# CHAPTER – 3

## MATHEMATICAL TECHNIQUE AND FORMULATION

In the present Work double-time retarded Green's function technique given by Zubarev (1960) is used as a mathematical tool for investigations. The Green's functions are the appropriate generalization of the concept of correlation functions and work as a propagator. They are connected with the evaluation of observed quantities and have well known advantages when equation are formulated and solved.

In many body problems, determining properties of the system by solving the exact many body eigen function is very complicated. In such case and many others, the Green's function technique turns out to be simple, direct and very useful.

In statistical mechanism different kinds of Green's functions are used. They are double time casual Green's function $G_c(t,t`)$ , retarded Green's function $G_a(t,t`)$ & Advanced Green's function $G_a(t,t`)$. But in the present work only double-time retarded green's function is used. It is defined as follows:

$$G_r(t,t') = \left\langle\left\langle A(t), B(t,t') \right\rangle\right\rangle_r = -i\theta(t-t')\left\langle [A(t), B(t')\right\rangle \tag{3.1}$$

Where, $A(t)$, $B(t')$ are the Heisenberg representation of operator $A$ & $B$, expressed in terms of a product of quantized field function ( or of particle creation and annihilation operators).

We know, $A(t) = e^{iHt} A(0)\, e^{-iHt}$ , H is Hamiltonian operator. $[A,B]_+$ & $[A,B]_-$ indicates the commutator or anti commutator respectively.

$[A,B]_\eta = AB - \eta BA$ ,where $\eta = +1$ for Bose operator

&, $\eta = -1$ for fermi operator.

The symbol $T$ indicates the time order or $T$ product of operators, which is defined as-

$T\, A(t)\, B(t`) = \theta(t-t`)\, A(t)\, B(t`) + \eta\, \theta(t-t`)\, B(t`)\, A(t)$

And $\theta(t)$ is the unit step function, unity for positive $t$ and zero for negative $t$.

Differentiating retarded Green's function (3.1) with respect to time, we get:-

$$i\frac{dG_r}{dt} = i\frac{d}{dt}\langle\langle A|B\rangle\rangle_r = \frac{d\theta(t-t`)}{dt}\langle[A(t),B(t`)]\rangle - i\theta(t-t`)\left\langle\frac{idA(t)}{dt},B(t`)\right\rangle \tag{3.2}$$

Taking into account the relation between the discontinuous function *θ(t)* and the *δ*-function:-

$$\theta(t) = \int_{-\infty}^{t}\delta(t)\,dt$$

And the equation of motion is , $i\frac{dA}{dt} = [A,H]_-$

So, the equation (3.2) may be written as-

$$i\frac{dG_r}{dt} = \delta(t-t`)\langle[A(t),B(t`)]\rangle + \langle\langle[A(t),H]|B(t`)\rangle\rangle \tag{3.3}$$

Taking the fourier transformation of this equation (3.3)-

$$\omega\langle\langle A|B\rangle\rangle_\omega = \frac{1}{2\pi}\langle[A,B]_\eta\rangle + \langle\langle[A,H]|B\rangle\rangle_\omega$$

here, $\langle\langle A|B\rangle\rangle_\omega = \langle\langle A|B\rangle\rangle_\omega^+$ if $I_m\ \omega > 0$

$= \langle\langle A|B\rangle\rangle_\omega^-$ if $I_m\ \omega < 0$

The correlation function $\langle B(t`), A(t)\rangle$ is related to Green's function by

$$\langle B(t`),A(t)\rangle = i\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty}\frac{[\langle\langle A|B\rangle\rangle_{\omega+i\varepsilon} - \langle\langle A|B\rangle\rangle_{\omega-i\varepsilon}]}{e^{\frac{\omega}{K_BT}}+1}e^{i\omega(t-t`)}\,d\omega \tag{3.4}$$

Where, $K_B$ is Boltzmann constant.

In this present work, two problems have been taken and solved using the advantage of this Green's function technique. First problem is described for the high $T_C$ cuprate superconductors and the second one is for Iron Pnictide Superconductors. The mathematical formulation has been divided in two parts.

## 3.1 HIGH $T_C$ CUPRATES SUPERCONDUCTORS

The Hamiltonian for high $T_C$ cuprate superconductor can be described as:-

$$H = \sum_{k\sigma} E_k a^+_{k\sigma} a_{k\sigma} - V \sum_{kk'} a^+_{k'\uparrow} a^+_{-k'\downarrow} a_{-k\downarrow} a_{k\uparrow} + \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma}$$
$$+ U \sum_{l} a^+_{l\uparrow} a_{l\uparrow} a^+_{l\downarrow} a_{l\downarrow} - \sum_{lm\,\sigma\sigma'} J_{lm} a^+_{l\sigma} a^+_{m\sigma'} a_{l\sigma'} a_{m\sigma}$$
$$+ \sum_{klm} \tau^{lm}_{k} ( a^+_{l\uparrow} a^+_{m\downarrow} a_{-k\downarrow} a_{k\uparrow} + a^+_{k\uparrow} a^+_{-k\downarrow} a_{m\downarrow} a_{l\uparrow} ) \tag{3.5}$$

Where, $a^+_{k\sigma}$ , $a_{k\sigma}$ denoted the fermion creation & annihilation operator for conduction electrons and $a^+_{l\sigma}$ , $a^+_{m\sigma}$ & $a_{l\sigma}$ , $a_{m\sigma}$ denoted the fermion creation & annihilation operator for localized electrons respectively. σ is spin index for fermions. In equation (3.5) the first term is the energy of the free charge carriers within the $CuO_2$ planes. The second term describes BCS type interlayer pairing and $V$ represent the attractive interlayer interactions between conduction electrons. $E_l$ is the energy of the localized electrons, $U$ is the intrasite interaction energy of localized electrons, $J_{lm}$ is the spin exchange interaction between localized electrons and $\tau^{lm}_{k}$ is the spin exchange interaction between localized and conduction electrons.

We consider two Green function's for conduction layers, which are define as:

$$G^{\uparrow\uparrow}_{qq} = \langle\langle a_{q\uparrow} , a^+_{q\uparrow} \rangle\rangle \tag{3.6}$$

$$G^{\downarrow\uparrow}_{-qq} = \langle\langle a^+_{-q\downarrow} , a^+_{q\uparrow} \rangle\rangle \tag{3.7}$$

Using the model Hamiltonian equation (3.5) and Green's function defined by (3.6) & (3.7), we obtain the following two equation of motion:

$$(\omega - E_q) G^{\uparrow\uparrow}_{qq} = \frac{1}{2\pi} + (\Delta - \phi_{ml}) G^{\downarrow\uparrow}_{-qq} \tag{3.8}$$

$$(\omega + E_q) G^{\downarrow\uparrow}_{-qq} = (\Delta - \phi_{ml}) G^{\uparrow\uparrow}_{qq} \tag{3.9}$$

Here, $\phi_{ml} = \sum_{lm} \tau_q^{lm} \langle a_{m\uparrow} a_{l\downarrow} \rangle$

And, $\Delta = \sum_q V \langle C_{-q\downarrow} C_{q\uparrow} \rangle$

After solving equation (3.8) & (3.9), we get two Green's functions:

$$G_{qq}^{\uparrow\uparrow} = \frac{(\omega + E_q)}{2\pi[\omega^2 - E_q^2 + (\Delta - \phi_{ml})^2]} \tag{3.10}$$

$$G_{-qq}^{\downarrow\uparrow} = \frac{-(\Delta - \phi_{ml})}{2\pi[\omega^2 - E_q^2 + (\Delta - \phi_{ml})^2]} \tag{3.11}$$

The correlation function $\langle C_{-q\downarrow} C_{q\uparrow} \rangle$ is related to Green's function (3.7), as:

$$\langle C_{-q\downarrow} C_{q\uparrow} \rangle = i \int_{-\infty}^{\infty} \frac{[G_{-qq}^{\downarrow\uparrow}(\omega + i\varepsilon) - G_{-qq}^{\downarrow\uparrow}(\omega - i\varepsilon)]}{e^{\beta\omega} - 1} d\omega \tag{3.12}$$

After solving equation (3.11) & (3.12), we get the correlation function:

$$\langle C_{-q\downarrow} C_{q\uparrow} \rangle = \frac{(\Delta - \phi_{ml})}{2\sqrt{E_q^2 - (\Delta - \phi_{ml})^2}} \tan h \frac{\sqrt{E_q^2 - (\Delta - \phi_{ml})^2}}{2KT} \tag{3.13}$$

The superconducting order parameter $\Delta$ is related to this correlation function $\langle C_{-q\downarrow} C_{q\uparrow} \rangle$ as:

$$\Delta = \sum_q V \langle C_{-q\downarrow} C_{q\uparrow} \rangle \tag{3.14}$$

By Putting the correlation function $\langle C_{-q\downarrow} C_{q\uparrow} \rangle$ in this equation (3.14), we get the expression of superconducting order parameter $\Delta$ as:

$$\Delta = \sum_q V \frac{(\Delta - \phi_{ml})}{2\sqrt{E_q^2 - (\Delta - \phi_{ml})^2}} \tan h \frac{\sqrt{E_q^2 - (\Delta - \phi_{ml})^2}}{2KT} \tag{3.15}$$

Now, we introduce a Green's function for localized sites, defining as-

$$G_{l'l'}^{\uparrow\uparrow} = \langle\langle a_{l'\uparrow}, a_{l'\uparrow}^{+} \rangle\rangle \tag{3.16}$$

and writing equation of motion as-

$$\omega G_{l'l'}^{\uparrow\uparrow} = \frac{1}{2\pi} + \left\langle\left\langle [a_{l'\uparrow}, H], a_{l'\uparrow}^{+} \right\rangle\right\rangle \tag{3.17}$$

Now, evaluating the commutator $[a_{l'\uparrow}, H]$ using the Hamiltonian (3.5), we get the commutative relation :

$$[a_{l'\uparrow}, H] = E_{l'}a_{l'\uparrow} + Ua_{l'\uparrow}a_{l'\downarrow}^{+}a_{l'\downarrow} + \sum_{m} J_{l'm}a_{m\downarrow}^{+}a_{l'\downarrow}a_{m\uparrow} - \sum_{l} J_{ll'}a_{l\downarrow}^{+}a_{l\uparrow}a_{l'\downarrow}$$
$$+ \sum_{km} \tau_{k}^{l'm} a_{m\downarrow}^{+} a_{-k\downarrow} a_{-k\downarrow} a_{k\uparrow}$$

Putting the value of commutator $[a_{l'\uparrow}, H]$ in the equation (3.17) we get-

$$\omega G_{l'l'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{l'}\left\langle\left\langle a_{l'\uparrow}; a_{l'\uparrow}^{+}\right\rangle\right\rangle - U\left\langle a_{l'\uparrow}a_{l'\downarrow}\right\rangle\left\langle\left\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle - \sum_{m'} J_{l'm'}\left\langle a_{m'\uparrow}a_{l'\downarrow}\right\rangle\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle$$
$$-\sum_{m'} J_{m'l'}\left\langle a_{m'\uparrow}a_{l'\downarrow}\right\rangle\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle + \sum_{km'} \tau_{k}^{l'm'}\left\langle a_{-k\downarrow}a_{k\uparrow}\right\rangle\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle \tag{3.18}$$

Now we introduce the superconducting order parameter $\Delta_k$ and magnetic order parameter $\phi_{l'l'}$ for same localized site and $\phi_{l'm'}$ for different localized site such as-

$$\Delta_k = \sum_k V\left\langle a_{-k\downarrow}a_{k\uparrow}\right\rangle$$
$$\Delta_k = \sum_k V\left\langle a_{k\uparrow}^{+}a_{-k\downarrow}^{+}\right\rangle \quad , \quad \phi_{l'l'} = U\left\langle a_{l'\uparrow}a_{l'\downarrow}\right\rangle$$
$$\phi_{l'l'} = U\left\langle a_{l'\downarrow}^{+}a_{l'\uparrow}^{+}\right\rangle$$

$$\phi_{l'm'} = \tau_{k}^{l'm'}\left\langle a_{l'\uparrow}a_{m'\downarrow}\right\rangle$$

And $$\phi_{l'm'} = \tau_{k}^{l'm'}\left\langle a_{m'\downarrow}^{+}a_{l'\uparrow}^{+}\right\rangle$$

Substituting these order parameters in equation (3.18), we obtained the equation:-

$$\omega G_{l'l'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{l'}\left\langle\left\langle a_{l'\uparrow}; a_{l'\uparrow}^{+}\right\rangle\right\rangle - \phi_{l'l'}\left\langle\left\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle - \sum_{m'} \frac{J_{l'm'}}{\tau_{k}^{l'm'}}\phi_{l'm'}\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle$$
$$-\sum_{m'} \frac{J_{m'l'}}{\tau_{k}^{l'm'}}\phi_{l'm'}\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle + \sum_{m'} \frac{\tau_{k}^{l'm'}}{V}\Delta_k\left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\right\rangle\right\rangle \tag{3.19}$$

Now introducing two Green's functions:

$$G_{l'l'}^{\downarrow\uparrow} = \left\langle\left\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+} \right\rangle\right\rangle \tag{3.20}$$

$$G_{m'l'}^{\downarrow\uparrow} = \left\langle\left\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+} \right\rangle\right\rangle \tag{3.21}$$

Substituting these Green function's in equation (3.19), we get-

$$\omega G_{l'l'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{l'} G_{l'l'}^{\uparrow\uparrow} - \phi_{l'l'} G_{l'l'}^{\downarrow\uparrow} - 2\sum_{m'} \frac{J_{l'm'}}{\tau_k^{l'm'}} \phi_{l'm'} G_{m'l'}^{\downarrow\uparrow} + \sum_{m'} \frac{\tau_k^{l'm'}}{V} \Delta_k G_{m'l'}^{\downarrow\uparrow} \tag{3.22}$$

By taking Fourier transformation of equation (3.22) and after solving, finally we get the equation:

$$(\omega - E_{l'}) G_{kk}^{\uparrow\uparrow}(l'l') = \frac{1}{2\pi} - \beta G_{kk}^{\downarrow\uparrow}(l'l') + (\eta - \lambda) G_{kk}^{\downarrow\uparrow}(m'l') \tag{3.23}$$

Where, $\beta = \phi_{l'l'}$, $\lambda = 2\frac{J_{l'm'}}{\tau_k^{l'm'}} \phi_{l'm'} Z_J \gamma_J$ and $\eta = \frac{\tau_k^{l'm'}}{V} \Delta_k Z_\tau \gamma_\tau$ .

Here $Z$ and $\gamma$ are the constants for a Crystal unit cell.

The Green's function (3.21) may be written in term of equation of motion as:-

$$\omega G_{l'l'}^{\downarrow\uparrow} = \left\langle\left\langle \left[ a_{l'\downarrow}^{+}, H \right]; a_{l'\uparrow}^{+} \right\rangle\right\rangle \tag{3.24}$$

Now, evaluating the commutator $[a_{l'\downarrow}^{+}, H]$ using the Hamiltonian (3.5), we get:

$$[a_{l'\downarrow}^{+}, H] = -E_{l'} a_{l'\downarrow}^{+} - U a_{l'\uparrow}^{+} a_{l'\uparrow} a_{l'\downarrow}^{+} + \sum_{m'} J_{l'm'} a_{l'\uparrow}^{+} a_{m'\downarrow}^{+} a_{m'\uparrow} - \sum_{m'} J_{m'l'} a_{m'\downarrow}^{+} a_{l'\uparrow}^{+} a_{m'\uparrow}$$
$$+ \sum_{km'} \tau_k^{m'l'} a_{k\downarrow}^{+} a_{-k\downarrow}^{+} a_{m'\uparrow}$$

Putting the value of commutator $[a_{l'\downarrow}^{+}, H]$ in the equation (3.24) we get-

$$\omega G_{l'l'}^{\downarrow\uparrow} = -E_{l'} \left\langle\left\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+} \right\rangle\right\rangle - U \left\langle a_{l'\downarrow}^{+} a_{l'\downarrow}^{+} \right\rangle \left\langle\left\langle a_{l'\uparrow}; a_{l'\uparrow}^{+} \right\rangle\right\rangle - 2\sum_{m'} J_{l'm'} \left\langle a_{m'\downarrow}^{+} a_{l'\uparrow}^{+} \right\rangle \left\langle\left\langle a_{m'\uparrow}; a_{l'\uparrow}^{+} \right\rangle\right\rangle$$
$$+ \sum_{km'} \tau_k^{l'm'} \left\langle a_{k\uparrow}^{+} a_{-k\downarrow}^{+} \right\rangle \left\langle\left\langle a_{m'\uparrow}; a_{l'\uparrow}^{+} \right\rangle\right\rangle \tag{3.25}$$

By substituting the superconducting and magnetic order parameters in equation (3.25), we obtained the equation:-

$$\omega G_{l'l'}^{\downarrow\uparrow} = -E_{l'}\left\langle\left\langle a_{l'\downarrow}^{+};a_{l'\uparrow}^{+}\right\rangle\right\rangle - \phi_{l'l'}\left\langle\left\langle a_{l'\uparrow};a_{l'\uparrow}^{+}\right\rangle\right\rangle - 2\sum_{m'}\frac{J_{l'm'}}{\tau_k^{l'm'}}\phi_{l'm'}\left\langle\left\langle a_{m'\uparrow};a_{l'\uparrow}^{+}\right\rangle\right\rangle$$

$$+\sum_{m'}\frac{\tau_k^{l'm'}}{V}\Delta_k\left\langle\left\langle a_{m'\uparrow};a_{l'\uparrow}^{+}\right\rangle\right\rangle \tag{3.26}$$

Now introducing another Green's function:

$$G_{l'm'}^{\uparrow\uparrow} = \left\langle\left\langle a_{m'\uparrow};a_{l'\uparrow}^{+}\right\rangle\right\rangle \tag{3.27}$$

Now equation (3.26) becomes-

$$\omega G_{l'l'}^{\downarrow\uparrow} = -E_{l'}G_{l'l'}^{\downarrow\uparrow} - \phi_{l'l'}G_{l'l'}^{\uparrow\uparrow} - 2\sum_{m'}\frac{J_{l'm'}}{\tau_k^{l'm'}}\phi_{l'm'}G_{l'm'}^{\uparrow\uparrow} + \sum_{m'}\frac{\tau_k^{l'm'}}{V}\Delta_k G_{l'm'}^{\uparrow\uparrow} \tag{3.28}$$

By taking Fourier transformation of equation (3.28) and after solving, finally we get the equation:

$$(\omega + E_{l'})G_{kk}^{\downarrow\uparrow}(l'l') = -\beta G_{kk}^{\uparrow\uparrow}(l'l') + (\eta - \lambda)G_{kk}^{\uparrow\uparrow}(m'l') \tag{3.29}$$

Now taking Green's function (3.27) and written in term of equation of motion as:-

$$\omega G_{m'l'}^{\uparrow\uparrow} = \left\langle\left\langle\left[a_{m'\uparrow}, H\right]; a_{l'\uparrow}^{+}\right\rangle\right\rangle \tag{3.30}$$

Now, evaluating the commutator $[a_{m'\uparrow}, H]$ using the Hamiltonian (3.5), we get -

$$[a_{m'\uparrow}, H] = E_{m'}a_{m'\uparrow} - Ua_{m'\uparrow}a_{m'\downarrow}^{+}a_{m'\downarrow} - 2\sum_{l'}J_{l'm'}a_{l'\downarrow}^{+}a_{l'\uparrow}a_{m'\downarrow} + \sum_{kl'}\tau_k^{m'l'}a_{l'\downarrow}^{+}a_{-k\downarrow}a_{k\uparrow}$$

Putting the value of commutator $[a_{m'\uparrow}, H]$ in the equation (3.30) we get-

$$\omega G_{m'l'}^{\uparrow\uparrow} = -E_{m'}G_{m'l'}^{\uparrow\uparrow} - \phi_{l'l'}G_{m'l'}^{\downarrow\uparrow} - 2\sum_{m'}\frac{J_{l'm'}}{\tau_k^{l'm'}}\phi_{l'm'}G_{l'l'}^{\downarrow\uparrow} + \sum_{m'}\frac{\tau_k^{l'm'}}{V}\Delta_k G_{l'l'}^{\downarrow\uparrow} \tag{3.31}$$

By taking Fourier transformation of equation (3.31) and after solving, finally we get the equation:

$$(\omega - E_{m'})G_{kk}^{\uparrow\uparrow}(m'l') = -\beta G_{kk}^{\downarrow\uparrow}(m'l') + (\eta - \lambda)G_{kk}^{\downarrow\uparrow}(l'l') \tag{3.32}$$

Now taking Green's function (3.21) and written in term of equation of motion as:-

$$\omega G^{\downarrow\uparrow}_{m'l'} = \left\langle\left\langle \left[a^{+}_{m'\downarrow}, H\right]; a^{+}_{l'\uparrow}\right\rangle\right\rangle \tag{3.33}$$

Now, evaluating the commutator $[a^{+}_{m'\downarrow}, H]$ using the Hamiltonian (3.5), we get -

$$[a^{+}_{m'\downarrow}, H] = -E_{m'}a^{+}_{m'\downarrow} - Ua^{+}_{m'\uparrow}a_{m'\uparrow}a^{+}_{m'\downarrow} - 2\sum_{l'} J_{l'm'}a^{+}_{l'\downarrow}a^{+}_{m'\uparrow}a_{l'\uparrow} + \sum_{kl'}\tau_k^{l'm'}a^{+}_{k\uparrow}a^{+}_{-k\downarrow}a_{l\uparrow}$$

Putting the value of commutator $[a^{+}_{m'\downarrow}, H]$ in the equation (3.33) we get-

$$\omega G^{\downarrow\uparrow}_{m'l'} = -E_{m'}G^{\downarrow\uparrow}_{m'l'} - \phi_{l'l'}G^{\uparrow\uparrow}_{m'l'} - 2\sum_{m'}\frac{J_{l'm'}}{\tau_k^{l'm'}}\phi_{l'm'}G^{\uparrow\uparrow}_{l'l'} + \sum_{m'}\frac{\tau_k^{l'm'}}{V}\Delta_k G^{\uparrow\uparrow}_{l'l'} \tag{3.34}$$

By taking Fourier transformation of equation (3.34) and after solving, finally we get the equation:

$$(\omega + E_{m'})G^{\downarrow\uparrow}_{kk}(m'l') = -\beta G^{\uparrow\uparrow}_{kk}(m'l') + (\eta - \lambda)G^{\uparrow\uparrow}_{kk}(l'l') \tag{3.35}$$

So, finally four equations are obtained containing four Green's functions:

$$(\omega - E_{l'})G^{\uparrow\uparrow}_{kk}(l'l') = \frac{1}{2\pi} - \beta G^{\downarrow\uparrow}_{kk}(l'l') + (\eta - \lambda)G^{\downarrow\uparrow}_{kk}(m'l')$$

$$(\omega + E_{l'})G^{\downarrow\uparrow}_{kk}(l'l') = -\beta G^{\uparrow\uparrow}_{kk}(l'l') + (\eta - \lambda)G^{\uparrow\uparrow}_{kk}(m'l')$$

$$(\omega - E_{m'})G^{\uparrow\uparrow}_{kk}(m'l') = -\beta G^{\downarrow\uparrow}_{kk}(m'l') + (\eta - \lambda)G^{\downarrow\uparrow}_{kk}(l'l')$$

$$(\omega + E_{m'})G^{\downarrow\uparrow}_{kk}(m'l') = -\beta G^{\uparrow\uparrow}_{kk}(m'l') + (\eta - \lambda)G^{\uparrow\uparrow}_{kk}(l'l')$$

After solving these equations, we can get the Green's function $G^{\downarrow\uparrow}_{kk}(l'l')$ as:

$$G^{\downarrow\uparrow}_{kk}(l'l') = \frac{-\beta\left[\omega^2 - E^2 - \beta^2 + (\eta-\lambda)^2\right]}{2\pi\left[\omega^2 - E^2 - \beta^2 - (\eta-\lambda)^2 - 2\beta(\eta-\lambda)\right]\left[\omega^2 - E^2 - \beta^2 - (\eta-\lambda)^2 + 2\beta(\eta-\lambda)\right]} \tag{3.36}$$

Here, $E^2 = E^2_{l'} = E^2_{m'}$,

Now, the magnetic order parameter for intrasite may be written as:

$$\phi_{l'l'} = U\left\langle a^{+}_{l'\downarrow} a^{+}_{l'\uparrow} \right\rangle \tag{3.37}$$

Here, the correlation function $\left\langle a^{+}_{l'\downarrow} a^{+}_{l'\uparrow} \right\rangle$ may be defined as:

$$\left\langle a^{+}_{l'\downarrow} a^{+}_{l'\uparrow} \right\rangle = i \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} \frac{[G^{\downarrow\uparrow}_{kk}(\omega + i\varepsilon) - G^{\downarrow\uparrow}_{kk}(\omega - i\varepsilon)]}{e^{\frac{\omega}{K_B T}} + 1} e^{i\omega(t-t')} d\omega \tag{3.38}$$

After solving the Green's function (3.36), and putting in equation (3.38), we get the correlation function:

$$\begin{aligned} \left\langle a^{+}_{l'\downarrow} a^{+}_{l'\uparrow} \right\rangle = & \frac{1}{2\pi N} \sum_k \left\{ \frac{\beta - (\eta - \lambda)}{\sqrt{E^2 + \beta^2 + (\eta - \lambda)^2 - 2\beta(\eta - \lambda)}} \tanh \frac{\sqrt{E^2 + \beta^2 + (\eta - \lambda)^2 - 2\beta(\eta - \lambda)}}{2K_B T} \right\} \\ & - \frac{1}{2\pi N} \sum_k \left\{ \frac{\beta + (\eta - \lambda)}{\sqrt{E^2 + \beta^2 + (\eta - \lambda)^2 + 2\beta(\eta - \lambda)}} \tanh \frac{\sqrt{E^2 + \beta^2 + (\eta - \lambda)^2 + 2\beta(\eta - \lambda)}}{2K_B T} \right\} \end{aligned} \tag{3.39}$$

By putting the correlation function (3.39) in equation (3.37), we get the expression for intrasite magnetic order parameter $\phi_{l'l'}$ as:

$$\phi_{l'l'} = \frac{U}{2\pi N} \sum_k \left\{ \frac{\beta - (\eta - \lambda)}{\sqrt{\chi - 2\beta(\eta - \lambda)}} \tanh \frac{\sqrt{\chi - 2\beta(\eta - \lambda)}}{2K_B T} - \frac{\beta + (\eta - \lambda)}{\sqrt{\chi + 2\beta(\eta - \lambda)}} \tanh \frac{\sqrt{\chi + 2\beta(\eta - \lambda)}}{2K_B T} \right\} \tag{3.40}$$

Where, $\chi = [E^2 + \beta^2 + (\eta - \lambda)^2]$

Equation (3.40) represent the expression for intrasite magnetic order parameter $\phi_{l'l'}$. Using this equation, we can evaluate the interplay between magnetism and superconductivity in high $T_C$ cuprate superconductors.

## 3.2 IRON PNICTIDE SUPERCONDUCTORS (OXYPNICTIDES)

For iron pnictides, we are considered the model Hamiltonian which can be written as:

$$H = J_1 \sum_{ij} S_{ia} S_{jb} - J_2 \sum_{ij} S_{ia} S_{ja} - J_2 \sum_{ij} S_{ib} S_{jb} + J_3 \sum_{ij} S_{ia} S_{jb} + J_\perp \sum_{ij} S_{ia} S_{jc} - J_\perp \sum_{ij} S_{ib} S_{jc} \tag{3.41}$$

Where, the first and Fourth term is the Heisenberg term for the antiferromagnetic spin Coupling between two localized sites *a* & *b* for nearest and first nearest Fe atoms. Second and third term represent the ferromagnetic onsite spin coupling between nearest Fe atoms. The last two terms represent the antiferromagnetic and ferromagnetic spin coupling between nearest As atom of localized site c and Fe atoms of sites *a* & *b* respectively. $J_1$ is the antiferromagnetic spin exchange interaction between nearest Fe – Fe atoms of stripe *a* and *b*. $J_3$ is the spin exchange interaction between first nearest Fe – Fe atoms of stripe *a* and *b*, which is antiferromagnetic in nature. $J_2$ is the spin exchange interaction between nearest Fe – Fe atom of the same stripe, which is ferromagnetic in nature. $J_\perp$ is the spin exchange interaction of Fe atoms with the As atoms.

Let us take the following Green's function to investigate the model,

$$G_{fg}^{aa} = \left\langle \left\langle S_{fa}^{+}; S_{ga}^{-} \right\rangle \right\rangle \tag{3.42}$$

Taking Fourier transformation and then writing the equation of motion of equation (3.42), we get:

$$\omega G_{fg}^{aa} = \frac{\left\langle S_{fa}^{z} \right\rangle}{\pi} \delta_{fg} + \left\langle \left\langle \left[ S_{fa}^{+}, H \right]; S_{ga}^{-} \right\rangle \right\rangle \tag{3.43}$$

Evaluating the commutator $\left[S_{fa}^{+}, H\right]$ using the Hamiltonian (3.41):

$$\left[S_{fa}^{+}, H\right] = J_1\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle S_{f+\delta,b}^{+} - J_1\sum_{\delta}\left\langle S_{f+\delta,b}^{z}\right\rangle S_{fa}^{+} - 2J_2\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle S_{f+\delta,a}^{+} + 2J_2\sum_{\delta}\left\langle S_{f+\delta,a}^{z}\right\rangle S_{fa}^{+}$$
$$+ J_3\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle S_{f+\delta,b}^{+} - J_3\sum_{\delta}\left\langle S_{f+\delta,b}^{z}\right\rangle S_{fa}^{+} + 2J_{\perp}\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle S_{f+\delta,c}^{+} - 2J_{\perp}\sum_{\delta}\left\langle S_{f+\delta,c}^{z}\right\rangle S_{fa}^{+}$$

Now, putting the value of commutator $\left[S_{fa}^{+}, H\right]$ in equation (3.43), we get:

$$\omega G_{fa}^{aa} = \frac{\left\langle S_{fa}^{z}\right\rangle}{\pi} + J_1\sum_{\delta}\left\langle\left\langle S_{fa}^{z}S_{f+\delta,b}^{+}; S_{ga}^{-}\right\rangle\right\rangle - J_1\sum_{\delta}\left\langle\left\langle S_{f+\delta,b}^{z}S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle - 2J_2\sum_{\delta}\left\langle\left\langle S_{fa}^{z}S_{f+\delta,a}^{+}; S_{ga}^{-}\right\rangle\right\rangle$$
$$+ 2J_2\sum_{\delta}\left\langle\left\langle S_{f+\delta,a}^{z}S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle + J_3\sum_{\delta}\left\langle\left\langle S_{fa}^{z}S_{f+\delta,b}^{+}; S_{ga}^{-}\right\rangle\right\rangle - J_3\sum_{\delta}\left\langle\left\langle S_{f+\delta,b}^{z}S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle$$
$$+ 2J_{\perp}\sum_{\delta}\left\langle\left\langle S_{fa}^{z}S_{f+\delta,c}^{+}; S_{ga}^{-}\right\rangle\right\rangle - 2J_{\perp}\sum_{\delta}\left\langle\left\langle S_{f+\delta,c}^{z}S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle \qquad (3.44)$$

Using the RPA decoupling scheme:

$\left\langle\left\langle S_{f+\delta}^{z}S_{f}^{+}; S_{g}^{-}\right\rangle\right\rangle = \left\langle S_{f+\delta}^{z}\right\rangle\left\langle\left\langle S_{f}^{+}; S_{g}^{-}\right\rangle\right\rangle$, and

$\left\langle\left\langle S_{f}^{z}S_{f+\delta}^{+}; S_{g}^{-}\right\rangle\right\rangle \approx \left\langle S_{f}^{z}\right\rangle\left\langle\left\langle S_{f+\delta}^{+}; S_{g}^{-}\right\rangle\right\rangle$

Now using the above approximations, equation (3.44) becomes:

$$\omega G_{fa}^{aa} = \frac{\left\langle S_{fa}^{z}\right\rangle}{\pi} + J_1\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,b}^{+}; S_{ga}^{-}\right\rangle\right\rangle - J_1\sum_{\delta}\left\langle S_{f+\delta,b}^{z}\right\rangle\left\langle\left\langle S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle - 2J_2\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,a}^{+}; S_{ga}^{-}\right\rangle\right\rangle$$
$$- 2J_2\sum_{\delta}\left\langle S_{f+\delta,a}^{z}\right\rangle\left\langle\left\langle S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle + J_3\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,b}^{+}; S_{ga}^{-}\right\rangle\right\rangle - J_3\sum_{\delta}\left\langle S_{f+\delta,b}^{z}\right\rangle\left\langle\left\langle S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle$$
$$+ 2J_{\perp}\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,c}^{+}; S_{ga}^{-}\right\rangle\right\rangle - 2J_{\perp}\sum_{\delta}\left\langle S_{f+\delta,c}^{z}\right\rangle\left\langle\left\langle S_{fa}^{+}; S_{ga}^{-}\right\rangle\right\rangle \qquad (3.45)$$

Now, taking the Spatial Fourier transform of equation (3.45), we get:

$$\omega G_{k}^{aa} = \frac{\bar{S}}{\pi} + J_1\bar{S}Z_1\gamma_1(k)G_k^{ba} + J_1\bar{S}Z_1G_k^{aa} - 2J_2\bar{S}Z_2\gamma_2(k)G_k^{aa} + 2J_2\bar{S}Z_2G_k^{aa}$$
$$+ J_3\bar{S}Z_3\gamma_3(k)G_k^{ba} + J_3\bar{S}Z_3G_k^{aa} + 2J_{\perp}\bar{S}Z_{\perp}\gamma_{\perp}(k)G_k^{ca} + 2J_{\perp}\bar{S}Z_{\perp}G_k^{aa} \qquad (3.46)$$

Where, $G_k^{aa}$ is the Green function when *f* and *g* sites are on the same sublattice *a*, $G_k^{ba}$ is the Green function when *f* and *g* sites are on the different sublattice *a* & *b*, and $G_k^{ca}$ is the Green function when *f* and *g* sites are on the different sublattice *a* & *c*.

$$Z_{ab} = \frac{\sum_\delta \left\langle S_{f+\delta}^z \right\rangle}{\left\langle S_f^z \right\rangle} \quad \text{and} \quad \gamma(k) = \frac{1}{Z_{ab}} \sum_\delta e^{ik\delta} \tag{3.47}$$

Equation (3.46) can be written as-

$$(\omega - \eta')G_k^{aa} = \frac{\bar{S}}{\pi} + \beta' G_k^{ba} + \lambda' G_k^{ca} \quad ,$$

(3.48)

Where, $\eta' = J_1 \bar{S} Z_1 - 2J_2 \bar{S} Z_2 \gamma_2 + J_2 \bar{S} Z_2 + J_3 \bar{S} Z_3 + 2J_\perp \bar{S} Z_\perp$ , (3.49)

$$\beta' = J_1 \bar{S} Z_1 \gamma_1 + J_3 \bar{S} Z_3 \gamma_3 \tag{3.50}$$

and $\lambda' = 2J_\perp \bar{S} Z_\perp \gamma_\perp$ (3.51)

Now, taking another Green's function:

$$G_{fg}^{ba} = \left\langle\left\langle S_{fb}^+ ; S_{ga}^- \right\rangle\right\rangle \tag{3.52}$$

Taking Fourier transformation and then writing the equation of motion of equation (3.52), we get:

$$\omega G_{fg}^{ba} = \left\langle\left\langle \left[S_{fb}^+, H\right]; S_{ga}^- \right\rangle\right\rangle \tag{3.53}$$

Evaluating the commutator $\left[S_{fb}^+, H\right]$ using the Hamiltonian (3.41):

$$\begin{aligned}\left[S_{fb}^+, H\right] = & J_1 \sum_\delta \left\langle S_{fb}^z \right\rangle S_{f+\delta,a}^+ - J_1 \sum_\delta \left\langle S_{f+\delta,a}^z \right\rangle S_{fb}^+ - 2J_2 \sum_\delta \left\langle S_{fb}^z \right\rangle S_{f+\delta,b}^+ + 2J_2 \sum_\delta \left\langle S_{f+\delta,b}^z \right\rangle S_{fb}^+ \\ & + J_3 \sum_\delta \left\langle S_{fb}^z \right\rangle S_{f+\delta,a}^+ - J_3 \sum_\delta \left\langle S_{f+\delta,a}^z \right\rangle S_{fb}^+ - 2J_\perp \sum_\delta \left\langle S_{fb}^z \right\rangle S_{f+\delta,c}^+ - 2J_\perp \sum_\delta \left\langle S_{f+\delta,c}^z \right\rangle S_{fb}^+\end{aligned}$$

Now, putting the value of commutator $\left[S_{fb}^+, H\right]$ in equation (3.53), we get:

$$\omega G_{fa}^{ba} = J_1 \sum_{\delta} \langle\langle S_{fb}^{z} S_{f+\delta,a}^{+}; S_{ga}^{-} \rangle\rangle - J_1 \sum_{\delta} \langle\langle S_{f+\delta,a}^{z} S_{fb}^{+}; S_{ga}^{-} \rangle\rangle - 2J_2 \sum_{\delta} \langle\langle S_{fb}^{z} S_{f+\delta,b}^{+}; S_{ga}^{-} \rangle\rangle$$

$$+2J_2 \sum_{\delta} \langle\langle S_{f+\delta,b}^{z} S_{fb}^{+}; S_{ga}^{-} \rangle\rangle + J_3 \sum_{\delta} \langle\langle S_{fb}^{z} S_{f+\delta,a}^{+}; S_{ga}^{-} \rangle\rangle - J_3 \sum_{\delta} \langle\langle S_{f+\delta,a}^{z} S_{fb}^{+}; S_{ga}^{-} \rangle\rangle$$

$$-2J_{\perp} \sum_{\delta} \langle\langle S_{fb}^{z} S_{f+\delta,c}^{+}; S_{ga}^{-} \rangle\rangle + 2J_{\perp} \sum_{\delta} \langle\langle S_{f+\delta,c}^{z} S_{fb}^{+}; S_{ga}^{-} \rangle\rangle \tag{3.54}$$

Now using the RPA decoupling approximations, equation (3.54) becomes :

$$\omega G_{fa}^{ba} = J_1 \sum_{\delta} \langle S_{fb}^{z} \rangle \langle\langle S_{f+\delta,a}^{+}; S_{ga}^{-} \rangle\rangle - J_1 \sum_{\delta} \langle S_{f+\delta,a}^{z} \rangle \langle\langle S_{fb}^{+}; S_{ga}^{-} \rangle\rangle - 2J_2 \sum_{\delta} \langle S_{fb}^{z} \rangle \langle\langle S_{f+\delta,b}^{+}; S_{ga}^{-} \rangle\rangle$$

$$+2J_2 \sum_{\delta} \langle S_{f+\delta,b}^{z} \rangle \langle\langle S_{fb}^{+}; S_{ga}^{-} \rangle\rangle + J_3 \sum_{\delta} \langle S_{fb}^{z} \rangle \langle\langle S_{f+\delta,a}^{+}; S_{ga}^{-} \rangle\rangle - J_3 \sum_{\delta} \langle S_{f+\delta,a}^{z} \rangle \langle\langle S_{fb}^{+}; S_{ga}^{-} \rangle\rangle$$

$$-2J_{\perp} \sum_{\delta} \langle S_{fb}^{z} \rangle \langle\langle S_{f+\delta,c}^{+}; S_{ga}^{-} \rangle\rangle + 2J_{\perp} \sum_{\delta} \langle S_{f+\delta,c}^{z} \rangle \langle\langle S_{fb}^{+}; S_{ga}^{-} \rangle\rangle \tag{3.55}$$

Now, taking the Spatial Fourier transform of equation (3.55), we get:

$$\omega G_{k}^{ba} = -J_1 \bar{S} Z_1 \gamma_1(k) G_k^{aa} - J_1 \bar{S} Z_1 G_k^{ba} + 2J_2 \bar{S} Z_2 \gamma_2(k) G_k^{ba} - 2J_2 \bar{S} Z_2 G_k^{ba}$$

$$- J_3 \bar{S} Z_3 \gamma_3(k) G_k^{aa} - J_3 \bar{S} Z_3 G_k^{ba} - 2J_{\perp} \bar{S} Z_{\perp} \gamma_{\perp}(k) G_k^{ca} - 2J_{\perp} \bar{S} Z_{\perp} G_k^{ba} \tag{3.56}$$

Putting the variables $\eta', \lambda'$ & $\beta'$ from equations (3.49), (3.50) and (3.51) in equation (3.56), we get the equation:

$$(\omega + \eta') G_k^{ba} = -\beta' G_k^{aa} - \lambda' G_k^{ca} \tag{3.57}$$

Let us take another Green's function:

$$G_{fg}^{ca} = \langle\langle S_{fc}^{+}; S_{ga}^{-} \rangle\rangle \tag{3.58}$$

Taking Fourier transformation and then writing the equation of motion of equation (3.58), we get:

$$\omega G_{fg}^{ca} = \langle\langle [S_{fc}^{+}, H]; S_{ga}^{-} \rangle\rangle \tag{3.59}$$

Evaluating the commutator $[S_{fc}^{+}, H]$ using the Hamiltonian (3.41):

$$\left[S_{fc}^{+},H\right]=2J_{\perp}\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle S_{f+\delta,a}^{+}-2J_{\perp}\sum_{\delta}\left\langle S_{f+\delta,a}^{z}\right\rangle S_{fc}^{+}-2J_{\perp}\sum_{\delta}\left\langle S_{fc}^{z}\right\rangle S_{f+\delta,b}^{+}+2J_{\perp}\sum_{\delta}\left\langle S_{f+\delta,a}^{z}\right\rangle S_{fc}^{+}$$

Now, putting the value of commutator $\left[S_{fc}^{+},H\right]$ in equation (3.59) and using the RPA decoupling approximations, we get:

Now, equation (3.54) becomes :

$$\omega G_{fa}^{ca}=2J_{\perp}\sum_{\delta}\left\langle S_{fa}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,a}^{+};S_{ga}^{-}\right\rangle\right\rangle-2J_{\perp}\sum_{\delta}\left\langle S_{fc}^{z}\right\rangle\left\langle\left\langle S_{f+\delta,b}^{+};S_{ga}^{-}\right\rangle\right\rangle \quad (3.60)$$

Now, taking the Spatial Fourier transform of equation (3.60), we get:

$$\omega G_{fa}^{ca}=-2J_{\perp}\bar{S}Z_{\perp}\gamma_{\perp}(k)G_{k}^{aa}+2J_{\perp}\bar{S}Z_{\perp}\gamma_{\perp}(k)G_{k}^{ba} \quad (3.61)$$

Putting the variable $\lambda$ from equation (3.51) in equation (3.61), we get the equation:

$$\omega G_{k}^{ca}=-\lambda' G_{k}^{aa}+\lambda' G_{k}^{ba} \quad (3.62)$$

After solving equations (3.48), (3.57) and (3.62), we get:

$$G_{k}^{aa}=\frac{\bar{S}}{\pi}\left[\frac{\omega+\eta'}{\omega^{2}-\left(\eta'^{2}-2\lambda'^{2}-\beta'^{2}\right)^{2}}+\frac{\lambda'^{2}}{\omega\left\{\omega^{2}-\left(\eta'^{2}-2\lambda'^{2}-\beta'^{2}\right)^{2}\right\}}\right] \quad (3.63)$$

Using equation (3.63) we get the correlation function

$$\left\langle S_{fa}^{-}S_{ga}^{+}\right\rangle=\frac{2\bar{S}}{N}\sum_{k}\left[-\left(1+\frac{\lambda'^{2}}{\left(\eta'^{2}-2\lambda'^{2}-\beta'^{2}\right)^{2}}\right)+\frac{\eta'}{\eta'^{2}-2\lambda'^{2}-\beta'^{2}}\coth\left(\frac{\eta'^{2}-2\lambda'^{2}-\beta'^{2}}{2K_{B}T}\right)\right]$$

(3.64)

The sublattice magnetization for spin ½ system will then be given by

$$\bar{S}=\frac{1}{2}-\left\langle S_{fa}^{-}S_{ga}^{+}\right\rangle \quad (3.65)$$

After substituting eq. (3.64) in eq. Eq. (3.65), we get:

$$\bar{S}=\frac{1}{2}-\frac{2\bar{S}}{N}\sum_{k}\left[-\left(1+\frac{\lambda'^{2}}{\left(\eta'^{2}-2\lambda'^{2}-\beta'^{2}\right)^{2}}\right)+\frac{\eta'}{\eta'^{2}-2\lambda'^{2}-\beta'^{2}}\coth\left(\frac{\eta'^{2}-2\lambda'^{2}-\beta'^{2}}{2K_{B}T}\right)\right]$$

(3.66)

The above expression gives the variation of sublattice magnetization with temperature. It can be reduced to give expression for Néel temperature.

As magnetization $\bar{S} \to 0, T \to T_N$ (Néel temperature).

By putting $\bar{S} = 0$ in equation (3.66), we get:

$$T_N = \frac{N}{4K_B \sum_k \frac{J_1 Z_1 + J_2 Z_2 (1-\gamma_2) + J_3 Z_3 + J_\perp Z_\perp}{[(J_1 Z_1 + J_2 Z_2 (1-\gamma_2) + J_3 Z_3 + J_\perp Z_\perp)^2 - 2J^2{}_\perp Z^2{}_\perp \gamma^2{}_\perp - (J_1 Z_1 \gamma_1 + J_3 Z_3 \gamma_3)^2]}}, \tag{3.67}$$

Equation (3.67) is the obtained expression of Néel temperature for the above considered problem.