CHAPTER II

THEORETICAL DEVELOPMENT

2.1 Perturbation Expansion

In quantum mechanics, we work with operators $H_o \psi_i = E_i^{(o)} \psi_i$ where H_o is the time independent Hamiltonian operator, ψ_i are the eigenstates of H_o and $E_i^{(o)}$ are the eigenvalues. We can define an operator $G_o(E) = \frac{1}{E - H_o}$. This operator is called the Green's function.[12,13] The expectation value of the Green's function is calculated as follows.

$$\left\langle \psi_i \left| \frac{1}{E - H_o} \right| \psi_i \right\rangle = \left\langle \psi_i \left| \frac{1}{E}\left(\frac{1}{1 - \frac{H_o}{E}} \right) \right| \psi_i \right\rangle$$

$$= \left\langle \psi_i \left| \frac{1}{E}\left\{ 1 + \frac{H_o}{E} + \left(\frac{H_o}{E}\right)^2 + \ldots \right\} \right| \psi_i \right\rangle \quad (2.1.1)$$

Since

$$(H_o)^n \left| \psi_i \right\rangle = (H_o)^{n-1} H_o \left| \psi_i \right\rangle$$

$$= (H_o)^{n-1} E_i^{(o)} \left| \psi_i \right\rangle$$

$$= E_i^{(o)} H_o^{n-1} \left| \psi_i \right\rangle$$

....

$$= E_i^{(o)^n} \left| \psi_i \right\rangle \quad (2.1.2)$$

So (2.1.1) becomes

$$\langle \psi_i | \frac{1}{E - H_o} | \psi_i \rangle = \langle \psi_i | \frac{1}{E} (1 + \frac{E_i^{(o)}}{E} + \frac{E_i^{(o)2}}{E^2} + \ldots + \frac{E_i^{(o)n}}{E^n} + \ldots) | \psi_i \rangle$$

$$= \langle \psi_i | \frac{1}{E} (\frac{1}{1 - \frac{E_i^{(o)}}{E}}) | \psi_i \rangle$$

$$= \langle \psi_i | \frac{1}{E - E_i^{(o)}} | \psi_i \rangle$$

$$= \frac{\langle \psi_i | \psi_i \rangle}{E - E_i^{(o)}}$$

$$= \frac{1}{E - E_i^{(o)}} \qquad (2.1.3)$$

where $| \psi_i \rangle$ are the eigenvectors of H_o with the eigenvalues $E_i^{(o)}$.

Let us now consider a system which is described by the Hamiltonian $H = H_o + \lambda V$, where V is a time independent perturbation operator, λ is a real parameter to be set equal to one at a later time, and H_o is the time independent Hamiltonian operator for a system without perturbation. The eigenvectors are no longer $| \psi_i \rangle$ and the eigenvalues are no longer $E_i^{(o)}$ but E_i.

$$E_i = E_i^{(o)} + \langle i | V | i \rangle + \sum_m \frac{|\langle i | V | m \rangle|^2}{E_i^{(o)} - E_m^{(o)}} + \ldots \qquad (2.1.4)$$

Of interest to us now are the two resolvents :

$$\langle i | \frac{1}{E - H_o} | i \rangle = G_o(E)$$

$$= \frac{1}{E - E_i^{(o)}} \qquad (2.1.5)$$

$$\left\langle i \left| \frac{1}{E - H_o - \lambda V} \right| i \right\rangle = \left\langle i \left| \frac{1}{E - H} \right| i \right\rangle$$

$$= G(E)$$

$$= \frac{1}{E - E_i} \qquad (2.1.6)$$

where E_i is the new energy of the system in the presence of the perturbation V.

$$E_i = E_i^{(o)} + \text{all perturbative corrections to the energy}$$

$$= E_i^{(o)} + \Sigma \qquad (2.1.7)$$

where Σ is the self energy correction. From (2.1.5), (2.1.6) and (2.1.7), we get

$$G(E) = \frac{1}{E - E_i}$$

$$= \frac{1}{E - E_i^{(o)} - \Sigma}$$

$$G^{-1}(E) = E - E_i^{(o)} - \Sigma$$

$$G^{-1}(E) = G_o^{-1}(E) - \Sigma \qquad (2.1.8)$$

Equation (2.1.8) is called Dyson's equation.[14] Thus the self energy Σ is the difference in the reciprocal of the two Green's functions. From Dyson's equation $G^{-1}(E) = G_o^{-1}(E) - \Sigma$, multiply from the right by G(E) and the left by $G_o(E)$, we get

$$G_o(E) = G(E) - G_o(E)\,\Sigma\, G(E)$$

or

$$G\,(E) = G_o(E) + G_o(E)\,\Sigma\, G(E) \qquad (2.1.9)$$

and substituting G(E) by (2.1.9) into G(E) of the right in (2.1.9)

$$G(E) = G_o(E) + G_o(E)\,\Sigma\, G_o(E) + G_o(E)\,\Sigma\, G_o(E)\,\Sigma\, G(E)$$

By iteration, we get

$$G(E) = G_o(E) + G_o(E)\,\Sigma\, G_o(E) + G_o(E)\,\Sigma\, G_o(E)\,\Sigma\, G_o(E) + G_o(E)\,\Sigma\, G_o(E)\,\Sigma\, G_o(E)\,\Sigma\, G_o(E) + \ldots \qquad (2.1.10)$$

which is the development of G(E) in terms of the self energy Σ

We shall now develop G(E) in terms of the perturbation V.

$$G(E) = \langle i | \frac{1}{E - H_o - \lambda V} | i \rangle$$

$$= \langle i | \frac{1}{E - H_o} \left(\frac{1}{1 - \frac{\lambda V}{E - H_o}} \right) | i \rangle$$

$$= \sum_j \langle i | \frac{1}{E - H_o} | j \rangle \langle j | \frac{1}{1 - \frac{\lambda V}{E - H_o}} | i \rangle ;$$

$$\left(\text{since } \sum_j | j \rangle \langle j | = 1 \right) \qquad (2.1.11)$$

Because of

$$\langle i | \frac{1}{E - H_o} | j \rangle = \frac{1}{E - E_j^{(o)}} \langle i | j \rangle$$

$$= \frac{1}{E - E_j^{(o)}} \delta_{ij}$$

(2.1.11) becomes

$$G(E) = \sum_j \langle i \,|\, \frac{1}{E - H_o} |j\rangle\langle j| \frac{1}{1 - \frac{\lambda V}{E - H_o}} |\, i \rangle$$

$$= \sum_j \frac{1}{E - E_j^{(o)}} \delta_{ij} \langle j| \frac{1}{1 - \frac{\lambda V}{E - H_o}} |\, i \rangle$$

$$= \frac{1}{E - E_i^{(o)}} \langle i \,|\, \frac{1}{1 - \frac{\lambda V}{E - H_o}} \,|\, i \rangle$$

$$= \langle i| \frac{1}{E - H_o} |i\rangle \langle i| \frac{1}{1 - \frac{\lambda V}{E - H_o}} |\, i \rangle$$

$$= G_o(E) \langle i \,|\, \frac{1}{1 - \frac{\lambda V}{E - H_o}} \,|\, i \rangle \qquad (2.1.12)$$

If λ is small and $E \neq H_o$ we can expand $\frac{1}{1 - \frac{\lambda V}{E - H_o}}$ in geometrical series.

$$G(E) = G_o(E) \left[\langle i \,|\, \{ 1 + \frac{\lambda V}{E - H_o} + \frac{\lambda^2 V^2}{(E - H_o)^2} + \ldots + \frac{\lambda^n V^n}{(E - H_o)^n} + \ldots \} \,|\, i \rangle \right] \qquad (2.1.13a)$$

the first term $= G_o(E) \langle i \,|\, i \rangle$

$= G_o(E)$ (2.1.13b)

the second term $= G_o(E)\ \lambda \langle i \,|\frac{V}{E - H_o}|\, i \rangle$

$= G_o(E)\ \lambda \sum_j \langle i \,|V|\, j \rangle \langle j| \frac{1}{E - H_o} |i\rangle$

$= G_o(E)\ \lambda \sum_j \langle i \,|V|\, j \rangle\ G_o(E)\ \delta_{ij}$

$= G_o(E)\ \lambda \langle i \,|V|\, i \rangle\ G_o(E)$ (2.1.13c) the third term $= G_o(E)\,\lambda^2 \langle i \,|\, \dfrac{V^2}{(E - H_o)^2} \,|i\rangle$

With this term, we have to be careful how we arrange terms. Let us look at the third term in the expansion $\langle i \,|\, \dfrac{V^2}{(E - H_o)^2} \,|\, i\rangle$

$$\langle i \,|\frac{V^2}{(E - H_o)^2}|\, i\rangle = \sum_{jj'j''} \langle i|\, V|\, j\rangle \langle j|\, V|\, j'\rangle \langle j'|\, \frac{1}{E - H_o}|\, j''\rangle \times \langle j'' \,|\frac{1}{E - H_o}|\, i\rangle$$

It makes no difference how we rearrange the operators V, V, $\dfrac{1}{E - H_o}$, $\dfrac{1}{E - H_o}$

$$\langle i|\, \frac{V^2}{(E - H_o)^2}|\, i\rangle = \sum_{jj'j''} \langle i|\, V|\, j\rangle \langle j|\, \frac{1}{E - H_o}|\, j'\rangle \times \langle j'|\, V\, |j''\rangle\langle j''\,|\, \frac{1}{E - H_o}|\, i\rangle$$

Because of $\langle j|\, \dfrac{1}{E - H_o}|\, j'\rangle = \dfrac{1}{E - E_{j'}^{(o)}}\, \delta_{jj'}$ and $\langle j''|\, \dfrac{1}{E - H_o}|\, i\rangle$

$$= \frac{1}{E - E_i^{(o)}}\, \delta_{j''i}$$

$$\langle i\, |\frac{V^2}{(E - H_o)^2}|\, i\rangle = \sum_{jj'j''} \langle i|\, V|\, j\rangle \frac{1}{E - E_{j'}^{(o)}}\, \delta_{jj'}\langle j'\,|\, V\, |j''\rangle \times \frac{1}{E - E_i^{(o)}}\, \delta_{j''i}$$

$$= \sum_{jj'} \langle i\, |V|\, j\rangle \frac{1}{E - E_{j'}^{(o)}}\, \delta_{jj'}\langle j'|\, V|\, i\rangle \frac{1}{E - E_i^{(o)}}$$

$$= \sum_{j} \langle i|\, V|\, j\rangle \frac{1}{E - E_j^{(o)}} \langle j|\, V|\, i\rangle\, \frac{1}{E - E_i^{(o)}}$$

$$= \sum_j \frac{\langle i|V|j\rangle\langle j|V|i\rangle}{E - E_j^{(o)}} G_o(E)$$

$$= \left(\sum_j \frac{|\langle i|V|j\rangle|^2}{E - E_j^{(o)}}\right) G_o(E)$$

If we replace $\sum_j$ by $\sum_j \delta_{ij} + \sum'_{j \neq i}$, we will get

$$\langle i|\frac{V^2}{(E - H_o)^2}|i\rangle = \langle i|V|i\rangle^2 \, G_o^2(E) + \left(\sum'_{j \neq i} \frac{|\langle i|V|j\rangle|^2}{E - E_j^{(o)}}\right) G_o(E)$$

therefore,

the third term = $G_o(E)\,\lambda^2 \langle i|V|i\rangle^2 \, G_o^{\,2}(E) + G_o(E)\,\lambda^2$

$$\times \sum'_{j \neq i} \frac{|\langle i|V|j\rangle|^2}{E - E_j^{(o)}} G_o(E) \qquad (2.1.13d)$$

the fourth term = $G_o(E)\,\lambda^3 \langle i|\frac{V^3}{(E - H_o)^3}|i\rangle$

Let's look at $\frac{V^3}{(E - H_o)^3}$

$$\langle i|\frac{V^3}{(E - H_o)^3}|i\rangle = \sum_{j_1 j_2 j_3 j_4 j_5} \langle i|V|j_1\rangle\langle j_1|\frac{1}{E - H_o}|j_2\rangle$$

$$\times \langle j_2|V|j_3\rangle\langle j_3|\frac{1}{E - H_o}|j_4\rangle\langle j_4|V|j_5\rangle\langle j_5|\frac{1}{E - H_o}|i\rangle$$

$$= \sum_{j_1 \ldots j_5} \langle i|V|j_1\rangle \frac{1}{E - E_2^{(o)}} \delta_{12} \langle j_2|V|j_3\rangle$$

$$\times \frac{1}{E - E_4^{(o)}} \delta_{34} \langle j_4|V|j_5\rangle \frac{1}{E - E_i^{(o)}} \delta_{5i}$$

$$= \sum_{j_1 j_3} \langle i | V | j_1 \rangle \frac{1}{E - E_1^{(o)}} \langle j_1 | V | j_3 \rangle$$

$$\times \frac{1}{E - E_3^{(o)}} \langle j_3 | V | i \rangle G_o(E)$$

$$= \sum_{j_1 j_3} \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_3 \rangle \langle j_3 | V | i \rangle}{(E - E_1^{(o)})\ (E - E_3^{(o)})}$$

$$\times\ G_o(E)$$

$$\langle i | \frac{V^3}{(E - H_o)^3} | i \rangle = \sum_{j_1 j_3} \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_3 \rangle \langle j_3 | V | i \rangle}{(E - E_1^{(o)})(E - E_3^{(o)})}$$

$$\times\ G_o(E)$$

If $j_1 = j_3 = i$; $\quad = \langle i | V | i \rangle^3 G_o^3(E)$

$j_1 = i,\ j_3 \neq i$; $\quad = \langle i | V | i \rangle G_o(E)$

$$\times \sum_{j_3 \neq i}' \frac{\langle i | V | j_3 \rangle \langle j_3 | V | i \rangle}{E - E_3^{(o)}} G_o(E)$$

$j_3 = i,\ j_1 \neq i$, $\quad = \langle i | V | i \rangle G_o(E)$

$$\times \sum_{j_1 \neq i}' \frac{\langle i | V | j_1 \rangle \langle j_1 | V | i \rangle}{E - E_1^{(o)}} G_o(E)$$

$j_1 = j_3 \neq i$;

$$= \sum_{j_3 \neq i}' \frac{|\langle i | V | j_3 \rangle|^2}{(E - E_3^{(o)})^2} \langle j_3 | V | j_3 \rangle G_o(E)$$

$j_1 \neq j_3 \neq i$;

$$= \sum_{j_1 j_3 \neq i}' \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_3 \rangle \langle j_3 | V | i \rangle}{(E - E_1^{(o)})(E - E_3^{(o)})}$$

$$\times\ G_o(E)$$

therefore ,

the fourth term $= G_o(E)\,\lambda^3 \langle i\,|\,V\,|\,i\rangle^3\, G_o^3\,(E)$

$$+ G_o(E)\,\lambda^3 \langle i\,|\,V\,|\,i\rangle\, G_o(E) \sum_{j_3 \neq i}{}' \frac{|\langle i\,|\,V\,|\,j_3\rangle|^2}{E - E_3^{(o)}}\, G_o(E)$$

$$+ G_o(E)\,\lambda^3 \langle i\,|V|\,i\rangle\, G_o(E) \sum_{j_1 \neq i}{}' \frac{|\langle i\,|\,V\,|\,j_1\rangle|^2}{E - E_1^{(o)}}\, G_o(E)$$

$$+ G_o(E)\,\lambda^3 \sum_{j_3 \neq i}{}' \frac{|\langle i\,|\,V\,|\,j_3\rangle|^2}{(E - E_3^{(o)})^2} \langle j_3\,|\,V\,|\,j_3\rangle\, G_o(E)$$

$$+ G_o(E)\,\lambda^3 \sum_{j_1 j_3 \neq i}{}' \frac{\langle i\,|\,V\,|\,j_1\rangle\langle j_1\,|\,V\,|\,j_3\rangle\langle j_3\,|\,V\,|\,i\rangle}{(E - E_1^{(o)})(E - E_3^{(o)})}\, G_o(E)$$

(2.1.13e)

If λ is equal to one and keeping only the first four terms, we have the perturbative series expansion from (2.1.13a-e)

$$\langle i\,|\frac{1}{E - H}|\,i\rangle = G_o(E)\,\{1 + \langle i\,|\,V\,|\,i\rangle G_o(E) + \langle i\,|\,V\,|\,i\rangle^2\, G_o^2(E)$$

$$+ \langle i\,|\,V\,|\,i\rangle^3\, G_o^3(E) + \sum_{j \neq i}{}' \frac{|\langle i\,|\,V\,|\,j\rangle|^2}{E - E_j^{(o)}}\, G_o(E)$$

$$+ 2\langle i\,|\,V\,|\,i\rangle\, G_o(E) \sum_{j \neq i}{}' \frac{|\langle i\,|\,V\,|\,j\rangle|^2}{E - E_j^{(o)}}\, G_o(E)$$

$$+ \sum_{j \neq i} \frac{|\langle i\,|\,V\,|\,j\rangle|^2}{(E - E_j^{(o)})^2} \langle j\,|\,V\,|\,j\rangle G_o(E)$$

$$+ \sum_{j_1 j_3 \neq i}{}' \frac{\langle i\,|\,V\,|\,j_1\rangle\langle j_1|\,V\,|\,j_3\rangle\langle j_3\,|\,V\,|\,i\rangle}{(E - E_1^{(o)})\,(E - E_3^{(o)})}\, G_o(E)\quad + \ldots\} \tag{2.1.14}$$

From (2.1.10) , we have the self energy expansion.

$$\langle i | \frac{1}{E - H} | i \rangle = G_o(E) \{ 1 + \Sigma G_o(E) + \Sigma G_o(E) \Sigma G_o(E)$$

$$+ \Sigma G_o(E) \Sigma G_o(E) \Sigma G_o(E) + \ldots \}$$

$$= G_o(E) \{ 1 + (\Sigma + \Sigma G_o(E) \Sigma + \Sigma G_o(E) \Sigma G_o(E) \Sigma$$

$$+ \ldots) G_o(E) \} \quad (2.1.15)$$

Comparing the perturbative expansion (2.1.14) and the self energy expansion (2.1.15), we get the self energy

$$\text{Self energy} = \Sigma = \langle i | V | i \rangle + \sum_{j \neq i} \frac{|\langle i | V | j \rangle|^2}{E - E_j^{(o)}}$$

$$+ \sum_{j \neq i} \frac{|\langle i | V | j \rangle|^2 \langle i | V | i \rangle}{(E - E_j^{(o)})^2}$$

$$+ \sum_{j_1 j_2 \neq i} \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_2 \rangle \langle j_2 | V | i \rangle}{(E - E_1^{(o)}) (E - E_2^{(o)})}$$

plus terms coming from the higher order perturbative correction (2.1.16)

In perturbative expansion, if we compared with self energy expansion, we will find that

$\langle i | V | i \rangle^2 G_o(E)$ comes from $\Sigma G_o(E) \Sigma$ where

$$\Sigma G_o(E) \Sigma = (\langle i | V | i \rangle + \ldots) G_o(E) (\langle i | V | i \rangle + \ldots)$$

$\langle i | V | i \rangle^3 G_o^2(E)$ comes from $\Sigma G_o(E) \Sigma G_o(E) \Sigma$ where

$$\Sigma G_o(E) \Sigma G_o(E) \Sigma = (\langle i | V | i \rangle + \ldots) G_o(E) (\langle i | V | i \rangle + \ldots)$$

$$\times G_o(E) (\langle i | V | i \rangle + \ldots)$$

$2 \langle i | V | i \rangle G_o(E) \sum_{j \neq i} \frac{|\langle i | V | j \rangle|^2}{E - E_j^{(o)}}$ comes from $\Sigma G_o(E) \Sigma$ by crossing terms which gives

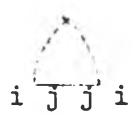
$$\Sigma\, G_o(E)\, \Sigma = \left(\langle i|\, V|\, i\rangle + \sum_{j \neq i}{}' \frac{|\langle i|\, V\, |j\rangle|^2}{E - E_j^{(o)}} + \ldots\right) G_o(E)$$

$$\times \left(\langle i\, |V\, |\, i\rangle + \sum_{j \neq i}{}' \frac{|\langle i\, |\, V\, |\, j\rangle|^2}{E - E_j^{(o)}} + \ldots\right)$$

2.2 Diagram Expansion

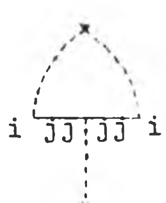
We will represent perturbative expansion with diagram expansion. Let us adopt the following convention.

$$= \langle i\, |\, V\, |\, i\rangle \qquad (2.2.1)$$



$$= \sum_{j \neq i}{}' \frac{\langle i\, |\, V\, |\, j\rangle \langle j\, |\, V\, |\, i\rangle}{E - E_j^{(o)}} \qquad (2.2.2)$$

$$= \sum_{j_1 j_2 \neq i} \frac{\langle i\, |\, V\, |\, j_1\rangle \langle j_1\, |\, V\, |\, j_2\rangle \langle j_2\, |\, V\, |\, i\rangle}{(E - E_{j_1}^{(o)})\ (E - E_{j_2}^{(o)}\ )} \qquad (2.2.3)$$



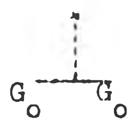
$$= \sum_{j \neq i}{}' \frac{\langle i\, |\, V\, |\, j\rangle \langle j\, |\, V\, |\, j\rangle \langle j\, |\, V\, |\, i\rangle}{(E - E_j^{(o)})^2} \qquad (2.2.4)$$

etc.

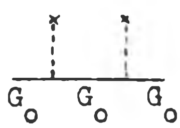
We will represent the free exciton propagator $\frac{1}{E - E_j^{(o)}}$ by a horizontal solid line as was done by Chatuporn.[15] Each vertex is associated with a polynomial $P_n(c)$ (where n equals to the number of interaction lines V which represented by a dash line) connecting the impurity (represented by a cross) and the exciton propagator line.

A horizontal solid line can be inside or partially inside. If it is inside, it must be summed over.

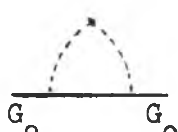
We shall now going to look at the diagrammatic interpretation of the perturbative series.[16] Perturbative series beyond the first term can be rewritten as $G_o(E)\ \Sigma\ G_o(E)$. The first term of $G_o(E)\ \Sigma\ G_o(E)$ is $G_o(E) \langle i\,|V|\,i\rangle G_o(E)$. Perturbative series beyond the first term can be represented by the diagrams (or graphs)



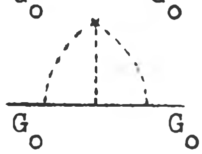
$$= G_o(E) \langle i\,|V|\,i\rangle G_o(E) \qquad (2.2.5)$$



$$= G_o(E) \langle i\,|V|\,i\rangle G_o(E) \langle i\,|V|\,i\rangle G_o(E) \qquad (2.2.6)$$

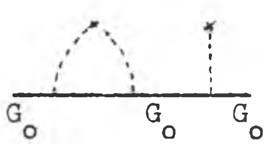


$$= G_o(E) \sum_{j \neq i}{}' \frac{|\langle i\,|V|\,j\rangle|^2}{E - E_j^{(o)}} G_o(E) \qquad (2.2.7)$$



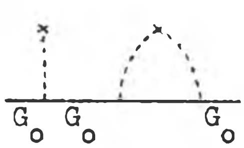
$$= G_o(E) \sum_{j_1 j_2 \neq i}{}' \frac{\langle i\,|V|\,j_1\rangle \langle j_1\,|V|\,j_2\rangle}{(E - E_{j_1}^{(o)})\ (E - E_{j_2}^{(o)})}$$

$$\times \langle j_2|\,V\,|\,i\rangle G_o(E) \qquad (2.2.8)$$



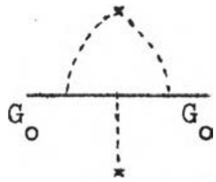
$$= G_o(E) \sum_{j \neq i}{}' \frac{|\langle i\,|V|\,j\rangle|^2}{E - E_j^{(o)}} G_o(E)$$

$$\times \langle i\,|V|\,i\rangle G_o(E) \qquad (2.2.9)$$



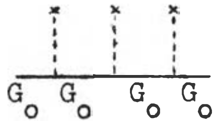
$$= G_o(E) \langle i\,|V|\,i\rangle G_o(E) \sum_{j \neq i}{}' \frac{|\langle i\,|V|\,j\rangle|^2}{E - E_j^{(o)}}$$

$$\times\ G_o(E) \qquad (2.2.10)$$



$$= G_o(E) \sum_{j \neq i}' \frac{\langle i | V | j \rangle \langle j | V | j \rangle \langle j | V | i \rangle}{(E - E_j^{(o)})^2}$$

$$\times\, G_o(E) \qquad (2.2.11)$$



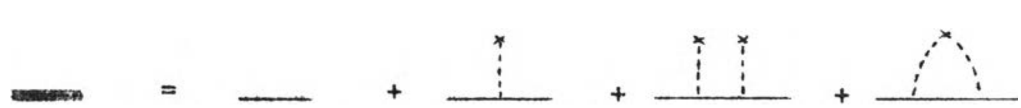
$$= G_o(E) \langle i | V | i \rangle G_o(E) \langle i | V | i \rangle G_o(E)$$

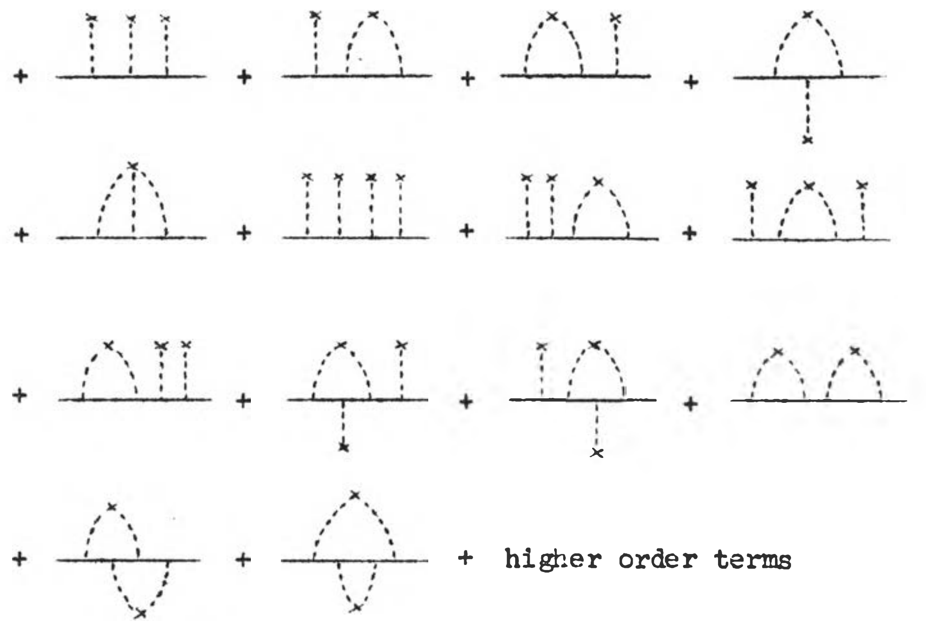
$$\times \langle i | V | i \rangle G_o(E) \qquad (2.2.12)$$

etc.

We now attempt to generalize to higher orders. The n - th order correction has n interaction V (¦) lines and it has n + 1 propagators of the type $\frac{1}{E - E_j^{(o)}}$ at least two of these are $G_o(E)$. The total number of terms arising in the n - th order perturbative series is the total number of distinct pictures having n - interaction lines and the correspondence is one - to - one. We obtain the n - th order correction when we write down the analytic expressions for all the distinct graphs we can draw with n - interaction lines.

If we represent $\langle i | \frac{1}{E - H} | i \rangle$ by ▬ (fat line) and $\langle i | \frac{1}{E - H_o} | i \rangle$ by —— (thin line), the perturbative series is graphically represented as





+ higher order terms

(2.2.13)

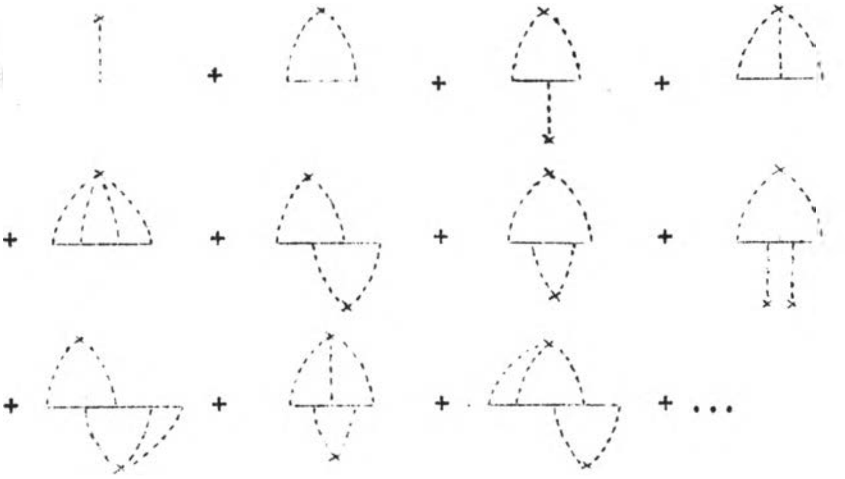
The graphs can be divided into two groups.

1. Reducible graphs : these are the graphs which can be separated into two parts by cutting one propagation line (horizontal line).

2. Irreducible graphs : these are the graphs which cannot be separated into two parts by cutting one propagation line.

The self energy Σ are the summation of all irreducible graphs in (2.2.13) by cutting G_o at the first and the end of graphs thus

Σ =



(2.2.14)

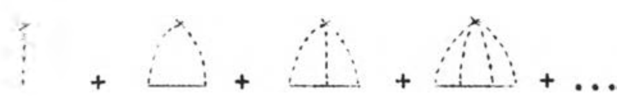
The self energy = Monomer series + Dimer series + Trimer series +...

(2.2.15a)

$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_3 + \ldots \qquad (2.2.15b)$$

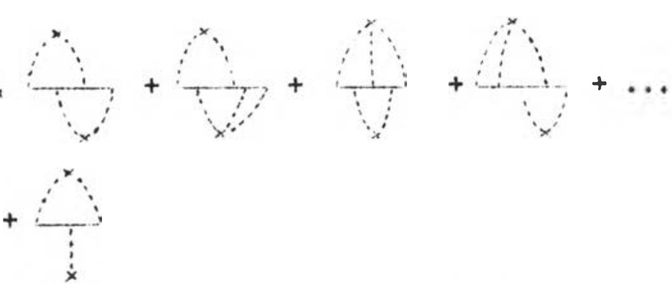
where Σ_1 is the monomer series, Σ_2 is the dimer series,... which are the summation of all irreducible graphs have one vertex, two vertex,... respectively.

Σ_1 =



(2.2.16)

Σ_2 =



(2.2.17)

We shall discuss Σ_1 and Σ_2 in the next section .

2.3 Monomers

From the monomer series expansion by diagram approach of the self - energy in previous section, the analytical expression can be expressed as (where Δ is equivalent to V)

$$\Sigma_1 = (\Delta/N)NP_1(c) + (\Delta/N)^2 NP_2(c) \sum_{k'} G_o(k') + (\Delta/N)^3 NP_3(c) \sum_{k'}\sum_{k''} G_o(k') G_o(k'') + \ldots \quad (2.3.1)$$

N is the total number of molecules or states. $P_n(c)$ is a polynomial given by the following generating function :

$$\ln(1 - c + c\, e^{\alpha}) = \sum_{n=1}^{\infty} \frac{P_n(c)\, \alpha^n}{n!} \quad (2.3.2)$$

Hong and Kopelman's result[7] is obtained when c is substituted for $P_n(c)$ in (2.3.1). This substitution leads to

$$\Sigma_1 = (\Delta/N)Nc\{1 + \Delta G_o(E) + \Delta^2 G_o^2(E) + \ldots\} \quad (2.3.3)$$

where $G_o(E) = \frac{1}{N}\sum_{k'} G_o(k')$. Notice that Σ_1 has no $\vec{k}$ dependence. Using the geometric power series expansion :

$$\frac{1}{1-x} = 1 + x + x^2 + \ldots \quad (2.3.4)$$

So (2.3.3) can be written as

$$\Sigma_1 = \frac{c\Delta}{1 - \Delta G_o(E)} \quad (2.3.5)$$

It has been shown by Hong and Robinsion that, within the restricted Frenkel limit, the mixed crystal Green's function can be written in Dyson's form as

$$\langle G(\vec{k})\rangle = G_o(\vec{k}) + G_o(\vec{k})\ \Sigma\ (k) \langle G(\vec{k})\rangle \tag{2.3.6}$$

or it can be written as

$$\langle G(\vec{k})\rangle = \{G_o^{-1}(\vec{k}) - \Sigma\ (\vec{k})\}^{-1}$$

$$\text{or } \langle G(\vec{k})\rangle = \{E - \varepsilon(\vec{k}) - \Sigma(\vec{k})\}^{-1} \tag{2.3.7}$$

By taking the imaginary part of each side in (2.3.7) . we get

$$\text{Im}\langle G(\vec{k})\rangle = \frac{\text{Im}\ \Sigma(\vec{k})}{\{E - \varepsilon(\vec{k}) - \text{Re}\ \Sigma\ (\vec{k})\}^2 + \{\text{Im}\ \Sigma(\vec{k})\}^2} \tag{2.3.8}$$

$$\left(\text{since if } X = \frac{1}{A - iB} \Longrightarrow \text{Im } X = \frac{B}{A^2 + B^2}\right)$$

Since at low concentration $\Sigma(\vec{k})$ is very small, we can put

$$\text{Im}\langle G(\vec{k})\rangle \simeq \frac{\text{Im}\ \Sigma(\vec{k})}{\{E - \varepsilon\ (\vec{k})\}^2} \tag{2.3.9}$$

In other words, the poles of $\langle G(\vec{k})\rangle$ outside the band are the same as the poles of $\Sigma\ (\vec{k})$ and the residues of these two functions at their common poles are related through (2.3.9)

It follows immediately from (2.3.5) and (2.3.9) that the monomer energy, E(1), must satisfy ($\Sigma \rightarrow \Sigma_1$)

$$1 - \Delta G_o(E) = 0$$

$$\text{or} \int \frac{\rho_o(E')dE'}{E(1) - E'} = \frac{1}{\Delta} \tag{2.3.10}$$

which is the familiar Koster and Slater equation.

The optical spectrum can also be obtained by using the following relationship

$$I_b^o(E) = \frac{1}{\pi} \text{Im} \langle G(\vec{k}^+ = 0) \rangle$$

and $$I_{ac}^o(E) = \frac{1}{\pi} \text{Im} \langle G(\vec{k}^- = 0) \rangle \qquad (2.3.11)$$

where b and ac refer to the branches of the spectrums. For convenience, Hong and Kopelman worked with $I_b\{E(1)\}$ and $I_{ac}\{E(1)\}$, defined as the total intensity attributable to the monomer impurity integrated over the neighborhood ε of E(1) defined as

$$I_b\{E(1)\} = \int_{E(1)-\varepsilon}^{E(1)+\varepsilon} I_b^o(E)dE,$$

and $$I_{ac}\{E(1)\} = \int_{E(1)-\varepsilon}^{E(1)+\varepsilon} I_{ac}^o(E)dE \qquad (2.3.12)$$

By using (2.3.9),(2.3.11), and (2.3.12), we get

$$I_b\{E(1)\} = \frac{1}{\pi} \int_{E(1)-\varepsilon}^{E(1)+\varepsilon} \frac{\text{Im}\,\Sigma_1(\vec{k}^+ = 0)dE'}{\{E' - \varepsilon_b\}^2}$$

$$= \frac{\text{res}\ \Sigma_1\{E' = E(1)\}}{\{E(1) - \varepsilon_b\}^2} \qquad (2.3.13)$$

where $\varepsilon_b = \varepsilon(\vec{k}^+ = 0)$. Since Σ_1 is $\vec{k}$ independent (and branch independent), $\Sigma_1(\vec{k}^+ = 0) = \Sigma_1(\vec{k}^- = 0)$. Similarly we get

$$I_{ac}\{E(1)\} = \frac{\text{res}\,\Sigma_1\{E' = E(1)\}}{\{E(1) - \varepsilon_{ac}\}^2} \qquad (2.3.14)$$

where $\varepsilon_{ac} = \varepsilon(\vec{k} = 0)$. The polarization ratio P(b/ac), which is simply equal to $\frac{I_b \cdot |\mu_b|^2}{I_{ac} \cdot |\mu_{ac}|^2}$, can be rewritten as

$$P(b/ac) = \frac{\{E(1) - \varepsilon_{ac}\}^2 \cdot |\mu_b|^2}{\{E(1) - \varepsilon_b\}^2 \cdot |\mu_{ac}|^2} \qquad (2.3.15)$$

where μ_b and μ_{ac} are the transition moments to the two Davydov components. This result has come to be known as the Rashba effect. Furthermore, the residue of Σ_1 at E(1) can be evaluated from (2.3.5) and substituted into (2.3.13) and (2.3.14). We find that

$$I_b\{E(1)\} = \frac{1}{\{E(1) - \varepsilon_b\}^2} \cdot \frac{1}{\left[\frac{d}{dE}\Sigma_1^{-1}\right]_{E = E(1)}}$$

$$= \frac{c}{\{E(1) - \varepsilon_b\}^2} \left[\frac{\rho_o(E')\, dE'}{\{E(1) - E'\}^2}\right]^{-1}$$

$$= \frac{c}{\{E(1) - \varepsilon_b\}^2} \Delta^2 \frac{dE(1)}{d\Delta}$$

$$= \frac{c\,\Delta^2}{\{E(1) - \varepsilon_b\}^2} \left\{\frac{dE(1)}{d\Delta}\right\} \qquad (2.3.16)$$

$$\left[\text{Since} \left[\int \frac{\rho_o(E')\, dE'}{\{E(1) - E'\}^2}\right]^{-1} = \Delta^2 \frac{dE(1)}{d\Delta}\right]$$

and similarly

$$I_{ac}\{E(1)\} = \frac{c\,\Delta^2}{\{E(1) - \varepsilon_{ac}\}^2} \left\{\frac{dE(1)}{d\Delta}\right\} \qquad (2.3.17)$$

These results were also derived by Craig and Philpott, based on the Koster and Slater formalism.

From these results Hong and Kopelman were able to explain some of the observed properties of mixed naphthalene crystal.

Later Chatuporn and Tang[15,16] extend the theory to crystals containing the higher concentrations of impurities. The modification consists essentially of replacing the approximation $P_n(c) = c$ for all n by a form of $P_n(c)$ used by Leath and Goodman for treating lattice vibration in disordered binary system.

Leath and Goodman pointed out that $P_n(c)$ can be written as

$$P_n(c) = \sum_{m=1}^{n} (-1)^{m-1} (m-1)!\, S(n,m)\, c^m \qquad (2.3.18)$$

where S(n,m) are Stirling numbers of the second kind. A combinatorial interpretation is that S(n,m) is the number of ways that n distinct objects can be put into m indistinguishable boxes with no box empty. Or it is the number of ways of partitioning a set of n elements into m non - empty subset.

Stirling numbers of the second kind can be defined in terms of the binomial coefficient as[17]

$$S(n,m) = S_n^{(m)} \quad \text{(notation in the Handbooks)}$$

$$= \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} k^n \qquad (2.3.19)$$

Substitution of (2.3.19) into (2.3.18) gives

$$P_n(c) = \sum_{m=1}^{n} (-1)^{m-1} \quad (m-1)! \quad c^m \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \frac{m!}{(m-k)!\,k!} k^n \tag{2.3.20}$$

The coefficients of the N^{th} power of c in the n^{th} function $P_n(c)$ can be obtained by the relationship

$$\text{Coefficient of } c^N \text{ in } P_n(c) = \frac{1}{N!} \frac{\partial^N}{\partial c^N} P_n(c) \Big|_{c=0} \tag{2.3.21}$$

where $n > N$

Substituting (2.3.20) into (2.3.21), we get the coefficient of c^N in $P_n(c)$ equal to

$$\frac{1}{N} \sum_{m=n}^{n} (-1)^{m-1} (m-1)! \frac{m!}{(m-N)!} c^{m-N} \Big|_{c=0}$$

$$\times \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \frac{m!}{(m-k)!\,k!} k^n$$

$$= \frac{1}{N!} \sum_{m=N}^{n} (-1)^{m-1} (m-1)! \frac{m!}{(m-N)!} \delta_{mN} \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \frac{m!}{(m-k)!\,k!} k^n$$

$$= \frac{1}{N!} (-1)^{N-1} (N-1)!\, N! \frac{1}{N!} \sum_{k=0}^{N} (-1)^{N-k} \frac{N!}{(N-k)!\,k!} k^n$$

$$= (N-1)! \sum_{k=0}^{N} (-1)^{k+1} \frac{1}{(N-k)!\,k!} k^n \tag{2.3.22}$$

Again it should be emphasized that the n appearing in (2.3.22) is the subscript of P(c) function while N is the power of c in $P_n(c)$

We are now in a position of being able to sum the self - energy arising from the monomer contribution. The summing of Σ_1 is accomplished by summing those contribution from each diagram which are proportional to c, then summing those parts which are proportional to c^2, then those proportional to c^3 and so forth. For example, the contribution of the L^{th} diagram to the series which is proportional to c^N is

$$(N - 1)!\,\Delta \sum_{k=0}^{N} (-1)^{k+1} \frac{k^L \Delta^{L-1} G_o^{L-1}}{(N-k)!\,k!} \qquad (2.3.23)$$

Equation (2.3.23) is the product of (2.3.22) and the Green's function equivalent of L interactions connected to the impurity with the propagator G(E) without the probability factor $P_n(c)$ present.

Putting everything together, we find that the self-energy is

$$\Sigma_1 = c\Delta\,(1 + \Delta G_o + \Delta^2 G_o^2 + \ldots + \Delta^n G_o^n + \ldots) + \Sigma^{(2)} \qquad (2.3.24)$$

where

$$\Sigma^{(2)} = \Delta \sum_{N=2}^{\infty} c^N \sum_{n=N}^{\infty} (N-1)! \sum_{k=0}^{N} (-1)^{k+1} \frac{k^n \Delta^{n-1} G_o^{n-1}}{(N-k)!\,k!} \qquad (2.3.25a)$$

The first summation in $\Sigma^{(2)}$ represents summation over all the orders of c, the second summation represents the summing of all the contributions which are proportional to c^N, while the last summation arises from the definition of n^{th} contribution. By rearranging the terms in the last two summations, we get

$$\Sigma^{(2)} = \Delta \sum_{N=2}^{\infty} \frac{c^N}{N} \sum_{n=N}^{\infty} \sum_{k=0}^{N} (-1)^{k+1} \binom{N}{k} k^n \Delta^{n-1} G_o^{n-1} \qquad (2.3.25b)$$

where $\binom{N}{k}$ is the binomial coefficient. If we now adopt a convention that $\binom{N}{k} = 0$ for $k > N$, the summation over k can be extended to infinity. This allow us to interchange the two summation over n and k. The summation over n can now be carried out as follows.

$$\sum_{n=N}^{\infty} k^n \Delta^{n-1} G_o^{n-1} = \Delta^{-1} G_o^{-1} \sum_{n=N}^{\infty} k^n \Delta^n G_o^n$$

$$= \Delta^{-1} G_o^{-1} k^N \Delta^N G_o^N \sum_{n=0}^{\infty} k^n \Delta^n G_o^n$$

$$= \frac{k^N \Delta^{N-1} G_o^{N-1}}{1 - k\Delta G_o} \qquad (2.3.26)$$

where $k \Delta G_o < 1$

Thus the second part of the self-energy becomes

$$\Sigma^{(2)} = \Delta \sum_{N=2}^{\infty} \frac{c^N}{N} \sum_{k=0}^{\infty} (-1)^{k+1} \binom{N}{k} \frac{k^N \Delta^{N-1} G_o^{N-1}}{1 - k\Delta G_o}$$

(2.3.27a)

$$= G_o^{-1} \sum_{N=2}^{\infty} \frac{c^N \Delta^N G_o^N}{N} \sum_{k=0}^{\infty} (-1)^{k+1} \binom{N}{k} \frac{k^N}{1 - k\Delta G_o}$$

(2.3.27b)

$$= \Sigma_1^{(2)} + \Sigma_2^{(2)} + \Sigma_3^{(2)} + \Sigma_4^{(2)} + \ldots \qquad (2.3.28)$$

where

$$\Sigma_1^{(2)} = G_o^{-1} \sum_{N=2}^{\infty} \frac{1}{N} \binom{N}{1} \frac{c^N \Delta^N G_o^N}{1 - \Delta G_o} \qquad (2.3.29a)$$

$$\Sigma_2^{(2)} = -G_o^{-1} \sum_{N=2}^{\infty} \frac{1}{N}\binom{N}{2}\frac{(2c\,\Delta\,G_o)^N}{1-2\,\Delta\,G_o} \tag{2.3.29b}$$

$$\Sigma_3^{(2)} = G_o^{-1} \sum_{N=3}^{\infty} \frac{1}{N}\binom{N}{3}\frac{(3c\,\Delta\,G_o)^N}{1-3\,\Delta\,G_o} \tag{2.3.29c}$$

and where the general expression is

$$\Sigma_L^{(2)} = G_o^{-1} \sum_{N=L}^{\infty} (-1)^{L+1} \frac{1}{N}\binom{N}{L}\frac{(Lc\,\Delta\,G_o)^N}{1-L\,\Delta\,G_o} \tag{2.3.29d}$$

By writting out the binomial coefficient, (2.3.29a) to (2.3.29d) become

$$\Sigma_1^{(2)} = \frac{c^2\,\Delta^2\,G_o}{1-\Delta G_o}\quad\frac{1}{1-c\,\Delta\,G_o} \tag{2.3.30a}$$

$$\Sigma_2^{(2)} = \frac{-c\,\Delta}{1-2\,\Delta G_o}\quad\sum_{n=0}^{\infty} n(2c\,\Delta\,G_o)^n \tag{2.3.30b}$$

$$\Sigma_3^{(2)} = \frac{c\,\Delta}{1-3\,\Delta G_o}\quad\sum_{n=0}^{\infty}\frac{n(n-1)}{2}\,(3c\,\Delta G_o)^n \tag{2.3.30c}$$

$$\Sigma_L^{(2)} = (-1)^{L+1}\,\frac{c\,\Delta}{1-L\,\Delta\,G_o} \times \sum_{n=0}^{\infty}\frac{n(n-1)\,(n-2)\ldots(n-L+2)\,(Lc\,\Delta G_o)^n}{(L-1)!} \tag{2.3.30d}$$

The summation over n in (2.3.30b) to (2.3.30d) can be carried out by noting that

$$\sum_{k=0}^{\infty} kX^{k} = \frac{X}{(1 - X)^{2}} \qquad (2.3.31)$$

Dividing both sides of eq. (2.3.31) By X, we get

$$\sum_{k=0}^{\infty} kX^{k-1} = \frac{1}{(1 - X)^{2}} \qquad (2.3.32)$$

By differentiating (2.3.32) with respect to X, we get

$$\sum_{k=0}^{\infty} k(k - 1)\, X^{k-2} = \frac{2}{(1 - X)^{3}} \qquad (2.3.33)$$

Again by differentiating (2.3.33)with respect to X,we get

$$\sum_{k=0}^{\infty} k(k - 1)\,(k - 2)\, X^{k-3} = \frac{2.3}{(1 - X)^{4}} \qquad (2.3.34)$$

Repeating the differentiation N - 2 times , we get

$$\sum_{k=0}^{\infty} k(k - 1)\,(k - 2)\ldots(k - N + 2)\, X^{k-(N-1)} = \frac{(N - 1)!}{(1 - X)^{N}} \qquad (2.3.35)$$

Multiplying (2.3.35) the both sides by $X^{(N-1)}$, we get

$$\sum_{k=0}^{\infty} k(k - 1)\,(k - 2)\ldots(k - N + 2)\, X^{k} = \frac{(N - 1)!\, X^{(n-1)}}{(1 - X)^{N}} \qquad (2.3.36)$$

Putting the general result (2.3.36) in (2.3.30d) , we find that

$$\Sigma_{L}^{(2)} = (-1)^{L+1} \frac{c\Delta}{1 - L\Delta G_{o}} \frac{(Lc\Delta G_{o})^{L-1}}{(1 - Lc\Delta G_{o})^{L}} \qquad (2.3.37)$$

Summing over all values of the variables L of (2.3.37) and replacing $1 + \Delta G_o + \Delta^2 G_o^2 + \ldots$ by its sum, we find that the self-energy due to the monomer contribution is

$$\begin{aligned}\Sigma_1 &= \frac{c\,\Delta}{1 - \Delta G_o} + \frac{c\Delta}{(1 - \Delta G_o)}\,\frac{c\Delta G_o}{(1 - c\,\Delta G_o)} \\ &+ \sum_{L=2}^{\infty} (-1)^{L+1} \frac{c\Delta}{1 - L\,\Delta G_o}\,\frac{(Lc\,\Delta G_o)^{L-1}}{(1 - Lc\,\Delta G_o)^L} \\ &= \frac{c\,\Delta}{1 - \Delta G_o}\,\frac{1}{(1 - c\,\Delta\,G_o)} \\ &+ \sum_{L=2}^{\infty} (-1)^{L+1} \frac{c\,\Delta}{1 - L\,\Delta\,G_o}\,\frac{(Lc\Delta\,G_o)^{L-1}}{(1 - Lc\Delta\,G_o)^L} \\ &= c\,\Delta \sum_{L=1}^{\infty} (-1)^{L+1} \frac{c\Delta}{1 - L\,\Delta\,G_o}\,\frac{(Lc\,\Delta\,G_o)^{L-1}}{(1 - Lc\,\Delta\,G_o)^L}\end{aligned} \tag{2.3.38}$$

It should be noted that as $c \to 0$, (2.3.38) reduces to the self-energy, (2.3.5), derived by Hong and Kopelman on the basis of the substitution $P_n(c) = c$ for all values of n.

2.4 Dimers

In the two-impurity problem, we are interested in the so-called translationally equivalent pairs and interchange pairs. As we have already mentioned, the nature of a lattice structure implies that, corresponding to any arbitrary molocule, there is a molecule in every other unit cell with exactly the same orientation and exactly the same relative position in the unit cell. These molecules are called translationally equivalent pairs. Interchange molecules have different crystal orientations, that is, different translationally equivalent pairs.

2.4.1 Hong and Kopelman's results[7]

Let us now consider the pair problem. Σ_2 is $\vec{k}$ dependent and much more complicated to derive. The following procedure is an adaptation of Yonezawa and Matsubara's method[18] to the multiple branched exciton band.

We first define :

$$f_1(\vec{R}) = \sum_{\vec{k}^+} \exp(i\vec{k}^+ . \vec{R})\, G_o(\vec{k}^+) + \sum_{\vec{k}^-} \exp(i\vec{k}^- . \vec{R})\, G_o(\vec{k}^-) \tag{2.4.1a}$$

$$f_2(\vec{R}) = \sum_{\vec{k}^+} \exp(i\vec{k}^+ . \vec{R})\, G_o(\vec{k}^+) - \sum_{\vec{k}^-} \exp(i\vec{k}^- . \vec{R})\, G_o(\vec{k}^-) \tag{2.4.1b}$$

and

$$\rho_{\vec{R}}(E') = N^{-1}\Big[\sum_{\vec{k}^+} \exp(i\vec{k}^+ . \vec{R})\, \delta\{E' - E(\vec{k}^+)\} \pm \sum_{\vec{k}^-} \exp(i\vec{k}^- . \vec{R})\, \delta\{E' - E(\vec{k}^-)\}\Big] \tag{2.4.2}$$

where $\rho_{\vec{R}}(E')$ is the off-diagonal density of states function. The upper sign must be used for the translationally equivalent pair and the lower sign must be used for the interchange equivalent pair.

The diagonal density of states function $\rho_o(E')$ for naphthalene crystal in its ${}^1B_{2u}$ state can be written as

$$\rho_o(E') = N^{-1}\left[\sum_{\vec{k}^+} \delta\{E' - E(\vec{k}^+)\} + \sum_{\vec{k}^-} \delta\{E' - E(\vec{k}^-)\} \right]$$

(2.4.3)

and the density of states $\rho_o(E')$ is connected to the Green's function for the pure crystal

$$G_o(E) = N^{-1}\{ \sum_{\vec{k}^+} G_o(\vec{k}^+) + \sum_{\vec{k}^-} G_o(\vec{k}^-) \} \quad (2.4.4)$$

by the relationship

$$G_o(E) = \int \frac{\rho_o(E')}{E - E'} dE' \quad (2.4.5)$$

From (2.4.1a), (2.4.1b), (2.4.2), (2.4.3), (2.4.4) and (2.4.5) we have

$$f_1(0)/N = G_o(E)$$

$$= \int \frac{\rho_o(E')}{E - E'} dE' \quad (2.4.6a)$$

$$f_1(\vec{R}_e)/N = \int \frac{\rho_{\vec{R}e}(E')}{E - E'} dE' \quad (2.4.6b)$$

$$f_2(\vec{R}_i)/N = \int \frac{\rho_{\vec{R}_i}(E')}{E - E'} dE' \quad (2.4.6c)$$

where $\vec{R}_e$ is the pair distance between two translationally equivalent molecules and $\vec{R}_i$ is the pair distance between two interchange equivalent molecules.

We must define a new type of delta function $\bar{\delta}$ which is peculiar to the problem of multiple-branched exciton bands. As was stressed by Hong and Robinson, the "selection rules" for exciton scattering by impurities in multiple-branched exciton bands contain not only the conservation of quasimomentum (associated with translational symmetry) but also the retention of interchange symmetry (associated with factor group symmetry). Mathematically, we have

$$\bar{\delta}(\vec{P}_1 + \vec{P}_2 + \vec{P}_3 + \ldots + \vec{P}_s) = \delta(\vec{P}_1 + \vec{P}_2 + \vec{P}_3 + \ldots + \vec{P}_s)\, H\{(-1)^m\} \tag{2.4.7}$$

where $\vec{P}_1 = \vec{k} - \vec{k}'$, $\vec{P}_2 = \vec{k}' - \vec{k}''$, etc., are the momentum transfers between the impurities and the "exciton" in each encounter. $H\{(-1)^m\}$ is the Heaviside step function and m is the number of times an exciton is scattered from one branch of the band to the other; so

$$H\{(-1)^m\} = 0 \;, \quad \text{if} \quad m = \text{odd},$$
$$H\{(-1)^m\} = 1 \;, \quad \text{if} \quad m = \text{even}$$

It is noted that only those scattering routes included in Fig. 2.4.1a are to be summed over all the routes would be legitimate from a simple momentum consideration.

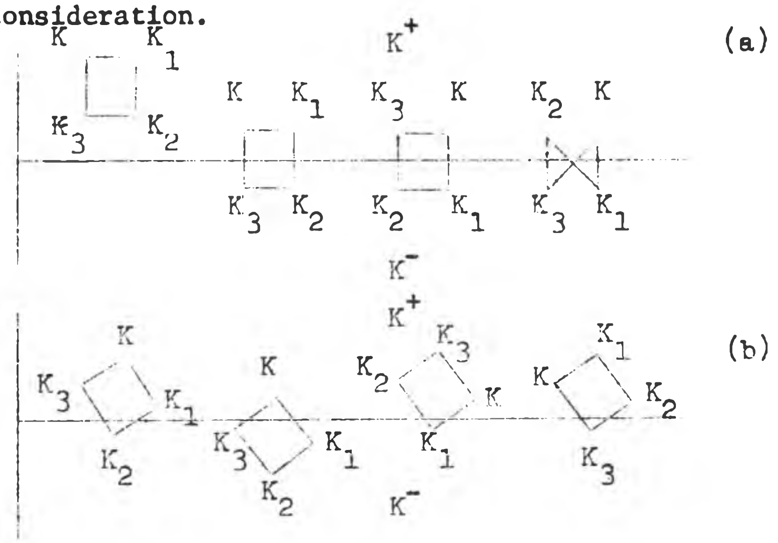


Fig. 2.4.1 Possible scattering routes given by $\bar{\delta}(\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3)$ $\times\ \bar{\delta}(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k})$ according to our definition of the delta functions. Terms to be summed are those in (a) and terms not to be summed are those in (b)

We will now examine the diagrams in Fig. 2.4.2

Σ_2 =

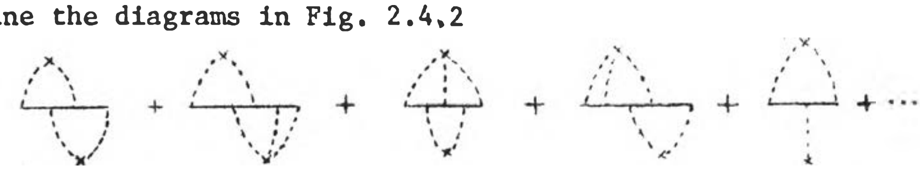


Fig.2.4.2 Diagrams included in the second-order self-energy part $\Sigma_2(\vec{k})$ which yields the resonance pair levels.

The first diagram in Fig. 2.4.2 can be rewritten in terms of $f_1(\vec{R}_e)$ and $f_2(\vec{R}_i)$ { putting $P_n(c) = c$ for small c }

$$(\Delta/N)^4 N^2 c^2 \sum_{k_1} \sum_{k_2} \sum_{\vec{k}_3} \bar{\delta}(\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3) . \bar{\delta}(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k})$$

$$\times\ G_o(\vec{k}_1)\ G_o(\vec{k}_2)\ G_o(\vec{k}_3) \quad = \quad (\Delta/N)^4 Nc^2 \{ \sum_{R_e} \exp(-i\vec{k}^{\pm} . \vec{R}_e)$$

$$\times\ f_1(\vec{R}_e)\ |f_1(\vec{R}_e)|^2$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm} , \vec{R}_i)\ f_2(\vec{R}_i)\ |f_2(\vec{R}_i)|^2 \} \qquad (2.4.8)$$

The upper sign should be used if the initial states are in the plus branch ($|\vec{k}^+ >$'s) and the lower sign should be used if they are in the minus branch ($|\vec{k}^- >$'s). In deriving this, we have used the following equality :

$$\sum_{\vec{R}_e} \exp \{- i(\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3) \cdot \vec{R}_e \}$$

$$+ (- 1)^m \sum_{\vec{R}_i} \exp \{- i(\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3) \cdot \vec{R}_i \}$$

$$= N \bar{\delta} (\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3) \quad , \qquad (2.4.9)$$

where $\bar{\delta}$ and m have been defined in (2.4.7)

Next we consider the third diagram in Fig. 2.4.2 (the second and forth diagrams are actually variations of the same type, generalized from the first diagram). This term can also be rewritten in terms of $f_1(\vec{R}_e)$ and $f_2(\vec{R}_i)$ { again $P_n(c) = c$ }

$$(\Delta/N)^5 N^2 c^2 \sum_{\vec{k}_1} \sum_{\vec{k}_2} \sum_{\vec{k}_3} \sum_{\vec{k}_4} \bar{\delta} (\vec{k} - \vec{k}_1 + \vec{k}_2 - \vec{k}_3 + \vec{k}_4 - \vec{k})$$

$$\times \bar{\delta} (\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4) \quad G_o(\vec{k}_1) G_o(\vec{k}_2) G_o(\vec{k}_3) G_o(\vec{k}_4)$$

$$= (\Delta/N)^5 N c^2 \{ \sum_{\vec{R}_e} | f_1(\vec{R}_e) |^4 + \sum_{\vec{R}_i} | f_2(\vec{R}_i)|^4 \} \qquad (2.4.10)$$

In general, it is easy to see that terms represented by diagrams of the type in Fig. 2.4.3 (these would include, for example, the second and fourth diagrams of Fig. 2.4.2) can be written as { until $P_n(c) = c$ }

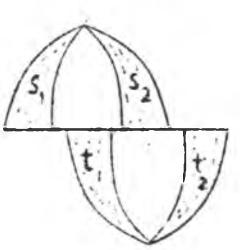


Fig.2.4.3 Typical diagrams included in $\Sigma_2(\vec{k})$. For convenience, diagrams of this type were summed up to form the partial sum that is represented by the first diagram in Fig.2.4.2

$$(\Delta/N)^4 Nc^2\{ \sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm} \cdot \vec{R}e)\, f_1(\vec{R}_e)|\, f_1(\vec{R}_e)\,|^2$$

$$\pm \sum_{\vec{R}_1} \exp(-i\vec{k}^{\pm} \cdot \vec{R}_1)\, f_2(\vec{R}_1)\,|f_2(\vec{R}_1)|^2\}\{(\Delta/N)\, f_1(0)\}^{s-2}$$

$$x\{(\Delta/N)\, f_1(0)\}^{t-2} \qquad (2.4.11)$$

where $s = s_1 + s_2$, $t = t_1 + t_2$ (in reference to Fig.2.4.3) are the total numbers of interaction lines associated with each guest. Similarly, for diagrams of the type given in Fig.2.4.4, we have

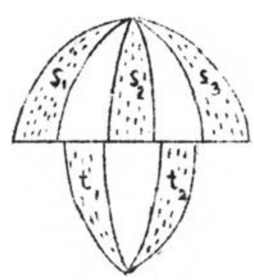


Fig.2.4.4 Typical diagrams included in $\Sigma_2(\vec{k})$. For convenience, diagrams of this type were summed up to form the partial sum that is represented by the third diagram in Fig.2.4.2

$$(\Delta/N)^5 Nc^2\{ \sum_{R_e} |f_1(\vec{R}_e)|^4 + \sum_{\vec{R}_1} |f_2(\vec{R}_1)|^4\}\{(\Delta/N)\, f_1(0)\}^{s-3}$$

$$x\{(\Delta/N)\, f_1(0)\}^{t-2}, \qquad (2.4.12)$$

where $s = s_1 + s_2 + s_3$, and $t = t_1 + t_2$. These expressions can be derived from (2.4.1), (2.4.6) and (2.4.9).

It is appearent that diagrams with the same values of s and t but different values of s_1, s_2, s_3, t_1, t_2, etc., are actually equal and can be lumped together. The problem is, then to calculate the number possible partitions of s and t interaction lines into two or three groups. This general problem was treated by Yonezawa and Matsubara. We will use their results here. If we denote the number of all possible partitions of s interaction lines into r groups as $B_{s,r}$, we have

$$B_{s,r} = (s-1)!\ /\ (s-r)!\ (r-1)! \qquad (2.4.13)$$

or alternatively, $B_{s,r}$ can be given by a generating function :

$$\left(\frac{x}{1-x}\right)^r = \sum_{s=r}^{\infty} B_{s,r}\, x^s \qquad (2.4.14)$$

Infinite sums over all diagrams of the type represented in Fig.2.4.3 or Fig.2.4.4 can now be performed with the aid of (2.4.13) and (2.4.14). Denoting these sums as $S_{2,2}$ or $S_{3,2}$ (subscripts referring to the number of groups of interaction lines associated with the first and the second guest, repectively), we have, from (2.4.11)

$$S_{2,2} = (\Delta/N)^4 Nc^2 \{ \sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm} \cdot \vec{R}_e)\, f_1(\vec{R}_e) |\, f_1(\vec{R}_e)|^2$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm} \cdot \vec{R}_i)\, f_2(\vec{R}_i) |\, f_2(\vec{R}_i)|^2 \}$$

$$\times \left[\sum_{s=2}^{\infty} B_{s,2} \{(\Delta/N)\, f_1(0)\}^{s-2} \right.$$

$$\left. \{ \sum_{t=2}^{\infty} B_{t,2} \{(\Delta/N)\, f_1(0)\}^{t-2} \right]$$

$$= Nc^2 \{ \sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm} . \vec{R}_e)\, f_1(\vec{R}_e) |\, f_1(\vec{R}_e)|^2$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm} . \vec{R}_i)\, f_2(\vec{R}_i) |\, f_2(\vec{R}_i)|^2 \}$$

$$\times \left[(\Delta/N) / \{1 - (\Delta/N)\, f_1(0)\} \right] \tag{2.4.15a}$$

Similarly, from (2.4.12)

$$S_{3,2} = (\Delta/N)^5\, Nc^2 \{ \sum_{\vec{R}_e} |f_1(\vec{R}_e)|^4 + \sum_{\vec{R}_i} |f_2(\vec{R}_i)|^4 \}$$

$$\left[\sum_{s=3}^{\infty} B_{s,3} \{(\Delta/N)\, f_1(0)\}^{s-3} \right] \left[\sum_{t=2}^{\infty} B_{t,2} \{(\Delta/N)\, f_1(0)\}^{t-2} \right]$$

$$= Nc^2 \{ \sum_{\vec{R}_e} |f_1(\vec{R}_e)|^4 + \sum_{\vec{R}_i} |f_2(\vec{R}_i)|^4 \} \left[(\Delta/N)/\{1 - (\Delta/N)\, f_1(0)\} \right]^5 \tag{2.4.15b}$$

These two partial sums are represented by the first two diagrams in Fig.2.4.5 where the second-order self-energy, Σ_2, is written as a sum of these partial sums (each one of them, in turn, is an infinite sum).

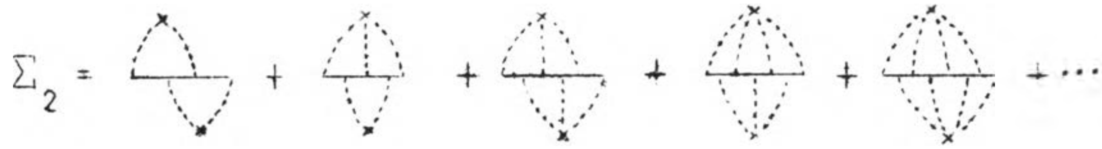


Fig.2.4.5 Diagrams representing the expansion of $\Sigma_2(\vec{k})$ in terms of partial sums.

From the above discussion, a generalization can now be made concerning other partial sums in Fig.2.4.5. In general, the odd - numbered partial sums {i.e.,the (2r-3) th diagram in Fig.2.4.5, for r ≥ 2 } contain terms of the type:

$$(\Delta/N)^{2r}\, Nc^2\{\sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)\, f_1(\vec{R}_e)|\, f_1(\vec{R}_e)|^{2(r-1)}$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)\, f_2(\vec{R}_i)|\, f_2(\vec{R}_i)|^{2(r-1)}\}$$

$$\times\left[\sum_{s=r}^{\infty} B_{s,r}\{(\Delta/N)\, f_1(0)\}^{s-r}\right]\left[\sum_{t=r}^{\infty} B_{t,r}\{(\Delta/N)\, f_1(0)\}^{t-r}\right]$$

(2.4.16a)

which are summed to give

$$S_{r,r} = Nc^2\{\sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)\, f_1(\vec{R}_e)|f_1(\vec{R}_e)|^{2(r-1)}$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)\, f_2(\vec{R}_i)|\, f_2(\vec{R}_i)|^{2(r-1)}\}\left\{\frac{\Delta/N}{1-(\Delta/N)f_1(0)}\right\}^{2r}$$

(2.4.16b)

Similarly, the even-numbered partial sums{ corresponding to the (2r-2) th diagram in Fig.2.4.5 } contain terms of the type:

$$(\Delta/N)^{2r+1}\ Nc^2\{\sum_{\vec{R}_e}|f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i}|f_2(\vec{R}_i)|^{2r}\}$$

$$\times\left[\sum_{s=r+1}^{\infty} B_{s,r+1}\{(\Delta/N)\ f_1(0)\}^{s-r-1}\right]$$

$$\times\left[\sum_{t=r}^{\infty} B_{t,r}\{(\Delta/N)\ f_1(0)\}^{t-r}\right] \qquad (2.4.17a)$$

which are summed, again, to give

$$S_{r+1,r} = Nc^2\{\sum_{\vec{R}_e}|f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i}|f_2(\vec{R}_i)|^{2r}\}\left\{\frac{\Delta/N}{1-(\Delta/N)\ f_1(0)}\right\}^{2r+1}$$

(2.4.17b)

We are now in a position to perform the summation in Fig.2.4.5. So, finally, we have

$$\Sigma_2(\vec{k}^{\pm}) = \sum_{r=2}^{\infty}(S_{r,r} + S_{r+1,r})$$

$$= \frac{(\Delta/N)^4\ Nc^2}{\{1-(\Delta/N)\ f_1(0)\}^3}$$

$$\times\left[\sum_{\vec{R}_e}\frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)\ f_1(\vec{R}_e)|f_1(\vec{R}_e)|^2\{1-(\Delta/N)\ f_1(0)\} + \frac{(\Delta)}{N}|f_1(\vec{R}_e)|^4}{\{1-(\Delta/N)\ f_1(0)\}^2 - |(\Delta/N)\ f_1(\vec{R}_e)|^2}\right.$$

$$\left. \pm\sum_{\vec{R}_i}\frac{\pm\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)\ f_2(\vec{R}_i)|f_2(\vec{R}_i)|^2\{1-(\Delta/N)\ f_1(0)\} + (\Delta/N)|f_2(\vec{R}_i)|^4}{\{1-(\Delta/N)\ f_1(0)\}^2 - |(\Delta/N)\ f_2(\vec{R}_i)|^2}\right]$$

(2.4.18)

It can be seen that for general $\vec{k}^+$ and $\vec{k}^-$, the second-order self-energy contains poles which correspond to the energy states of resonance pairs with varying separations ($\vec{R}_e$ and $\vec{R}_i$). Furthermore, these pairs are equally probable (c^2 dependence).

At the poles, the following equations are satisfied :
For translationally equivalent pairs,

$$\{1 - (\Delta/N)\, f_1(0)\}^2 - |(\Delta/N)\, f_1(\vec{R}_e)|^2 = 0 \qquad (2.4.19a)$$

and for interchange equivalent pairs,

$$\{1 - (\Delta/N)\, f_1(0)\}^2 - |(\Delta/N)\, f_2(\vec{R}_i)|^2 = 0 \qquad (2.4.19b)$$

As we noted earlier, $f_1(\vec{R}_e)$ and $f_2(\vec{R}_i)$ are usually real. The solutions to (2.4.19a) and (2.4.19b) are then

$$\{f_1(0)/N\} \pm \{f_2(\vec{R}_e)/N\} = \frac{1}{\Delta} \qquad (2.4.20a)$$

and

$$\{f_1(0)/N\} \pm \{f_2(\vec{R}_i)/N\} = \frac{1}{\Delta} \qquad (2.4.20b)$$

As for the optical spectrum, we simply put $\vec{k}^\pm = 0$. Thus for translationally equivalent pairs, we have from (2.4.18)

$$\Sigma_2(\vec{k}^+ = 0) = \Sigma_2(\vec{k}^- = 0)$$
$$= \frac{(\Delta/N)^4\, Nc^2 f_1(\vec{R}_e)\, |f_1(\vec{R}_e)|^2}{\{1 - (\Delta/N)f_1(0)\}^3\left[\{1 - (\Delta/N)f_1(0)\} - \{(\Delta/N)f_1(\vec{R}_e)\}\right]} \qquad (2.4.21a)$$

so that only one state E_+ is optically allowed. Again f_1 is real and at the pole, we have

$$\Sigma_2(\vec{k}^+ = 0) = \Sigma_2(\vec{k}^- = 0) = \frac{\Delta c^2}{\{1 - (\Delta/N) f_1(0)\} - \{(\Delta/N) f_1(\vec{R}_e)\}} \tag{2.4.21b}$$

The spectral functions I_b and I_{ac} which have been discussed before in connection with the optical properties of the monomer can also be found.

$$I_b(E_+) = \frac{1}{(E_+ - E_b)^2} \left[\frac{d}{dE} \left(\frac{1}{\Sigma_2} \right) \right]^{-1}_{E = E_+}$$

$$= \frac{c^2}{(E_+ - E_b)^2} \left[\int \frac{\rho_o(E') + \rho_{\vec{R}_e}(E')}{(E_+ - E')^2} dE' \right]^{-1},$$

where $\left[\int \frac{\{\rho_o(E') \pm \rho_{\vec{R}_e}(E')\} dE'}{(E_\pm - E')^2} \right]^{-1} = \Delta^2 \frac{dE_\pm}{d\Delta}$

$$I_b(E_+) = \frac{c^2 \Delta^2}{(E_+ - E_b)^2} \left(\frac{dE_+}{d\Delta} \right) \tag{2.4.22a}$$

Similarly,

$$I_{ac}(E_+) = \frac{c^2 \Delta^2}{(E_+ - E_{ac})^2} \left(\frac{dE_+}{d\Delta} \right) \tag{2.4.22b}$$

For interchange equivalent pairs, the situation is slightly different. $\Sigma_2(\vec{k}^+ = 0)$ and $\Sigma_2(\vec{k}^- = 0)$ are, in this case, no longer the same. From (2.4.18) we note that $\Sigma_2(\vec{k}^+ = 0)$ has a pole at E_+, whereas $\Sigma_2(\vec{k}^- = 0)$ has a pole at E_-. In other words, both E_+ and E_-

are optically allowed and uniquely and oppositely polarized. We have

$$\text{at } E_+,\ \Sigma_2(\vec{k}^+ = 0) = \frac{\Delta c^2}{\{1 - (\Delta/N)f_1(0)\} - (\Delta/N)f_2(\vec{R}_i)} \qquad (2.4.23a)$$

$$\text{at } E_-,\ \Sigma_2(\vec{k}^- = 0) = \frac{\Delta c^2}{\{1 - (\Delta/N)f_1(0) + (\Delta/N)f_2(\vec{R}_i)} \qquad (2.4.23b)$$

The corresponding spectral functions I_b, I_{ac} are found to be

$$I_b(E_+) = \{ c^2/(E_+ - E_b)^2 \} \times \left[\int \frac{\{\rho_o(E') + \rho_{\vec{R}_i}(E')\}\, dE'}{(E_+ - E')^2} \right]^{-1}$$

$$= \{ c^2\Delta^2 / (E_+ - E_b)^2 \} \left(\frac{dE_+}{d\Delta} \right) \qquad (2.4.24a)$$

$$I_{ac}(E_-) = \{ c^2/(E_- - E_b)^2 \} \times \left[\int \frac{\{\rho_o(E') - \rho_{\vec{R}_i}(E')\}\, dE'}{(E_- - E')^2} \right]^{-1}$$

$$= \{ c^2\Delta^2 / (E_- - E_{ac})^2 \} \left(\frac{dE_-}{d\Delta} \right) \qquad (2.4.24b)$$

2.4.2 Suporn's Results.[19]

In her research, she replaces c^2 in (2.4.16a) by $P_s(c)\ P_t(c)$, and she gets

$$S_{r,r} = (\Delta/N)^{2r}\, N\, P_s(c)\, P_t(c)$$

$$\times \Big\{ \sum_{\vec{R}_e} \exp(-i\vec{k}.\vec{R}_e)\, f_1(\vec{R}_e)\, |f_1(\vec{R}_e)|^{2(r-1)} \pm \sum_{\vec{R}_i} \exp(-i\vec{k}.\vec{R}_i)\, f_2(\vec{R}_i)\, |f_2(\vec{R}_i)|^{2(r-1)} \Big\}$$

$$\times \left[\sum_{s=r}^{\infty} B_{s,r} \{ (\Delta/N)\, f_1(0) \}^{s-r} \right]$$

$$\times \left[\sum_{t=r}^{\infty} B_{t,r} \{ (\Delta/N)\, f_1(0) \}^{t-r} \right] \qquad (2.4.25a)$$

$$= \sum_{s=r}^{\infty} P_s(c)\, B_{s,r} \{ (\Delta/N)\, f_1(0) \}^{s-r}$$

$$\times \left[\sum_{t=r}^{\infty} P_t(c)\, B_{t,r} \{ (\Delta/N)\, f_1(0) \}^{t-r} (\Delta/N)^{2r}\, N \right]$$

$$\times \Big\{ \sum_{\vec{R}_e} \exp(-i\vec{k}.\vec{R}_e)\, f_1(\vec{R}_e)\, |f_1(\vec{R}_e)|^{2(r-1)} \pm \sum_{\vec{R}_i} \exp(-i\vec{k}.\vec{R}_i)\, f_2(\vec{R}_i)\, |f_2(\vec{R}_i)|^{2(r-1)}$$

(2.4.25b)

Now $\sum_{s=r}^{\infty} B_{s,r} P_s(c) \{ (\Delta/N)f_1(0) \}^{s-r} \sum_{t=r}^{\infty} P_t(c) B_{t,r} \{ (\Delta/N)f_1(0) \}^{t-r}$

$$= y^{-2r} \{ \sum_{s=r}^{\infty} \sum_{t=r}^{\infty} B_{s,r} P_s(c) y^s B_{t,r} P_t(c) y^t \}, \qquad (2.4.25c)$$

where $y = (\Delta/N)f_1(0)$

and $P_s(c)\ P_t(c) = \{ \sum_{m=1}^{s} (-1)^{m-1}(m-1)!\ c^m \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} k^s \}$

$$\times \{ \sum_{n=1}^{t} (-1)^{n-1}(n-1)!\, c^n \frac{1}{n!} \sum_{q=0}^{n} (-1)^{n-q} \binom{n}{q} q^t$$

$$= \sum_{m=1}^{s} \sum_{n=1}^{t} (-1)^{2m-1}(-1)^{2n-1} \frac{1}{m\ n} c^m\ c^n$$

$$\times \sum_{k=0}^{m} \{ \sum_{q=0}^{n} (-1)^{-(q+k)} \binom{m}{k} \binom{n}{q} k^s\ q^t \} \qquad (2.4.25d)$$

and $$B_{s,r} = \frac{(s-1)!}{(s-r)!\ (r-1)!} = \binom{s-1}{r-1} \qquad (2.4.25e)$$

$$B_{t,r} = \frac{(t-1)!}{(t-r)!\ (r-1)!} = \binom{t-1}{r-1} \qquad (2.4.25f)$$

Substituting (2.4.25d), (2.4.25e) and (2.4.25f) into (2.4.25c), we get

$$\sum_{s=r}^{\infty} B_{s,r} P_s(c) y^{s-r} \sum_{t=r}^{\infty} B_{t,r} P_t(c) y^{t-r}$$

$$= y^{-2r}\{ \sum_{s=r}^{\infty} \sum_{t=r}^{\infty} \binom{s-1}{r-1}\binom{t-1}{r-1} \sum_{m=1}^{n} \sum_{n=1}^{t} (-1)^{2m-1} (-1)^{2n-1}$$

$$\frac{1}{m\,n} c^m c^n \sum_{k=0}^{n} \sum_{q=0}^{n} (-1)^{-(q+k)} \binom{m}{k}\binom{n}{q} k^s q^t y^s y^t$$

$$= y^{2r} \sum_{s=r}^{\infty} \sum_{t=r}^{\infty} \binom{s-1}{r-1}\binom{t-1}{r-1} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m\,n} c^m c^n$$

$$\sum_{k=0}^{\infty} \sum_{q=0}^{\infty} (-1)^{-(q+k)} \binom{m}{k}\binom{n}{q} (ky)^s (qy)^t \qquad (2.4.25g)$$

The summations over s and t in (2.4.25 g) can be summed by using the fact that[20]

$$\sum_{s=r}^{\infty} \binom{s-1}{r-1} (ky)^s = \left(\frac{ky}{1-ky}\right)^r \quad \text{and} \quad \sum_{t=r}^{\infty} \binom{t-1}{r-1} (qy)^t \quad \left(\frac{qy}{1-qy}\right)^r$$

(2.4.25g) becomes

$$\sum_{s=r}^{\infty} B_{s,r} P_s(c) y^{s-r} \sum_{t=r}^{\infty} B_{t,r} P_t(c) y^{t-r}$$

$$= y^{-2r}\{ \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m\,n} c^m c^n$$

$$\sum_{k=0}^{\infty} \sum_{q=0}^{\infty} (-1)^{-(q+k)} \binom{m}{k}\binom{n}{q} \left(\frac{ky}{1-ky}\right)^r \left(\frac{qy}{1-qy}\right)^r \}$$

$$\sum_{s=r}^{\infty} B_{s,r} P_s(c) y^{s-r} \sum_{t=r}^{\infty} B_{t,r} P_s(c) y^{t-r}$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{mn} c^m c^n \sum_{k=0}^{\infty} \left[\sum_{q=0}^{\infty} (-1)^{-(q+k)} \binom{m}{k} \binom{n}{q} \left\{ \frac{kq}{(1-ky)(1-qy)} \right\}^r \right] \tag{2.4.25h}$$

$$\sum_{r=2}^{\infty} S_{r,r} = N \left[\sum_{r=2}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m.n} c^m c^n \right.$$

$$\left. \sum_{k=0}^{\infty} \sum_{q=0}^{\infty} (-1)^{-(q+k)} \binom{m}{k} \binom{n}{q} \left\{ \frac{kq}{(1-ky)(1-qy)} \right\}^r \left(\frac{\Delta}{N} \right)^{2r} \right]$$

$$\times \sum_{\vec{R}_e} \exp(-i\vec{k}^{\pm} \cdot \vec{R}_e) f_1(\vec{R}_e) \, |f_1(\vec{R}_e)|^{2(r-1)}$$

$$\pm \sum_{\vec{R}_i} \exp(-i\vec{k}^{\pm} \cdot \vec{R}_i) \, f_2(\vec{R}_i) |f_2(\vec{R}_i)|^{2(r-1)} \Big\} \tag{2.4.25i}$$

We also have

$$\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{mn} c^m c^n \binom{m}{k} \binom{n}{q} = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{mn} c^m c^n \binom{m}{k} \frac{n!}{(n-q)!\,q!}$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m} \binom{m}{k} c^m \frac{1}{q} \binom{n-1}{q-1} c^n$$

$$= \sum_{m=1}^{\infty} \frac{1}{m} \binom{m}{k} c^m \frac{1}{q} \left(\frac{c}{1-c} \right)^q$$

$$= \frac{1}{q} \left(\frac{c}{1-c} \right)^q \sum_{m=1}^{\infty} \frac{1}{k} \binom{m-1}{k-1} c^m$$

$$= \frac{1}{q} \left(\frac{c}{1-c} \right)^q \frac{1}{k} \left(\frac{c}{1-c} \right)^k$$

$$= \frac{1}{q\,k}\left(\frac{c}{1-c}\right)^{q+k} \qquad (2.4.25j)$$

Substituting (2.4.25j) into (2.4.25i) , (2.4.25i) becomes

$$\sum_{r=2}^{\infty} S_{r,r} = N\left[\sum_{r=2}^{\infty}\sum_{k=0}^{\infty}\sum_{q=0}^{\infty}(-1)^{-(q+k)}\frac{1}{q\,k}\left(\frac{c}{1-c}\right)^{q+k}\left\{\frac{kq}{(1-ky)(1-qy)}\right\}^{r}\left(\frac{\Delta}{N}\right)^{2r}\right]$$

$$\times\left\{\sum_{\vec{R}_e}\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)f_1(\vec{R}_e)\,|f_1(\vec{R}_e)|^{2(r-1)}\right.$$

$$\left.\pm\sum_{\vec{R}_i}\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)f_2(\vec{R}_i)\,|f_2(\vec{R}_i)|^{2(r-1)}\right\} \qquad (2.4.25k)$$

Also

$$\sum_{r=2}^{\infty}\left\{\frac{kq}{(1-ky)(1-qy)}\right\}^{r}\left(\frac{\Delta}{N}\right)^{2r}\left\{\sum_{\vec{R}_e}\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)f_1(\vec{R}_e)\right.$$

$$|f_1(\vec{R}_e)|^{2(r-1)}$$

$$\left.\pm\sum_{\vec{R}_i}\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)\,f_2(\vec{R}_i)|f_2(\vec{R}_i)|^{2(r-1)}\right\}$$

$$= \sum_{\vec{R}_e}\sum_{r=2}^{\infty}\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)f_1(\vec{R}_e)|f_1(\vec{R}_e)|^{2(r=1)}$$

$$\left\{\frac{kq}{(1-ky)(1-qy)}\right\}^{r}\left(\frac{\Delta}{N}\right)^{2r}$$

$$\pm \sum_{\vec{R}_i} \sum_{r=2}^{\infty} \exp(-i\vec{k}^{\pm}\cdot\vec{R}_i) f_2(\vec{R}_i) \left|f_2(\vec{R}_i)\right|^{2(r-1)}$$

$$\left\{\frac{kq}{(1-ky)(1-qy)}\right\}^r \frac{\Delta}{N}^{2r}$$

$$= \sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)}{f_1(\vec{R}_e)} \sum_{r=2}^{\infty} \left\{\frac{kq\Delta^2 \left|f_1(\vec{R}_e)\right|^2}{(1-ky)(1-qy)N^2}\right\}^r$$

$$\pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)}{f_1(R_i)} \sum_{r=2}^{\infty} \left\{\frac{kq\Delta^2 \left|f_2(\vec{R}_i)\right|^2}{(1-ky)(1-qy)N^2}\right\}^r$$

$$= \sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot R_e)}{f_1(\vec{R}_e)} \left\{\frac{kq\Delta^2 \left|f_1(\vec{R}_e)\right|^2}{(1-ky)(1-qy)N^2}\right\}^2$$

$$\sum_{r'=0}^{\infty} \left\{\frac{kq\Delta^2 \left|f_1(\vec{R}_e)\right|^2}{(1-ky)(1-qy)N^2}\right\}^{r'}$$

$$\pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)}{f_2(\vec{R}_i)} \left\{\frac{kq\Delta^2 \left|f_2(\vec{R}_i)\right|^2}{(1-ky)(1-qy)N^2}\right\}^2$$

$$\sum_{r'=0}^{\infty} \left\{\frac{kq\Delta^2 \left|f_2(\vec{R}_i)\right|^2}{(1-ky)(1-qy)N^2}\right\}^{r'}$$

$$= \sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)}{f_1(\vec{R}_e)} \left\{\frac{kq\Delta^2 \left|f_1(\vec{R}_e)\right|^2}{(1-ky)(1-qy)N^2}\right\}^2$$

$$\left\{\frac{1}{1-\dfrac{kq\Delta^2 \left|f_2(\vec{R}_i)\right|^2}{(1-ky)(1-qy)N^2}}\right\}$$

$$\pm \sum_{\vec{R}_i} \frac{\exp(-\, i\vec{k}^{\pm} \cdot \vec{R}_i)}{f_2(R_i)} \left\{ \frac{kq\, \Delta^2 |f_2(\vec{R}_i)|^2}{(1 - ky)(1 - qy)N^2} \right\}^2$$

$$\left\{ \frac{1}{1 - \dfrac{kq\Delta^2 |f_2(\vec{R}_i)|^2}{(1 - ky)(1 - qy)N^2}} \right\}$$

$$= \sum_{\vec{R}_e} \exp(-\, i\vec{k}^{\pm} \cdot \vec{R}_e) |f_1(\vec{R}_e)|^3 \, (\Delta/N)^4 \left\{ \frac{kq}{(1 - ky)(1 - qy)} \right\}^2$$

$$\left\{ \frac{1}{1 - \dfrac{kq\, \Delta^2 |f_1(\vec{R}_e)|^2}{(1 - ky)(1 - qy)N^2}} \right\}$$

$$\pm \sum_{\vec{R}_i} \exp(-\, i\vec{k}^{\pm} \cdot \vec{R}_i) |f_2(\vec{R}_i)|^3 (\Delta/N)^4 \left\{ \frac{kq}{(1 - ky)(1 - qy)} \right\}^2$$

$$\left\{ \frac{1}{1 - \dfrac{kq\Delta^2 |f_2(\vec{R}_i)|^2}{(1 - ky)(1 - qy)N^2}} \right\} \qquad (2.4.25\ell)$$

Substituting (2.4.25 ℓ) into (2.4.25k), (2.4.25k) becomes

$$\sum_{r=2}^{\infty} S_{r,r} = N(\Delta/N)^4 \left[\sum_{k=1}^{\infty} \sum_{q=1}^{\infty} (-1)^{-(q+k)} \frac{1}{qk} \left(\frac{c}{1 - c}\right)^{q+k} \left\{\frac{kq}{(1 - ky)(1 - qy)}\right\}^2 \right]$$

$$\times\left[\sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)|f_1(\vec{R}_e)|^3}{\{1-\frac{kq\Delta^2|f_1(R_e)|^2}{(1-ky)(1-qy)N^2}\}} \pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)|f_2(\vec{R}_i)|^3}{\{1-\frac{kq\Delta^2|f_2(R_i)|^2}{(1-ky)(1-qy)N^2}\}}\right]$$

$$= N(\Delta/N)^4\{\sum_{k=1}^{\infty}\sum_{q=1}^{\infty}(-1)^{-(q+k)}\, qk\left(\frac{c}{1-c}\right)^{q+k}\frac{1}{(1-ky)^2(1-qy)^2}\}$$

$$\times\left[\sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)|f_1(\vec{R}_e)|^3}{\{1-\frac{kq\Delta^2|f_1(\vec{R}_e)|^2}{(1-ky)(1-qy)N^2}\}} \pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)|f_2(\vec{R}_i)|^3}{\{1-\frac{kq\Delta^2|f_2(\vec{R}_i)|^2}{(1-ky)(1-qy)N^2}\}}\right]$$

$$= N(\Delta/N)^4\left[\sum_{p=2}^{\infty}\sum_{q=1}^{p-1}(-1)^{-p}\, q(p-q)\left(\frac{c}{1-c}\right)^{p}\frac{1}{\{1-(p-q)y\}^2(1-qy)^2}\right]$$

$$\times\left[\sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_e)|f_1(\vec{R}_e)|^3}{\left[1-\frac{(p-q)\Delta^2|f_1(\vec{R}_e)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]} \pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}\cdot\vec{R}_i)|f_2(\vec{R}_i)|^3}{\left[1-\frac{(p-q)\Delta^2|f_2(\vec{R}_i)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]}\right]$$

(2.4.26)

Next by replacing c^2 by $P_s(c)\,P_t(c)$ in (2.4.17b), we get

$$S_{r+1,r} = (\Delta/N)^{2r+1}\, N\, P_s(c)\, P_t(c)\{\sum_{\vec{R}_e}|f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i}|f_2(\vec{R}_i)|^{2r}\}$$

$$x\left[\sum_{s=r+1}^{\infty} B_{s,r+1}\{(\Delta/N)\ f_1(0)\}^{s-r+1}\right]$$

$$x\left[\sum_{t=r}^{\infty} B_{t,r}\{(\Delta/N)f_1(0)\}^{t-r}\right]$$

$$S_{r+1,r} = \left[\sum_{s=r+1}^{\infty} B_{s,r+1}\ P_s(c)\{(\Delta/N)f_1(0)\}^{s-r-1}\right.$$

$$\sum_{t=r}^{\infty} B_{t,r}\ P_t(c)\{(\Delta/N)f_1(0)\}^{t-r}$$

$$\left. x\ (\Delta/N)^{2r+1}\ N\right]\{\sum_{\vec{R}_e} |f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i} |f_2(\vec{R}_i)|^{2r}\} \qquad (2.4.27a)$$

Since $\sum_{s=r+1}^{\infty} B_{s,r+1}\ P_s(c)\{\ (\Delta/N)\ f_1(0)\}^{s-r-1}$

$$\sum_{t=r}^{\infty} B_{t,r}\ P_t(c)\{\ (\Delta/N)\ f_1(0)\}^{t-r}$$

$$= y^{-2r-1}\{\sum_{s=r+1}^{\infty}\ \sum_{t=r}^{\infty} B_{s,r+1}\ P_s(c)\ P_t(c)\ y^s y^t\} \qquad (2.4.27b)$$

where $y = (\Delta/N)\ f_1(0)$

and $$B_{s,r+1} = \frac{(s-1)!}{(s-r-1)!(r+1-1)!} = \binom{s-1}{r+1-1} \qquad (2.4.27c)$$

$$B_{t,r} = \frac{(t-1)!}{(t-r)!\ (r-1)!} = \binom{t-1}{r-1} \qquad (2.4.27d)$$

We get after substituting (2.4.25d), (2.4.27c) and (2.4.27d) into (2.4.27b)

$$\sum_{s=r+1}^{\infty} B_{s,r+1}\, P_s(c)\, \{(\Delta/N)\, f_1(0)\}^{s-r-1}$$

$$\times \sum_{t=r}^{\infty} B_{t,r}\, P_t(c)\, \{(\Delta/N)\, f_1(0)\}^{t-r}$$

$$= y^{-2r-1}\Big\{ \sum_{s=r+1}^{\infty} \sum_{t=r}^{\infty} \binom{s-1}{r+1-1}\binom{t-1}{r-1}$$

$$\sum_{m=1}^{s} \sum_{n=1}^{t} (-1)^{2m-1} (-1)^{2n-1} (-1)^{2n-1} \frac{1}{m\,n}\, c^m c^n$$

$$\times \sum_{k=0}^{m} \sum_{q=0}^{n} (-1)^{-(q+k)} \binom{m}{k}\binom{n}{q} (ky)^s\, (qy)^t \Big\} \qquad (2.4.27e)$$

Since

$$\sum_{s=r+1}^{\infty} \binom{s-1}{r+1-1} (ky)^s = \left(\frac{ky}{1-ky}\right)^{r+1}$$

$$\sum_{t=r}^{\infty} \binom{t-1}{r-1} (qy)^t = \left(\frac{qy}{1-qy}\right)^{r}$$

(2.4.27e) becomes

$$\sum_{s=r+1}^{\infty} B_{s,r+1}\, P_s(c)\, y^{s-r-1} \sum_{t=r}^{\infty} B_{t,r}\, P_t(c)\, y^{t-r}$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m.n}\, c^m c^n$$

$$\times \sum_{k=0}^{\infty} \sum_{q=0}^{\infty} (-1)^{-(q+k)} \binom{m}{k}\binom{n}{q} \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r}$$

(2.4.27f)

$$= \sum_{k=1}^{\infty} \sum_{q=1}^{\infty} (-1)^{-(q+1)} \frac{1}{q\,k} \left(\frac{c}{1-c}\right)^{q+k} \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r}$$

(2.4.27g)

$$\sum_{r=1}^{\infty} S_{r+1,r} = N \sum_{r=1}^{\infty} \left[\sum_{k=1}^{\infty} \sum_{q=1}^{\infty} (-1)^{-(q+k)} \left(\frac{c}{1-c}\right)^{q+k} \right.$$

$$\times \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r}$$

$$\left. \times \left(\frac{\Delta}{N}\right)^{2r+1} \left\{ \sum_{\vec{R}_e} |f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i} |f_2(\vec{R}_i)|^{2r} \right\} \right] \qquad (2.4.27h)$$

Since $\displaystyle \sum_{r=1}^{\infty} \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r} (\Delta/N)^{2r+1}$

$$\times \left\{ \sum_{\vec{R}_e} |f_1(\vec{R}_e)|^{2r} + \sum_{\vec{R}_i} |f_2(\vec{R}_i)|^{2r} \right\}$$

$$= \sum_{\vec{R}_e} \sum_{r=1}^{\infty} \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r} (\Delta/N)^{2r+1} |f_1(\vec{R}_e)|^{2r}$$

$$+ \sum_{\vec{R}_i} \sum_{r=1}^{\infty} \left(\frac{k}{1-ky}\right)^{r+1} \left(\frac{q}{1-qy}\right)^{r} (\Delta/N)^{2r+1} |f_2(\vec{R}_i)|^{2r}$$

$$= \left(\frac{k}{1-ky}\right) (\Delta/N) \left[\sum_{\vec{R}_e} \sum_{r=1}^{\infty} \left\{ \left(\frac{k}{1-ky}\right) \left(\frac{q}{1-qy}\right) (\Delta/N)^2 |f_1(\vec{R}_e)|^2 \right\}^{r} \right.$$

$$\left. + \sum_{\vec{R}_i} \sum_{r=1}^{\infty} \left\{ \left(\frac{k}{1-ky}\right) \left(\frac{q}{1-qy}\right) (\Delta/N)^2 |f_2(\vec{R}_i)|^2 \right\}^{r} \right]$$

$$=\left(\frac{k}{1-ky}\right)(\Delta/N)\left[\sum_{\vec{R}_e}\left\{\frac{kq\Delta^2|f_1(\vec{R}_e)|^2}{(1-ky)(1-qy)N^2}\right\}\sum_{r'=0}^{\infty}\left\{\frac{kq\Delta^2|f_1(R_e)|^2}{(1-ky)(1-qy)N^2}\right\}^{r'}\right.$$

$$\left.+\sum_{\vec{R}_i}\left\{\frac{kq\Delta^2|f_2(\vec{R}_i)|^2}{(1-ky)(1-qy)N^2}\right\}\sum_{r'=0}^{\infty}\left\{\frac{kq\Delta^2|f_2(\vec{R}_i)|^2}{(1-ky)(1-qy)N^2}\right\}^{r'}\right]$$

$$\times\sum_{r=1}^{\infty}\left(\frac{k}{1-ky}\right)^{r+1}\left(\frac{q}{1-qy}\right)^{r}(\Delta/N)^{2r+1}$$

$$\times\left\{\sum_{\vec{R}_e}|f_1(\vec{R}_e)|^{2r}+\sum_{\vec{R}_i}|f_2(\vec{R}_i)|^{2r}\right\}$$

$$=\left\{\frac{k^2q}{(1-ky)^2(1-qy)}\right\}(\Delta/N)^3\left[\sum_{\vec{R}_e}|f_1(\vec{R}_e)|^2\frac{1}{\left\{1-\frac{kq\Delta^2|f_1(\vec{R}_e)|^2}{(1-ky)(1-qy)N^2}\right\}}\right.$$

$$\left.+\sum_{\vec{R}_i}|f_2(\vec{R}_i)|^2\frac{1}{\left\{1-\frac{kq\Delta^2|f_2(\vec{R}_i)|^2}{(1-ky)(1-qy)N^2}\right\}}\right] \qquad (2.4.27i)$$

(2.4.27h) becomes,

$$\sum_{r=1}^{\infty}S_{r+1,r}=N(\Delta/N)^3\left\{\sum_{k=1}^{\infty}\sum_{q=1}^{\infty}(-1)^{-(q+k)}\left(\frac{c}{1-c}\right)^{q+k}\right.$$

$$\left.\times\frac{k}{(1-ky)^2(1-qy)}\right\}$$

$$\times\left[\sum_{\vec{R}_e}\frac{|f_1(\vec{R}_e)|^2}{\left\{1-\frac{kq\Delta^2|f_1(\vec{R}_e)|^2}{(1-ky)(1-qy)N^2}\right\}}+\sum_{\vec{R}_i}\frac{|f_2(\vec{R}_i)|^2}{\left\{1-\frac{kq\Delta^2|f_2(\vec{R}_i)|^2}{(1-ky)(1-qy)N^2}\right\}}\right]$$

$$= N(\Delta/N)^3 \left[\sum_{p=2}^{\infty} \sum_{q=1}^{p-1} (-1)^{-p}(p-q)\left(\frac{c}{1-c}\right)^p \right.$$

$$\left. \times \frac{1}{\{1-(p-q)y\}^2(1-qy)} \right]$$

$$\times \left[\sum_{\vec{R}_e} \frac{|f_1(\vec{R}_e)|^2}{\{1 - \frac{(p-q)q\Delta^2|f_1(\vec{R}_e)|^2}{\{1-(p-q)y\}(1-qy)N^2}\}} \right.$$

$$\left. + \sum_{\vec{R}_e} \frac{|f_2(\vec{R}_i)|^2}{\{1 - \frac{(p-q)q\Delta^2|f_2(\vec{R}_i)|^2}{\{1-(p-q)y\}(1-qy)N^2}\}} \right] \qquad (2.4.28)$$

Summing (2.4.26) and (2.4.28), we get

$$\Sigma_2(\vec{k}^{\pm}) = \left[N(\Delta/N)^3 \sum_{p=2}^{\infty} \sum_{q=1}^{p-1} (-1)^{-p}(p-q)\left(\frac{c}{1-c}\right)^p \right.$$

$$\left. \times \frac{1}{\{1-(p-q)y\}^2(1-qy)} \right]$$

$$\times \left[\sum_{\vec{R}_e} \frac{|f_1(\vec{R}_e)|^2}{\{1 - \frac{(p-q)q\Delta^2|f_1(\vec{R}_e)|^2}{\{1-(p-q)y\}(1-qy)N^2}\}} + \sum_{\vec{R}_i} \frac{|f_2(\vec{R}_i)|^2}{\{1 - \frac{(p-q)q\Delta^2|f_2(\vec{R}_i)|^2}{\{1-(p-q)y\}(1-qy)N^2}\}} \right.$$

$$+ (\Delta/N)\frac{q}{(1-qy)}\left[\sum_{\vec{R}_e} \frac{\exp(-i\vec{k}^{\pm}.\vec{R}_e)|f_1(\vec{R}_e)|^3}{\left[1 - \frac{(p-q)q\Delta^2|f_1(\vec{R}_e)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]} \right.$$

$$\left.\left. \pm \sum_{\vec{R}_i} \frac{\exp(-i\vec{k}^{\pm}.\vec{R}_i)\,|f_2(\vec{R}_i)|^3}{\left[1 - \frac{(p-q)q\Delta^2|f_2(\vec{R}_i)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]} \right]\right]$$

$$= \left[N(\Delta/N)^3 \sum_{p=2}^{\infty} \sum_{q=1}^{p-1} (-1)^{-p} (p-q) \left(\frac{c}{1-c}\right)^p \frac{1}{\{1-(p-q)y\}^2(1-qy)} \right.$$

$$\times \left[\sum_{\vec{R}_e} \frac{|f_1(\vec{R}_e)|^2 \{1 + (\Delta/N)(q/1-qy) \exp(-i\vec{k}^{\pm} . \vec{R}_e) f_1(\vec{R}_e)\}}{\left[1 - \frac{(p-q)q\Delta^2 |f_1(\vec{R}_e)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]} \right.$$

$$\left.\left. + \sum_{\vec{R}_i} \frac{|f_2(\vec{R}_i)|^2 \{1 \pm (\Delta/N)(q/1-qy) \exp(-i\vec{k}^{\pm} . \vec{R}_i) f_2(\vec{R}_i)\}}{\left[1 - \frac{(p-q)q\Delta^2 |f_2(\vec{R}_i)|^2}{\{1-(p-q)y\}(1-qy)N^2}\right]} \right] \right]$$

$$= \Delta^3 \sum_{p=2}^{\infty} \sum_{q=1}^{p-1} (-1)^{-p}(p-q)\left(\frac{c}{1-c}\right)^p$$

$$\times \left[\sum_{\vec{R}_e} \frac{|f_1(\vec{R}_e)|^2 \{1 + (\Delta/N)(q/1-qy) \exp(-i\vec{k}^{\pm} . \vec{R}_e) f_1(\vec{R}_e)\}}{\{1-(p-q)y\}^2 (1-qy)N^2 - \{1-(p-q)y\}(p-q)q\Delta^2 |f_1(\vec{R}_e)|^2} \right.$$

$$\left. + \sum_{\vec{R}_i} \frac{|f_2(\vec{R}_i)|^2 \{1 \pm (\Delta/N)(q/1-qy) \exp(-i\vec{k}^{\pm} . \vec{R}_i) f_2(\vec{R}_i)\}}{\{1-(p-q)y\}^2(1-qy)N^2 - \{1-(p-q)y\}(p-q)q\Delta^2 |f_2(\vec{R}_i)|^2} \right]$$

(2.4.29)

$\Sigma_2(\vec{k}^{\pm})$ is the second - order self energy part.

The poles of (2.4.29) are determined by the following equations : For translationally equivalent pairs,

$$\{1 - (p - q)y\}^2(1 - qy)N^2 - \{1 - (p - q)y\}(p - q)q\Delta^2|f_1(\vec{R}_e)|^2 = 0$$

(2.4.30a)

For interchange equivalent pairs,

$$\{1 - (p - q)y\}^2(1 - qy)N^2 - \{1 -(p - q)y\}(p - q)q\Delta^2|f_2(\vec{R}_i)|^2 = 0$$

(2.4.30b)

From (2.4.30a)

$$\{1 - (p - q)y\}^2(1 - qy)N^2 = \{1 - (p - q)y\}(p - q)q\Delta^2|f_1(\vec{R}_e)|^2$$

$$\{1 - (p - q)y\}(1 - qy)N = (p - q)q\Delta^2|f_1(\vec{R}_e)|^2$$

$$1 - py + q(p - q)y^2 = (p - q)q(\Delta/N)^2|f_1(\vec{R}_e)|^2$$

$$q(p - q)y^2 - py - (p - q)q(\Delta/N)^2|f_1(\vec{R}_e)|^2 + 1 = 0$$

$$\{q(p - q)\left|\frac{f_1(0)}{N}\right|^2 - q(p - q)\left|\frac{f_1(\vec{R}_e)}{N}\right|^2\}\Delta^2 - p\frac{f_1(0)}{N}\Delta + 1 = 0$$

$$\text{since } y = \frac{f_1(0)\Delta}{N}$$

$$q(p - q)\{\left|\frac{f_1(0)}{N}\right|^2 - \left|\frac{f_1(\vec{R}_e)}{N}\right|^2\} - p\frac{f_1(0)}{N}\frac{1}{\Delta} + \frac{1}{\Delta^2} = 0$$

(2.4.31a)

Similarly, from (2.4.30b), we get

$$q(p - q)\left\{ \left|\frac{f_1(0)}{N}\right|^2 - \left|\frac{f_2(\vec{R}_i)}{N}\right|^2 \right\} - p\,\frac{f_1(0)}{N} \quad \frac{1}{\Delta} + \frac{1}{\Delta^2} = 0$$

(2.4.31b)