

## CHAPTER I

### INTRODUCTION



#### 1.1 Approximation Methods.

In developing theories for the electronic properties of binary mixed crystals several important characteristic of these kind of objects have to be taken into consideration. Among them is a loss of lattice periodicity or the lack of crystal symmetry. For computing electronic properties such as the density of states which are associated with the entire system we can not use the standard statistical methods which are based on the translational symmetry of the crystal. To treat the disorder, various approximation methods have been used. These techniques are based on how we treat potential of electrons in mixed crystals. These methods have been developed for over fifty years. It should be remembered that each method has its own limitations.

(1)  
Nordheim introduced the method called virtual crystal approximation in 1931. This method assumes that the electrons in a binary systems behave identically, as far as macroscopic properties are concerned, to the electrons in a hypothetical ordered material in which the crystalline potential is the average of the potentials of the pure materials. This approximation represents the lowest order term in a perturbation expansion of the coherent potential  $W$  and is fairly successful in the case of the rigid band limit where the

perturbed wave functions are quite extended in space so that each electron sees nearly the average perturbation.

In 1958, Korringa<sup>(2)</sup> suggested the average T-matrix approximation, based on the assumption that the electrons in mixed crystals behave as if they were moving in a particular ordered system of localized potentials, the scattering matrix of which is the average of the scattering matrices of the localized potential corresponding to each constituent. This approximation was considered by Soven, who found that it was not a reasonable one for the case where the localized potentials have a strength approaching that found in transition metals.

In 1966, Yonezawa and Matsubara,<sup>(3)</sup> using what they called a 'cumulant expansion', gave a formal perturbation theory analysis leading to a systematic expansion of the coherent perturbation,

The method called the coherent potential approximation (CPA) was proposed by Soven<sup>(4)</sup> in 1967. The essential physical idea of this approach is to describe the system by an appropriate effective Hamiltonian. This Hamiltonian is defined by the condition that if it is employed, there is no further scattering from the individual sites on the average. If incorporates a potential such that with its use, a wave will propagate coherently through the material, To determine the coherent potential in the original and simplest form of this approximation, one requires that a single scatterer imbedded in this effective medium should produce no further scattering on the average, The attractive feature of the CPA is that only directly measurable physical quantities are required as input data when calculating the

excited electronic state of the mixed crystals. The pertinent parameters are the experimental density of states of the pure crystal and the difference of the single molecule excitation energies. The major shortcoming of the CPA involves an inadequate description of localized states.

## 1.2 Methods for Approximating Green's function $\langle G \rangle$ <sup>(5)</sup>

The various methods for calculating  $\langle G \rangle$  differ in the ways that the configuration average is inserted into the calculation. We begin by defining  $\langle G \rangle$  as

$$\langle G \rangle = \frac{1}{G_0^{-1} - W} \quad \text{I.1}$$

when

$$G_0 = \text{bare propagator of the system}$$

and

$$W = \text{correction due to the perturbation caused by the disordering and which also incorporates the configuration averaging}$$

### 1.2.1 Virtual Crystal Approximation (VCA).

As was pointed out in Virtual Crystal Approximation, it is assumed that the electrons in a binary mixed crystals behave identically, as far as macroscopic properties are concerned, to the electrons in a hypothetical ordered material in which the crystalline potential is the average of the potentials of the pure materials. Therefore the correction  $W$  is

$$W = \sum_i V_i \quad \text{I.2}$$

where

$$V_i = c_A V_i^A + c_B V_i^B \quad \text{I.3}$$

when

$$V_i^A = \text{potential for particle A at site } i$$

$$V_i^B = \text{potential for particle B at site } i$$

$$c_A = \text{concentration of particle A}$$

$$c_B = \text{concentration of particle B}$$

Substituting this equation (I.1), we get

$$\langle G \rangle = \frac{1}{G_0^{-1} - \sum_i V_i} \quad \text{I.4}$$

This approximation represents the lowest order term in a perturbation series of  $W$ .

### 1.2.2 Average t-Matrix Approximation (ATA).

We defined a single-site t-matrix to be

$$t_i = V_i + V_i G_0 t_i \quad \text{I.5}$$

$$= V_i \left( \frac{1}{1 - G_0 V_i} \right) \quad \text{I.6}$$

From this, we get

$$G_0 = G_0 \left( \frac{1}{1 - G_0 V} \right) \quad \text{I.7}$$

The Resolvent may be expressed by

$$\begin{aligned} G &= G_0 + \sum_i G_0 t_i G_0 + \\ &\sum_i \sum_{j \neq i} G_0 t_i G_0 t_j G_0 + \\ &\sum_i \sum_{j \neq i} \sum_{k \neq j} G_0 t_i G_0 t_j G_0 t_k G_0 + \dots \quad \text{I.8} \end{aligned}$$

Then the mean resolvent is

$$\begin{aligned} \langle G \rangle = & G_0 + \sum_i G_0 \langle t_i \rangle G_0 + \sum_i \sum_{j \neq i} G_0 \langle t_i G_0 t_j \rangle G_0 + \\ & \sum_i \sum_{j \neq i} \sum_{k \neq j} G_0 \langle t_i G_0 t_j G_0 t_k \rangle G_0 + \dots \end{aligned}$$

The restriction on the summation for the successive scatterings is because  $t$  contains all the scattering from a single site and further scattering must therefore be from another site.

By calculating the  $t_i$ -matrices  $t_i^A$  and  $t_i^B$  for scattering off the potential  $V_i^A$  and  $V_i^B$  respectively, then associating with each lattice site of the crystal the average t-matrix

$$\langle t_i \rangle = c_A t_i^A + c_B t_i^B$$

When on using the replacement of the average of products of t-matrices by the products of the average t-matrix, we get the approximation for  $\langle G \rangle$  as

$$\begin{aligned} \langle G \rangle = & G_0^{(1)} + \sum_i G_0 \langle t_i \rangle G_0 + \sum_i \sum_{j \neq i} G_0 \langle t_i \rangle G_0 \langle t_j \rangle G_0 \\ & + \sum_i \sum_{j \neq i} \sum_{k \neq j} G_0 \langle t_i \rangle G_0 \langle t_j \rangle G_0 \langle t_k \rangle G_0 + \dots \quad 1.9 \end{aligned}$$

This approximation is a single-site approximation and not reasonable for the case where the localized potentials have a strength approaching that found in transition metals.

### 1.2.3 The Coherent Potential Approximation (CPA).

This method developed by Taylor<sup>(6)</sup> and Soven<sup>(4)</sup> in 1967, introduce the concept of an coherent potential. The essential physical idea of this approach is to describe the system by an appropriate

effective Hamiltonian. This Hamiltonian is defined by the condition that if it is employed, there is no further scattering from the individual sites on the average. If incorporates a potential such that with its use, a wave will propagate coherently through the material. This method is equivalent to viewing the actual scattering potential as an impurity imbedded in an effective medium, whose propagator has a self-energy adjusted so that the t-matrix for scattering by a single site impurity in this medium is zero on the average.

In this approximation, we assume that there is an effective medium characterized by a resolvent  $G^{\circ}$  which is related to a coherent potential  $W$  through the Dyson equation

$$G^{\circ} = G_0 + G_0 W G^{\circ} \quad \text{I.10}$$

In the ordinary, or single-site CPA, the coherent potential is assumed to be site-diagonal, but in general there will be off-diagonal elements. Now we write equation (I.10) for  $G$  in terms of  $G^{\circ}$  eliminating  $G_0$  via equation (I.10) with the result

$$G = G^{\circ} + G^{\circ}(V - W)G \quad \text{I.11}$$

By iterating and averaging equation (I.11), we get

$$\langle G \rangle = G^{\circ} + G^{\circ} \langle V - W \rangle G^{\circ} + G^{\circ} \langle (V - W) G^{\circ} (V - W) \rangle G^{\circ} + \dots \quad \text{I.12}$$

There is an extra degree of freedom in that the coherent potential is arbitrary. Therefore, for the best improvement of the convergence of equation (I.12), we choose  $W$  to be the exact self-energy of  $\langle G \rangle$  in equation (I.10), then we would have  $\langle G \rangle = G^{\circ}$  and the scattering terms in equation (I.12) must cancel, that is the average T-matrix for the system must be zero. The CPA method is

to calculate  $\langle T \rangle$  in some approximation and set this to zero as a determining equation for  $W$ .

In the single-site CPA, one decouples  $\langle T \rangle$  into products of single-site  $t$ -matrices which are set to zero on average,

$$\begin{aligned} \langle t_i \rangle &= \langle (V_i - W) (1 - G^0 (V_i - W))^{-1} \rangle \\ &= 0 \end{aligned} \quad \text{I.13}$$

This equation is then solved simultaneously with equation (I.10) to find  $G^0$  as the approximation for  $\langle G \rangle$ .

#### 1.2.4 Cumulant Expansion Method.

From eq.(I.1)

$$\langle G \rangle = \frac{1}{G_0^{-1} - W}$$

when we replace  $W$  by potential  $V$  and expand in series we get

$$\begin{aligned} \langle G \rangle &= G_0 + G_0 \langle V \rangle G_0 + G_0 \langle V G_0 V \rangle G_0 \\ &\quad + G_0 \langle V G_0 V G_0 V \rangle G_0 + \dots \end{aligned}$$

By using the formulas of products of cumulant average such as

$$\langle A \rangle = \langle A \rangle^c$$

$$\langle AB \rangle = \langle A \rangle^c \langle B \rangle^c + \langle AB \rangle^c$$

or  $\langle AB \rangle^c = \langle AB \rangle - \langle A \rangle^c \langle B \rangle^c$

$$\begin{aligned} \langle ABC \rangle &= \langle A \rangle^c \langle B \rangle^c \langle C \rangle^c + \langle AB \rangle^c \langle C \rangle^c \\ &\quad + \langle A \langle B \rangle^c C \rangle^c + \end{aligned}$$

$$\langle A \rangle^c \langle BC \rangle^c + \langle ABC \rangle^c$$

or  $\langle ABC \rangle^c = \langle ABC \rangle - \langle A \rangle^c \langle B \rangle^c \langle C \rangle^c -$

$$\langle AB \rangle^c \langle C \rangle^c - \langle A \langle B \rangle^c C \rangle^c - \langle A \rangle^c \langle BC \rangle^c \quad \text{I.14}$$



and so forth. The suffix c indicates the 'cumulant average'. By use of this kind of average one gets

$$\begin{aligned}
 \langle G \rangle &= G_0 + G_0 \langle V \rangle^c G_0 + G_0 \langle V \rangle^c G_0 \langle V \rangle^c G_0 + \\
 &G_0 \langle VG_0 V \rangle^c G_0 + G_0 \langle V \rangle^c G_0 \langle V \rangle^c G_0 \langle V \rangle^c G_0 + \\
 &G_0 \langle VG_0 V \rangle^c G_0 \langle V \rangle^c G_0 + \\
 &G_0 \langle V \rangle^c G_0 \langle VG_0 V \rangle^c G_0 + \\
 &G_0 \langle VG_0 \langle V \rangle^c G_0 V \rangle^c G_0 + \\
 &G_0 \langle VG_0 V G_0 V \rangle^c G_0 + \dots \quad \text{I.15}
 \end{aligned}$$

This approximation includes all the effects of electron scattering caused by a single impurity, but does not take account of effects such that an electron scattered by an impurity is appreciably influenced by other impurities before the first scattering is completed.

### 1.2.5 Connection between Perturbation Expansion and Diagram

#### Approach.

For any system, we can define an operator  $\hat{G}_0(E) = \frac{1}{E - H_0}$

where  $H_0$  is the time independent Hamiltonian operator. The expectation value  $G_0(E)$  which is called Green's function (8) is calculated as follows.

$$\langle \psi_i | \hat{G}_0(E) | \psi_i \rangle = \langle \psi_i | \frac{1}{E - H_0} | \psi_i \rangle \quad \text{I.16}$$

As  $\psi_i$  are the eigenstates of  $H_0$ , and from equation(I.16)

$$\langle \psi_i | \frac{1}{E - H_0} | \psi_i \rangle = \langle \psi_i | \frac{1}{E} \left( \frac{1}{1 - \frac{H_0}{E}} \right) | \psi_i \rangle$$



$$= \langle \psi_i | \frac{1}{E} (1 + \frac{H_0}{E} + (\frac{H_0}{E})^2 + \dots) | \psi_i \rangle \quad \text{I.17}$$

$$\begin{aligned} \text{Since } (H_0)^n | \psi_i \rangle &= (H_0)^{n-1} H_0 | \psi_i \rangle \\ &= E_i (H_0)^{n-1} | \psi_i \rangle \\ &= E_i^n | \psi_i \rangle, \end{aligned}$$



equation (I.16) becomes

$$\begin{aligned} \langle \psi_i | \frac{1}{E-H_0} | \psi_i \rangle &= \langle \psi_i | \frac{1}{E} (1 + \frac{E_i}{E} + (\frac{E_i}{E})^2 + \dots + (\frac{E_i}{E})^n) | \psi_i \rangle \\ &= \langle \psi_i | \frac{1}{E} (\frac{1}{1 - \frac{E_i}{E}}) | \psi_i \rangle \\ &= \langle \psi_i | \frac{1}{E-E_i} | \psi_i \rangle \\ &= \frac{\langle \psi_i | \psi_i \rangle}{E-E_i} \\ &= \frac{1}{E-E_i} \\ &= G_0(E) \end{aligned} \quad \text{I.18}$$

Let us now consider a system with perturbation and which is described by the Hamiltonian  $H = H_0 + \lambda V$ , where  $\lambda$  is a real parameter to be set equal to one at a later time,  $V$  is a time independent perturbation operator. The eigenvectors of  $H_0 + V$  are no longer  $|\psi_i\rangle$  and the eigen energies are no longer  $E_i$  but  $E_i'$ .

$$\begin{aligned} E_i' &= E_i + \text{all perturbative corrections to the energy.} \\ &= E_i + \Sigma, \text{ where } \Sigma \text{ is the self energy correction.} \end{aligned}$$

Of interest to us now are the two expectation values

1. The expansion  $\langle i | \frac{1}{E-H} | i \rangle$  in terms of perturbation  $V$ , and

2. The expansion  $\langle i | \frac{1}{E-H} | i \rangle$  in terms of the self energy  $\Sigma$ ,

(Note that in both expansion,  $|i\rangle$  are the eigenvectors of  $H$ ) The

expansion  $\langle i | \frac{1}{E-H} | i \rangle$  in terms of perturbation  $V$  is obtained as follows :

$$\begin{aligned} \langle i | \frac{1}{E-H} | i \rangle &= \langle i | \frac{1}{E-H_0 - \lambda V} | i \rangle \\ &= \langle i | \frac{1}{E-H_0} \left( \frac{1}{1 - \frac{\lambda V}{E-H_0}} \right) | i \rangle \quad \text{I.19} \end{aligned}$$

Since  $\sum_j |j\rangle \langle j| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ , equation (I.19) becomes,

$$\begin{aligned} \langle i | \frac{1}{E-H} | i \rangle &= \sum_j \langle i | \frac{1}{E-H_0} | j \rangle \langle j | \frac{1}{1 - \frac{\lambda V}{E-H_0}} | i \rangle \\ &= \sum_j \frac{1}{E - E_j} \delta_{ij} \langle j | \frac{1}{1 - \frac{\lambda V}{E-H_0}} | i \rangle \\ &= \frac{1}{E - E_i} \langle i | \frac{1}{1 - \frac{\lambda V}{E-H_0}} | i \rangle \\ &= G_0(E) \langle i | \frac{1}{1 - \frac{\lambda V}{E-H_0}} | i \rangle \\ &= G_0(E) \left[ \langle i | \left( 1 + \lambda \frac{V}{E-H_0} + \lambda^2 \frac{V^2}{(E-H_0)^2} + \dots + \lambda^n \frac{V^n}{(E-H_0)^n} + \dots \right) | i \rangle \right] \quad \text{I.20} \end{aligned}$$

The second term in I.20 is  $\lambda \langle i | \frac{V}{E-H_0} | i \rangle$  which can be rewritten as follows.

$$\begin{aligned} \lambda \langle i | \frac{V}{E-H_0} | i \rangle &= \lambda \sum_j \langle i | V | j \rangle \langle j | \frac{1}{E-H_0} | i \rangle \\ &= \lambda \langle i | V | i \rangle G_0(E) \end{aligned}$$

The third term in equation (I.20) is  $\lambda^2 \langle i | \frac{V^2}{(E - H_0)^2} | i \rangle$ .

Expanding as before, we have

$$\begin{aligned}
 \lambda^2 \langle i | \frac{V^2}{(E - H_0)^2} | i \rangle &= \lambda^2 \sum_{j j' j''} \langle i | V | j \rangle \langle j | V | j' \rangle \langle j' | \frac{1}{E - H_0} | j'' \rangle \langle j'' | \frac{1}{E - H_0} | i \rangle \\
 &= \lambda^2 \sum_{j j' j''} \langle i | V | j \rangle \langle j | V | j' \rangle \frac{1}{E - E_{j''}} \delta_{j' j''} \frac{1}{E - E_i} \delta_{j'' i} \\
 &= \lambda^2 \sum_j \frac{\langle i | V | j \rangle \langle j | V | i \rangle}{E - E_i} \frac{1}{E - E_i} \\
 &= \lambda^2 \sum_j \frac{|\langle i | V | i \rangle|^2}{E - E_i} G_0(E) \\
 &= \lambda^2 \langle i | V | i \rangle^2 G_0^2(E)
 \end{aligned}$$

The fourth term in equation (I.20) is  $\lambda^3 \langle i | \frac{V^3}{(E - H_0)^3} | i \rangle$ .

Again expanding as before, we have

$$\begin{aligned}
 \lambda^3 \langle i | \frac{V^3}{(E - H_0)^3} | i \rangle &= \lambda^3 \sum_{j_1 j_2 j_3 j_4 j_5} \langle i | V | j_1 \rangle \langle j_1 | \frac{1}{E - H_0} | j_2 \rangle \langle j_2 | V | j_3 \rangle \\
 &\quad \langle j_3 | \frac{1}{E - H_0} | j_4 \rangle \langle j_4 | V | j_5 \rangle \langle j_5 | \frac{1}{E - H_0} | i \rangle \\
 &= \lambda^3 \sum_{j_1 j_2 j_3 j_4 j_5} \langle i | V | j_1 \rangle \frac{1}{E - E_{j_2}} \delta_{j_1 j_2} \langle j_2 | V | j_3 \rangle \frac{1}{E - E_{j_4}} \delta_{j_3 j_4} \\
 &\quad \langle j_4 | V | j_5 \rangle \frac{1}{E - E_i} \delta_{j_5 i} \\
 &= \lambda^3 \sum_{j_1 j_3} \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_3 \rangle \langle j_3 | V | i \rangle}{(E - E_{j_1})(E - E_{j_3})} G_0(E), \quad j_1 \neq j_3 \neq i
 \end{aligned}$$

$$\begin{aligned}
&= \lambda^3 \sum_{j_1 j_3} \frac{\langle i|V|j_1\rangle \langle j_1|V|j_3\rangle \langle j_3|V|i\rangle}{(E-E_{j_1})(E-E_{j_3})} G_0(E), j_1 \neq j_3 \neq i \\
&= \lambda^3 \langle i|V|i\rangle G_0(E) \sum_{j_1} \frac{\langle i|V|j_1\rangle \langle j_1|V|i\rangle}{E-E_{j_1}} G_0(E), j_1 \neq i, j_3=i \\
&= \lambda^3 \langle i|V|i\rangle G_0(E) \sum_{j_3} \frac{\langle i|V|j_3\rangle \langle j_3|V|i\rangle}{E-E_{j_3}} G_0(E) \\
&= \lambda^3 \sum_j \frac{|\langle i|V|j\rangle|^2 \langle i|V|j\rangle}{E-E_j} G_0(E) \\
&= \lambda^3 \langle i|V|i\rangle^3 G_0^3(E)
\end{aligned}$$

The other terms in equation (I.20) can be expanded in a similar manner. We add these terms together and now set  $\lambda$  equal to one. Thus equation (I.20) becomes

$$\begin{aligned}
\langle i|\frac{1}{E-H}|i\rangle &= G_0(E) \left[ 1 + \langle i|V|i\rangle G_0(E) \right. \\
&\quad + \sum_j \frac{\langle i|V|j\rangle \langle j|V|i\rangle}{E-E_j} G_0(E) \\
&\quad \left. + \sum_{j_1 j_3} \frac{\langle i|V|j_1\rangle \langle j_1|V|j_3\rangle \langle j_3|V|i\rangle}{(E-E_{j_1})(E-E_{j_3})} G_0(E) + \dots \right]
\end{aligned}$$

$$\begin{aligned}
&= G_0(E) \left[ \{ 1 + \langle i | V | i \rangle \right. \\
&\quad + \sum_j \frac{\langle i | V | j \rangle \langle j | V | i \rangle}{E - E_j} \\
&\quad + \sum_{j_1 j_3} \frac{\langle i | V | j_1 \rangle \langle j_1 | V | j_3 \rangle \langle j_3 | V | i \rangle}{(E - E_{j_1})(E - E_{j_3})} \\
&\quad + \dots \dots \dots G_0(E) \left. \right\} \quad ] \quad \text{I. 21}
\end{aligned}$$

Now consider the expansion  $\langle i | \frac{1}{E - H} | i \rangle$  in terms of the

self energy

$$\begin{aligned}
\text{Since } \langle i | \frac{1}{E - H} | i \rangle &= \frac{1}{E - E'_i}, \quad \text{where } E'_i = E_i + \Sigma \\
&= \frac{1}{E - E_i - \Sigma} \\
&= \langle G(E) \rangle \quad \text{I. 22}
\end{aligned}$$

$$\begin{aligned}
\text{Then } \langle G(E) \rangle^{-1} &= E - E_i - \Sigma \\
&= G_0^{-1}(E) - \Sigma \quad \text{I. 23}
\end{aligned}$$

Equation (I.23) is called Dyson's equation<sup>(9)</sup>. Multiply from the right by  $\langle G(E) \rangle$  and from the left by  $G_0(E)$ , we get

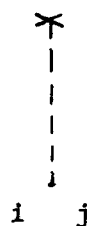
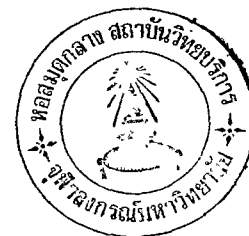
$$\begin{aligned}
G_0(E) &= \langle G(E) \rangle - G_0(E) \Sigma \langle G(E) \rangle \\
\langle G(E) \rangle &= G_0(E) + G_0(E) \Sigma \langle G(E) \rangle \\
&= G_0(E) + G_0(E) \Sigma G_0(E) + G_0(E) \Sigma G_0(E) \Sigma \langle G(E) \rangle \\
&= G_0(E) + G_0(E) \Sigma G_0(E) + G_0(E) \Sigma G_0(E) \Sigma G_0(E) \\
&\quad + G_0(E) \Sigma G_0(E) \Sigma G_0(E) \Sigma G_0(E) + \dots \\
&= G_0(E) \left[ 1 + \Sigma G_0(E) + \Sigma G_0(E) \Sigma G_0(E) \right. \\
&\quad \left. + G_0(E) \Sigma G_0(E) \Sigma G_0(E) + \dots \right] \\
&= G_0(E) \left[ 1 + \left\{ \Sigma + \Sigma G_0(E) \Sigma + \Sigma G_0(E) \Sigma G_0(E) \Sigma \right. \right. \\
&\quad \left. \left. + \Sigma G_0(E) \Sigma G_0(E) \Sigma G_0(E) \Sigma + \dots \right\} G_0(E) \right] \quad \text{I.24}
\end{aligned}$$

Comparing equation (I.21) and equation (I.24), we find the self-energy to be

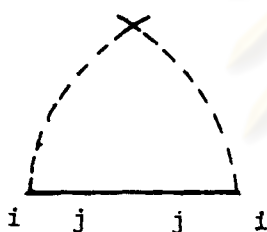
$$\begin{aligned}
\Sigma &= \langle i|V|i \rangle + \sum_j \frac{\langle i|V|j \rangle \langle j|V|j \rangle}{E - E_j} \\
&\quad + \sum_{j_1 j_3} \frac{\langle i|V|j_1 \rangle \langle j_1|V|j_3 \rangle \langle j_3|V|i \rangle}{(E - E_{j_1})(E - E_{j_3})} \\
&\quad + \text{terms coming from the higher order perturbative} \\
&\quad \text{correction} \quad \text{I.25}
\end{aligned}$$

We shall now look at the graphic interpretation of the perturbative series. We can represent the free propagator  $\frac{1}{E - E_j}$  by a horizontal line. Each vertex is associated with a polynomial  $P_n(c)$  where  $n$  equals the number of interaction lines (represented

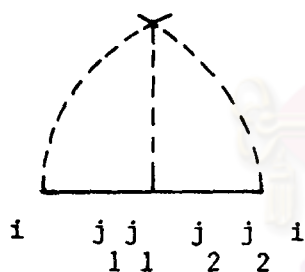
by a dash line) connecting the impurity (represented by a cross) and the exciton propagator line. Each interaction line is associated with a momentum transfer  $p$ . Of course the net momentum transfer to a single impurity must be zero. An example of graphical representation of few terms in the expansion are



for  $\langle i|V|j\rangle$



for  $\sum_j \frac{\langle i|V|j\rangle\langle j|V|i\rangle}{E-E_j}$



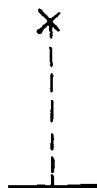
for  $\sum_{j_1 j_2} \frac{\langle i|V|j_1\rangle\langle j_1|V|j_2\rangle\langle j_2|V|i\rangle}{(E-E_{j_1})(E-E_{j_2})}$

etc

Let us now look at the graphs which represent each order correction in perturbative series.

A graph which represents the first order correction

$G_0(E) \langle i|V \left( \frac{1}{E-H_0} \right) |i\rangle$  is





Graphs which represent the second order correction

$$G_0(E) \langle i | V^2 \left( \frac{1}{E-H_0} \right)^2 | i \rangle \quad \text{are}$$

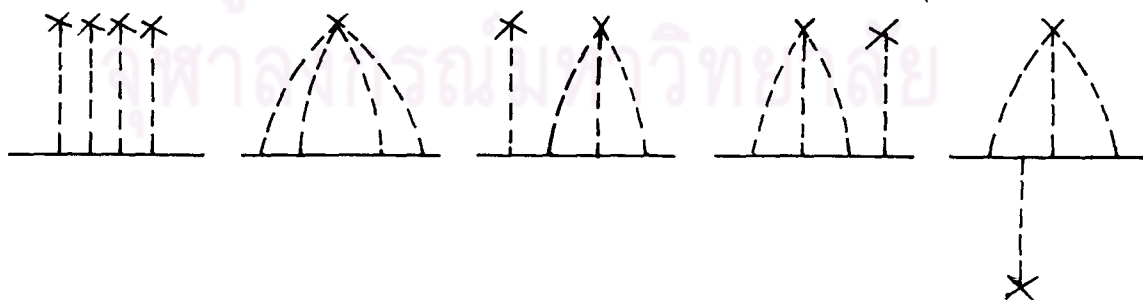


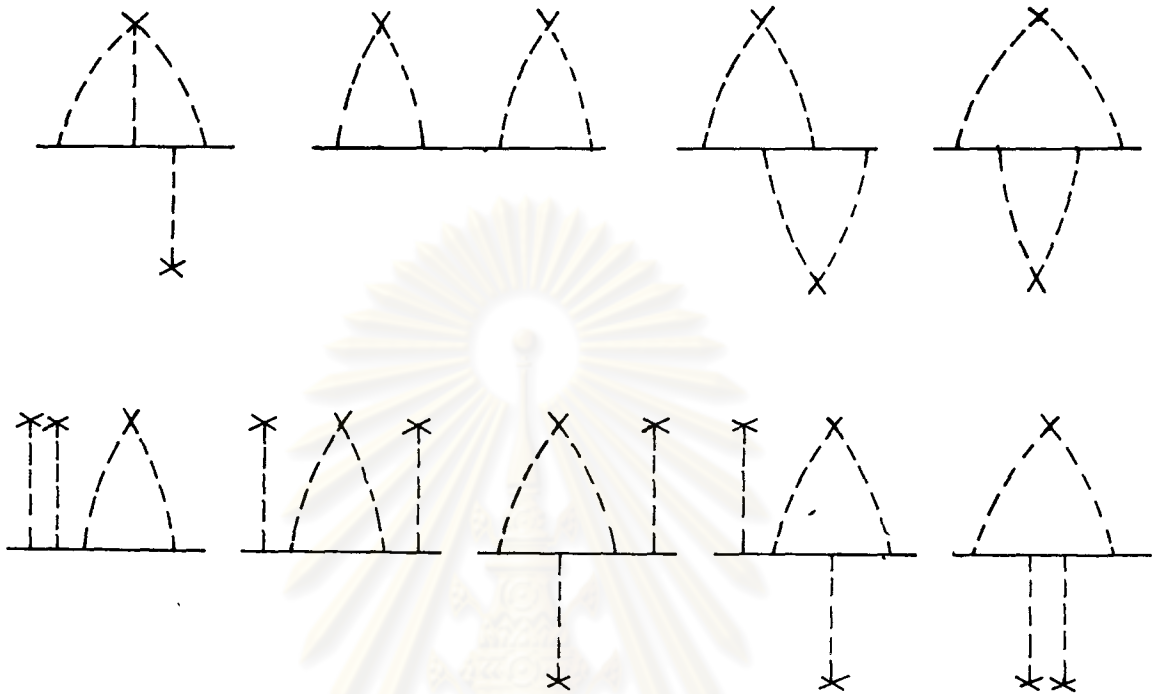
Graphs which represent the third order correction  $G_0(E) \langle i | V^3 \left( \frac{1}{E-H_0} \right)^3 | i \rangle$  are



Graphs which represent the fourth order correction

$$\text{are } G_0(E) \langle i | V^4 \left( \frac{1}{E-H_0} \right)^4 | i \rangle$$



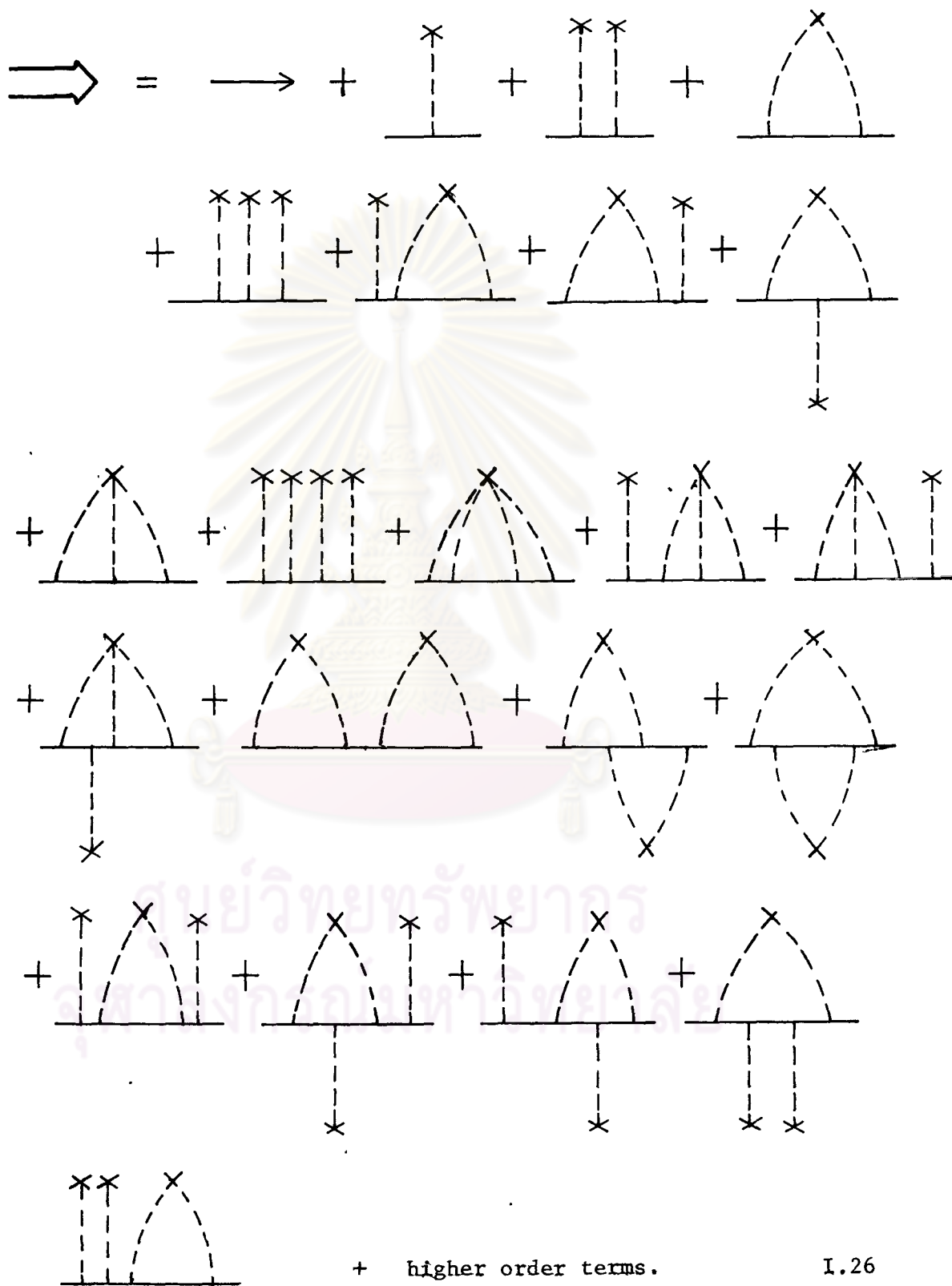


The generalization to  $n^{\text{th}}$  order correction which has 'n' interaction  $V$  (  $\overset{\times}{\vdots}$  ) lines and  $n + 1$  propagators of the type  $\frac{1}{E-E_j}$  (  $\text{---}$  ) lines is as follows,

The total number of terms arising in the  $n^{\text{th}}$  order perturbative series is the total number of distinct pictures having 'n' interaction lines and the correspondence is one-to-one, The  $n^{\text{th}}$  order correction is obtained when we write down the analytic expressions for all the distinct graphs we can draw with the n interaction lines,

If we now represent  $\langle i | \frac{1}{E-H_0} | i \rangle$  by  $\text{---}$  and  $\langle i | \frac{1}{E-H} | i \rangle$

by  $\implies$ , the perturbative series becomes graphically



These graphs can be divided into two groups.

1. Reducible graphs
2. Irreducible graphs

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

Irreducible graphs are the graph which cannot be cut into two parts by cutting propagation line.

The self-energy  $\Sigma$  are the summation of all irreducible graphs in equation (I.26)

Thus  $\Sigma =$

+ etc

I.27

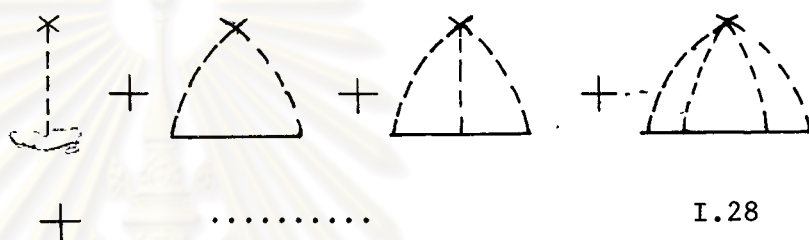
The self-energy  $\Sigma$  = one vertex series + two vertex series +  
three vertex series + .....

where the one vertex series are  $\Sigma_1$  , the two vertex series are  $\Sigma_2$  .

Thus

$$\Sigma_{\text{one vertex}} =$$

$$\Sigma_1 =$$



ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย