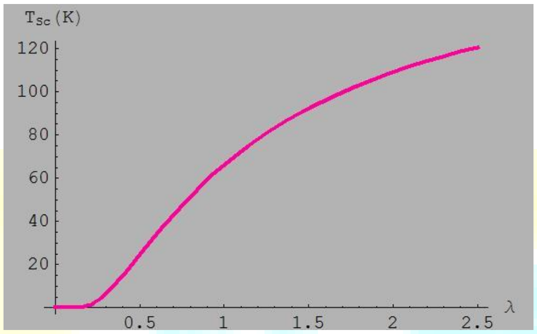

Fig2 Superconducting transition temperature versus coupling strength

The superconducting transition temperature increases as the coupling strength parameter increases and becomes slowly increase as the coupling strength parameter increases further

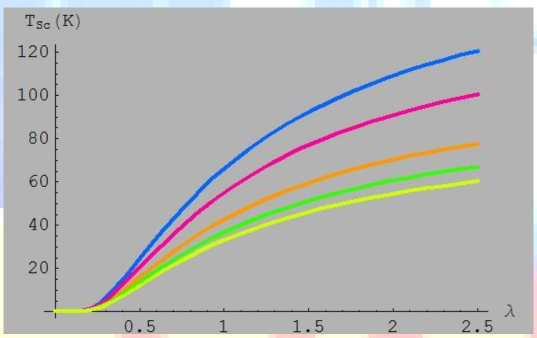

Fig3 Superconducting transition temperature versus coupling strength for different magnon frequency

5. Conclusion

In this paper, we have studied the high temperature superconductivity involving cuprate with the help of retarded Green function technique and Hamiltonian model. We have determined analytically the superconducting transition temperature for Y $Ba_2Cu_3O_{6:93}$ and the result is very close to the experiment result. We also observed that the superconducting order parameter decreases monotonically with the increasing temperature and disappear at the superconducting transition temperature for Y $Ba_2Cu_3O_{6:93}$.

Reference

[1] Heike Kammerling Onnes, Commn.Phys.Lab.Univ.Leiden, **12**,120(1911)

[2] J.Bardeen, L.N.Coopper and J.R.Scrieffer, Phys.Rev, 108, 1175(1957)

[3] J. Bednorz, and K.A. Muller, Z.Phys.B, **64**,189(1986)

[4] Schilling A.; Cantoni M.Guo, J.D.Ott, H, R.Nature, **363**, 56-58(1993)

[5] Gao.L.etal., Phys.Rev.B, **50**, 4260-4263(1994)

[6] Y.Kamihara ,etal., J.Am.Chem.Soc.**130**, 3296(2008)

[7] C.Wang.etal., Eurosphys.Lett.**83**, 67006(2001)

[8] Singh .P, Sinha K.P, J. Solid state communication, **73**, 45(1990)