Order parameter & interlayer interaction in high Tc superconductors

Sarita Khandka and Piyush Masih

Department of Physics, Allahabad Agricultural Institute
Deemed University, Allahabad, India
E-mail: saritakh@rediffmail.com

(Received May 05, 2008)

Abstract: Understanding the unusual physical properties of high Tc Cuprates superconductors continues to be one of the most challenging and exciting open problems in the solid state physics. These high Tc Cuprate superconductors contain CuO_2 layers which are very useful for conduction. The interlayer interactions between these layers are very important & useful for enhancement of Transition temperature. It has been found that interlayer interaction plays an important role in enhancement of Tc and stabilizes the superconducting order with respect to fluctuations. In this paper we observed by using Green's function technique that interlayer interaction helps to increase superconducting order parameter Δ and stabilize superconductivity.

1. Introduction

After 70 years from the discovery of superconductor by Kamerleingh Onnes[1], scientists were not able to push transition temperature above 23 K (for Nb_3Ge). But in 1986, decisive breakthrough in superconductivity research occurred, when Bednorz and Muller[2] discovered copper oxide compounds of the La-Ba-Cu-O system showed a transition temperature of about 30K. After that a series of high Tc cuprate superconductors are discovered. The highest transition temperature reached till date is 160K under extremely applied pressure for Hg-Ba-Ca-CuO_2.

Experimentally, it is known that the superconducting transition temperature (Tc) for multilayered high Tc superconductors does not monotonically increase with the number of CuO_2 layers n. The Tc increases with n up to n = 3, but then starts to drop for n > 4 [3–4].

This is in sharp contrast to the general expectation that Tc increases while n increases, suggesting that the charge carriers were not distributed equally in energy CuO_2 plane within a unit cell[5]. This is also confirmed by Cu – NMR experiment[6].

Interlayer interactions are found to increase Tc and stabilize superconducting order against fluctuations[7-9]. In view of above, here we try to investigate pairing gap taking interlayer interaction with in mean field theory irrespective of pairing mechanism responsible for it.

2. Mathematical Technique & Formulation

In the present work double-time retarded Green's function technique has been used as a mathematical tool for investigation of superconducting order parameter (Δ).

The Hamiltonian for our system can be described as:

$$H = \sum_{ik\sigma} E_k C^{+}_{ik\sigma} C_{ik\sigma} - \sum_{ikk'} V_{ii}(kk') C^{+}_{ik'\uparrow} C^{+}_{i-k'\downarrow} C_{i-k\downarrow} C_{ik\uparrow} - \sum_{ijkk'} V_{ij}(kk') C^{+}_{ik'\uparrow} C^{+}_{i-k'\downarrow} C_{j-k\downarrow} C_{jk\uparrow} \quad (1)$$

where $C^{+}_{ik\sigma}$, $C_{ik\sigma}$ denote the fermion creation & annihilation operator respectively, K is the wave vector and σ is spin index for fermions.

In equation (1), the first term is the energy of the free charge carriers within the CuO_2 planes. The second term describes BCS type intralayer attractive interaction originating from any proposed mechanism. And the third term represents interlayer pairing and V_{ij} represents the attractive interlayer interactions.

In our present analysis we use a Green's function, defining as:

$$G^{\uparrow\uparrow}_{rsqq} = \left\langle\left\langle C_{rq\uparrow}, C^{+}_{sq\uparrow} \right\rangle\right\rangle \quad (2)$$

and writing equation of motion as

$$\omega G^{\uparrow\uparrow}_{rsqq} = \frac{1}{2\pi} + \left\langle\left\langle [C_{rq\uparrow}, H], C^{+}_{sq\uparrow} \right\rangle\right\rangle \quad (3)$$

Now, evaluating the commutator [$C_{ik\uparrow}$, H] using the Hamiltonian (1), we get the commutative relation between $C_{ik\uparrow}$ & H , which is defined as follows:

$$[C_{rq\uparrow}, H] = E_q C_{rq\uparrow} - \sum_k V_{rr}(kq) C^{+}_{r-q\downarrow} C_{r-k\downarrow} C_{rk\uparrow} - \sum_{\substack{j,\,k \\ r\neq j}} V_{rj}(kq) C^{+}_{r-q\downarrow} C_{j-k\downarrow} C_{jk\uparrow}$$

Putting the value of commutator [$C_{ik\uparrow}$, H] in the equation (3), we get

$$\begin{aligned} \omega G^{\uparrow\uparrow}_{rsqq} &= \frac{1}{2\pi} + \left\langle\left\langle E_q C_{rq\uparrow}, C^{+}_{sq\uparrow} \right\rangle\right\rangle \\ &\quad - \sum_k V_{rr}(kq) \left\langle\left\langle C^{+}_{r-q\downarrow} C_{r-k\downarrow} C_{rk\uparrow}, C^{+}_{sq\uparrow} \right\rangle\right\rangle \\ &\quad - \sum_{\substack{j,k \\ r\neq j}} V_{rj}(kq) \left\langle\left\langle C^{+}_{r-q\downarrow} C_{j-k\downarrow} C_{jk\uparrow}, C^{+}_{sq\uparrow} \right\rangle\right\rangle \end{aligned} \quad (4)$$

Now we introduce the order parameter Δ such as:

$$\Delta_{rr} = \sum_k V_{rr}(kq)\left\langle C^+_{rk\uparrow}, C^+_{r-k\downarrow}\right\rangle$$

$$\Delta_{rj} = \sum_k V_{rj}(kq)\left\langle C^+_{jk\uparrow}, C^+_{j-k\downarrow}\right\rangle$$

Substituting these order parameters in equation (4), finally we obtained the equation:

(5) $$(\omega - E_q)G^{\uparrow\uparrow}_{rsqq} = \frac{1}{2\pi} - (\Delta_{rr} + \sum_{\substack{j \\ r\neq j}} \Delta_{rj})G^{\downarrow\uparrow}_{rs-qq}$$

where, $G^{\downarrow\uparrow}_{rs-qq}$ is another Green's function, which may be written as:

(6) $$G^{\downarrow\uparrow}_{rs-qq} = \left\langle\left\langle C^+_{r-q\downarrow}, C^+_{sq\uparrow}\right\rangle\right\rangle$$

This Green's function may also be written in term of equation of motion as:

(7) $$\omega G^{\downarrow\uparrow}_{rs-qq} = \left\langle\left\langle\left[C^+_{r-q\downarrow}, H\right], C^+_{sq\uparrow}\right\rangle\right\rangle$$

Evaluating the Commutator $[C^+_{r-q\downarrow}, H]$ using the Hamiltonian (1)

$$[C^+_{r-q\downarrow}, H] = [C^+_{r-q\downarrow}, \sum_{ik\sigma} E_k C^+_{ik\sigma} C_{ik\sigma}] - [C^+_{r-q\downarrow}, \sum_{ikk'} V_{ii}(kk')C^+_{ik'\uparrow} C^+_{i-k'\downarrow} C_{i-k\downarrow} C_{ik\uparrow}]$$

(8) $$-[C^+_{r-q\downarrow}, \sum_{ijkk'} V_{ij}(kk')C^+_{ik'\uparrow} C^+_{i-k'\downarrow} C_{j-k\downarrow} C_{jk\uparrow}]$$

Substituting the value of $[C^+_{r-q\downarrow}, H]$ in equation (7)

$$\omega G^{\downarrow\uparrow}_{rs-qq} = -E_{-q} G^{\downarrow\uparrow}_{rs-qq} - \sum_{k'} V_{rr}(qk')\left\langle C^+_{rk'\uparrow}, C^+_{r-k'\downarrow}\right\rangle\left\langle\left\langle C_{rq\uparrow}, C^+_{sq\uparrow}\right\rangle\right\rangle$$

$$-\sum_{\substack{k' \\ i\neq r}} V_{ir}(k'q)\left\langle C^+_{ik'\uparrow}, C^+_{i-k'\downarrow}\right\rangle\left\langle\left\langle C_{rq\uparrow}, C^+_{sq\uparrow}\right\rangle\right\rangle$$

But from the law of conservation of energy $E_{-q} = E_q$. So

(9) $$(\omega + E_q)G^{\downarrow\uparrow}_{rs-qq} = -(\Delta_{rr} + \sum_{i\neq r} \Delta_{ri})G^{\uparrow\uparrow}_{rsqq} ,$$

where Δ_{rr} & Δ_{ri} are order parameters which may be denoted as

(10) $$\Delta_{rr} = \sum_{k'} V_{rr}(qk')\left\langle C^+_{rk'\uparrow}, C^+_{r-k'\downarrow}\right\rangle$$

$$\Delta_{ir} = \sum_{k'} V_{ir}(k'q)\left\langle C^+_{ik'\uparrow}, C^+_{i-k'\downarrow}\right\rangle$$

Now, by the help of equation (5) & equation (9), we can calculate both Green's functions $G^{\uparrow\uparrow}_{rsqq}$ & $G^{\downarrow\uparrow}_{rs-qq}$.

(11) $$G^{\uparrow\uparrow}_{rsqq} = \frac{(\omega + E_q)}{2\pi[\omega^2 - E^2{}_q - (\Delta_{rr} + \sum\limits_{j\neq r}\Delta_{rj})(\Delta_{rr} + \sum\limits_{i\neq j}\Delta_{ri})]}$$

(12) $$G^{\downarrow\uparrow}_{rs-qq} = \frac{-(\Delta_{rr} + \sum\limits_{i\neq r}\Delta_{ri})}{2\pi[\omega^2 - E^2{}_q - (\Delta_{rr} + \sum\limits_{j\neq r}\Delta_{rj})(\Delta_{rr} + \sum\limits_{i\neq j}\Delta_{ri})]}$$

Using these Green's functions, we can obtain the expression for order parameter Δ_{ir} & correlation parameter γ.

The order parameter Δ_{ir} may be written as

(13) $$\Delta_{ir} = \sum_{k'} V_{ir}(k'q)\left\langle C^{+}_{ik'\uparrow}, C^{+}_{i-k'\downarrow}\right\rangle$$

Correlation function $\left\langle C^{+}_{ik'\uparrow}, C^{+}_{i-k'\downarrow}\right\rangle$ is related to Green's function $G^{\downarrow\uparrow}_{rs-qq}$ as

(14) $$\left\langle C^{+}_{ik'\uparrow}, C^{+}_{i-k'\downarrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty} \frac{G^{\downarrow\uparrow}_{rs-qq}(\omega+i\varepsilon) - G^{\downarrow\uparrow}_{rs-qq}(\omega-i\varepsilon)}{e^{\frac{\omega}{kT}} - \eta} d\omega$$

where η = -1, for fermion, K = Boltzmann constant & T = Temperature.

Green`s function $G^{\downarrow\uparrow}_{rs-qq}$(ω + iε) & $G^{\downarrow\uparrow}_{rs-qq}$(ω - iε) may be expressed as:

(15a) $$G^{\downarrow\uparrow}_{rs-qq}(\omega + i\varepsilon) = \frac{-(\Delta_{rr} + \sum\limits_{i\neq j}\Delta_{ri})}{2\pi[(\omega+i\varepsilon)^2 - Eq^2 - (\Delta_{rr} + \sum\limits_{j}\Delta_{rj})(\Delta_{rr} + \sum\limits_{i}\Delta_{ri})]}$$

(15b) $$G^{\downarrow\uparrow}_{rs-qq}(\omega - i\varepsilon) = \frac{-(\Delta_{rr} + \sum\limits_{i\neq j}\Delta_{ri})}{2\pi[(\omega-i\varepsilon)^2 - Eq^2 - (\Delta_{rr} + \sum\limits_{j}\Delta_{rj})(\Delta_{rr} + \sum\limits_{i}\Delta_{ri})]}$$

Substitute both Green's functions $G^{\downarrow\uparrow}_{rs-qq}$(ω + iε) & $G^{\downarrow\uparrow}_{rs-qq}$(ω - iε) from equation (15) and then after solving, we get correlation function:

$$\left\langle C^{+}_{ik'\uparrow}, C^{+}_{i-k'\downarrow} \right\rangle =$$

$$\frac{(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}} \tanh \frac{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}}{2KT}$$

Then we can obtain the expression of order parameter Δ_{ir} by substituting correlation function in equation (13)

(16) $\Delta_{ir} = \sum_{k'} V_{ir}(k'q)$

$$\frac{(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}} \tanh \frac{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}}{2KT}$$

Converting summation over k' into integration with cut-off energy $\pm\hbar\omega_D$ from the fermi level, we get:

(17) $\Delta_{ir} =$

$$N_0 \int_0^{\pm\hbar\omega_D} V_{ir} \frac{(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}} \tanh \frac{\sqrt{E_q^2 + (\Delta_{rr} + \sum_{\substack{j \\ r \neq j}} \Delta_{rj})(\Delta_{rr} + \sum_{i \neq r} \Delta_{ri})}}{2KT} \, dE_q$$

Thus, using the equation (17), we can calculate the order parameters of different layers with respect to temperature. We can also draw the curve between Δ versus T for different values of $1/N_0V_{ir}$.

3. Result & Discussion

Interlayer order parameter Δ_{12} is calculated numerically for different values of interlayer interaction from equation (17). Fig. 1 shows variation of Δ_{12} with temperature. It is clear from the graph that interlayer order parameter increases with increase in interlayer interaction. This is in the agreement with earlier results[5-7] which suggests increase in Tc with increasing interlayer interaction.

Further large order parameter implies more Tc, this with our result suggests that interlayer interaction increases Tc and helps to stabilize superconductivity. The results are relevant for La(Ba/Sr)CuO, YBaCuO, BiSrCaCuO and TlBaCaCuO, where layers of CuO_2 are present in a single unit cell.

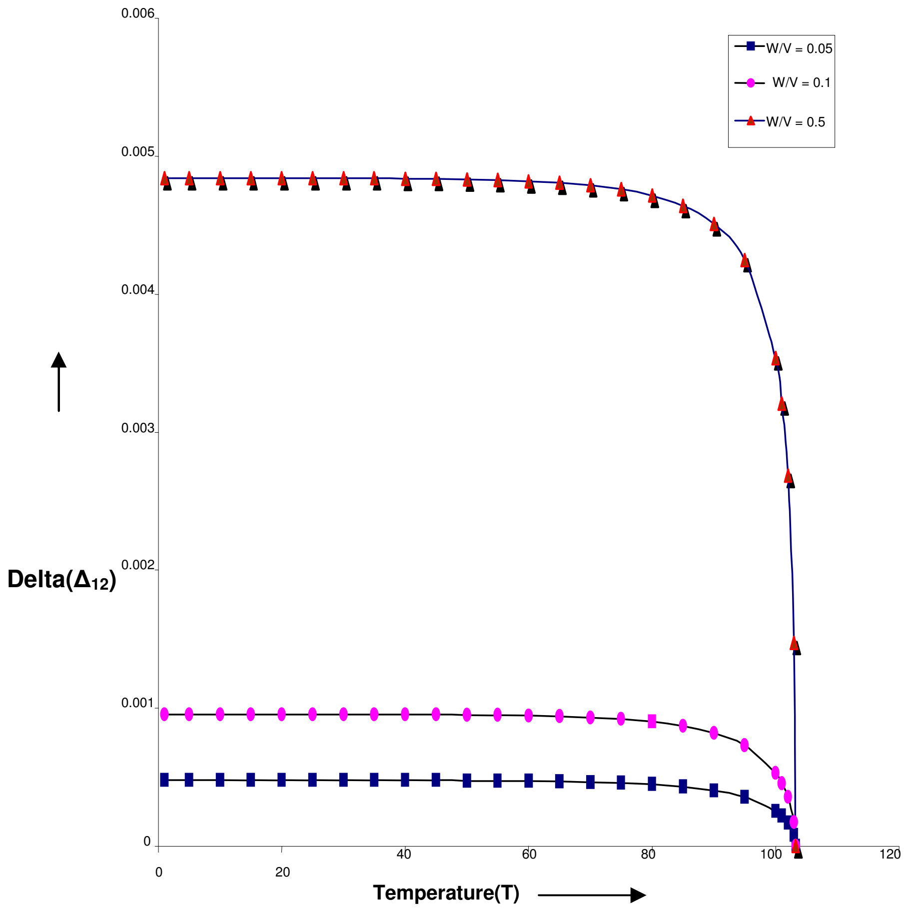

Fig. 1 Interlayer order parameter (**Δ_{12}**) Vs Temperature (**T**)

References

1. H. kamerliengh ones, *Akad. Van Wetenschappen* (Amsterdam) **14** (1911) 113, 818.
2. J. M. Bednorz and K. A. Muller, *Z. Phys.* **B64** (1986) 189.
3. H. Kotegawa. et al., *Phys. Rev.* **B63** (2001) 064508.
4. Y. Zhuo et al., *Phys. Rev.* **B 60** (1999) 13094.
5. S. L. Cooper and K. E. Gray, in physical properties of high temperature superconductors IV (World scientific, Singapore, 1994), 61.
6. H. Kotegawa. et al., *Phys. Rev.* **B64** (2001) 064515.
7. Z. Tesanovic, *Phys. Rev.* **B36** (1991) 2364.
8. U. Hofmann et al., *Solid State Communication* **70** (2001) 325.
9. A. R. Bishop et al., *Z. Phys.* **B7** (2001) 1020.