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THEORY OF NEUTRON SCATTERING IN DISORDERED ALLOYS*

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ABSTRACT

A comprehensive theory of thermal neutron scattering in disordered alloys is presented here. We consider in detail the case of substitutional random binary alloy with random changes in mass and force constants; and for all values of the concentration. The cluster CPA formalism in argumented space developed here is free from analytical difficulties for the Green function, performs correct averaging over random atomic scattering lengths and employs a self-consistent medium for the calculations. For easy computation, we describe the graphical representation of the resolvent where the approximation steps can be depicted as closed paths in augmented space. Our results for scattering cross sections, both coherent and incoherent, include new types of terms and these lead to asymmetric line shapes for the coherent scattering.

1. INTRODUCTION

The interaction between neutrons and condensed matter has yielded valuable information regarding elementary excitations. A proper theory of neutron scattering is essential to derive these informations. While such a theory in satisfactory form exists for perfect crystals [1),2),3)], the corresponding generalizations for randomly disordered systems have achieved limited success [4),5)]. The main problem is that the usual CPA methods for electronic structure [6)] of random alloys fail to handle random masses, random force constants and random scattering lengths at the same time. The additional difficulties due to force constant sum rule, herglotz properties of Green functions and self-consistent medium are beyond the capabilities of the usual CPA methods. For example, in the phonon problem, many workers [7)] have used special relations among force constants and examined small concentration limits in random binary alloys. Recently [8)] the augmented space method [9)] was used to overcome all the above difficulties in the phonon problem. The important difference between augmented space method and other methods lies in the fact that in the former method, one performs the averaging before approximating the physical quantities. Here we follow a similar approach to formulate a comprehensive theory of neutron scattering using the augmented space formalism.

Consider the scattering of a thermal neutron from state $\vec{k}$ to state $\vec{k}'$ with change of energy

$$E = \frac{h^2}{2M_n} (k^2 - k'^2) = \hbar w \tag{1a}$$

and change of wave vector

$$\vec{q} = \vec{k} - \vec{k}' + \vec{Q} \tag{1b}$$

Here $\vec{Q}$ is a reciprocal lattice vector for a perfect lattice. It is rather well established that thermal neutron interaction with condensed matter is

adequately described by Fermi pseudopotential

$$H_{int} = \sum_j \frac{2\pi\hbar^2}{m} b_j \delta[\vec{r} - \vec{x}_j] \tag{2}$$

where b_j is the scattering length of the j^{th} nucleus (for simplicity we assume one atom per unit cell). The position vector $\vec{x}_j$ can be written in terms of the equilibrium position $\vec{r}_j$ as

$$\underline{x}_j = \underline{r}_j + \underline{u}_j \tag{3}$$

where $\vec{u}_j$ are small displacement from $\vec{r}_j$. The coherent differential scattering cross-section in Born approximation is given [1] by

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar} \frac{k'}{k} \sum_{i,j} e^{i\vec{q}.(\vec{r}_i - \vec{r}_j)} \langle b_i^c \int e^{i\vec{q}.\vec{u}_i(t)} b_j^c e^{-i\vec{q}.\vec{u}_j(0)} \times e^{iwt} dt \rangle_{th} \tag{4}$$

Here the averaging indicated is the thermal averaging and b_i^c is the coherent scattering length obtained by averaging b_i over the nuclear spin states. For small $\vec{u}_i(t)$, the above equation becomes

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar} \frac{k'}{k} \int dt\, e^{iwt} \sum_{i,j} B_i B_j \langle [\vec{q}.\vec{u}_i(t)][\vec{q}.\vec{u}_j(0)] \rangle_{th} \times e^{i\vec{q}.(\vec{r}_i - \vec{r}_j)} \tag{5}$$

Here

$$B_i = b_i^c \exp[-\tfrac{1}{2} \langle [\vec{q}.\vec{u}_i]^2 \rangle_{th}] \tag{6}$$

and the Debye-Waller factor appears for obvious reasons. The incoherent scattering cross-section depends upon the correlations at the same site and may be written, using the incoherent scattering length β_j as

$$\frac{d^2\sigma_{inc}}{d\Omega dE} = \frac{1}{2\pi\hbar} \frac{k'}{k} \int dt\, e^{iwt} \sum_j \beta_j^2 \langle [\vec{q}.\vec{u}_j(t)][\vec{q}.\vec{u}_j(0)] \rangle_{th} \tag{7}$$

In disordered alloys the above formulae must be configuration averaged. To do so we write them in terms of the Green function defined by

$$G_{ij}^{\mu\nu}(w) = \int dt\, e^{iwt}\, i\theta(t) \langle [u_i^\mu(t)\, u_j^\nu(0)] \rangle_{th} \tag{8}$$

Here u_i^μ is thr x, y or z direction component of $\vec{u}_i$. The Green function satisfies the equation

$$\sum_{k,\nu} (m_i w^2 \delta_{ik}\delta_{\mu\nu} - \phi_{ik}^{\mu\nu})\, G_{kj}^{\nu\xi}(w) = \delta_{ij}\, \delta_{\mu\xi} \tag{9}$$

where ϕ is the force constant matrix [8].

The general formalism can be persued through steps analogous to that for a substitutional random binary alloy $A_c B_{1-c}$. In this the disorder is compositional with the solute A dissolving in the solvent B. The treatment of neutron scattering in this system by previous methods [4),5),7)] ran into several difficulties.

The first question to settle was how the formulae for the coherent and incoherent scattering cross-sections go over from the ordered to the disordered systems. It was mainly a question of separation into the coherent and incoherent parts in the presence of random scattering lengths. In the ideal crystal, the incoherent part describes the effect of spin or isotopic incoherence. The generalization of this is non-trivial and the diagramatic analysis [5)] seems to be one approach to this problem. Although suited for diagonal disorder, in this one separates the contributions from

connected diagrams to obtain the short range correlations in the form of incoherent scattering. This is almost independent of $\vec{q}$. The coherent part is of long range correlations.

The next step is the process of actual averaging and approximations. It is in this that the previous methods had difficulties. Configuration averaging by single site CPA has been done in many cases but physically such a method is highly inadequate. In general there are changes in mass and force constants and the absolute minimum requirement is a two-site CPA. Most difficult task has been to incorporate the force constant sum rules and the force constant $\phi(AB)$ themselves. So far the former has been completely ignored and the latter is forced to follow the linear superposition [5),7)] $\phi(AB) = \frac{1}{2}[\phi(AA) + \phi(BB)]$. In most of the cases, there is no physical reason for linear superposition of force constants. The method of conditionally averaged Green functions provides no better and even worse agreement with experiments.

Here we present the formalism to overcome the above mentioned difficulties. We describe how the combination of nuclear spin and configuration averages lead to the separation of coherent and incoherent scattering cross-section. Then we use the augmented space formalism [8),9)] for configuration averaging and describe the systematic approximation scheme for evaluating various quantities. The force constant sum rule will be built into the formalism. There are no restrictions whatsoever on $\rho(AB)$ or the concentration values. Finally the analytic properties of the Green functions will be always preserved. Completely self-consistent calculations (like CPA) are possible within this framework.

The formalism is described in the following section and we present the results for coherent and incoherent scattering cross-sections exhibiting new terms in Sec. 3. In Sec. 4, we describe the procedure for self-consistent two site cluster CPA and its generalizations. Finally in Sec. 5, we summarize the salient points of this work.

2. FORMALISM

We begin by writing the expression for the inelastic cross-section in terms of the Green function defined by Eq.(8). Thus

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar}\frac{k'}{k}\sum_{i,j,\mu,\nu} B_i B_j q^\mu q^\nu e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)} \operatorname{Im} G^{\mu\nu}_{ij}(w) \tag{10}$$

where the scattering lengths are

$$B_j = b_j^c \exp[-\tfrac{1}{2}\langle(\vec{q}\cdot\vec{u}_j)^2\rangle_{th}] \tag{11}$$

This equation is only approximate in nature because it has been written down in analogy with the perfect crystals. It is to be noted that both b_j and the Debye-Waller factor are random and depend upon the configuration. The observed differential cross-section will be the configuration average of Eq. (10). But an averaging of the product of scattering lengths $B_i B_j$ over nuclear spins must also be done. Thus we write

$$\left\langle\frac{d^2\sigma}{d\Omega dE}\right\rangle = \frac{1}{2\pi\hbar}\frac{k'}{k}\sum_{i,j,\mu,\nu} e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)} q^\mu q^\nu \operatorname{Im}\langle\overline{B_i B_j} G_{ij}\rangle \tag{12}$$

where $\overline{B_i B_j}$ denotes the average over nuclear spins and $\langle\ldots\rangle$ denotes configuration average.

In perfect crystals, it is $\overline{B_i}\,\overline{B_j}$ which leads to the coherent and incoherent scattering. In random alloys, both the averages contribute to the coherent and incoherent scatetrings. It is the configuration average that needs special techniques. One way to do it is by diagrammatic technique.. Such an attempt was made by Nowak and Diedericks [5)] using the diagrams of Yonezawa and Matsubara [10)]. A generalization of such diagrams in augmented space has been developed by Mookerjee [11)] and it also is applicable to the off diagonal disorder. But in this work we will describe an alternative

approach for configuration and nuclear spin averaging in Sec. 3.

Here we discuss the augmented space formalism for evaluating $\langle G_{ij}^{\alpha\nu} \rangle$ First we define the site occupation random variable n_i by

$$n_i = \begin{cases} 1 \text{ with probability } c \\ 0 \text{ with probability } 1-c \end{cases} \tag{13}$$

Then

$$m_i = m_B + (m_A - m_B)\, n_i \tag{14a}$$

and for $i \neq j$

$$\begin{aligned} \phi_{ij} &= \phi_{ij}^{AA} n_i n_j + \phi_{ij}^{BB}(1-n_i)(1-n_j) + \phi_{ij}^{AB}[n_i(1-n_j) + n_j(1-n_i)] \\ &= \phi_{ij}^{BB} + \phi_{ij}^{(1)} n_i n_j + \phi_{ij}^{(2)}(n_i+n_j) \end{aligned} \tag{14b}$$

with

$$\phi_{ij}^{(1)} = \phi_{ij}^{AA} + \phi_{ij}^{BB} - 2\phi_{ij}^{AB} \tag{14c}$$

and

$$\phi_{ij}^{(2)} = \phi_{ij}^{AB} - \phi_{ij}^{BB} \tag{14d}$$

Note that in general $\phi(1)$ is not zero. Thus the assumption in earlier work [4),5),7)] that force constants superimpose linearly amounts to vanishing $\phi(1)$ and omits some interesting off-diagonal disorder effects. One has also the sum rule

$$\sum_j \phi_{ij} = 0 \tag{15}$$

to take into account while evaluating $\langle G \rangle$. This is used to express $\phi_{ij}^{\alpha\nu}$ in terms of other force constants:

$$\phi_{ii} = -\sum_{j \neq i} \phi_{ij} \tag{16}$$

We introduce the projection and transfer operators $P_i = |\vec{r}_i\rangle\langle\vec{r}_i|$ and $T_{ij} = |\vec{r}_i\rangle\langle\vec{r}_j|$ to write Eq. (9) in the operator form

$$\underline{G} = [m_B w^2 \underline{I} - \underline{K}]^{-1} \tag{17}$$

with

$$\begin{aligned} \underline{K} = \underline{K}_B + \sum_i \Big\{ (m_A - m_B) w^2 n_i \underline{P}_i - \sum_{m \neq i} [\underline{\phi}_{im}^{(2)}(n_i+n_m) + \underline{\phi}_{im}^{(1)} n_i n_m] \underline{P}_i \Big\} \\ + \sum_{i \neq j} \underline{\phi}_{ij}^{(2)}(n_i+n_j)\, \underline{T}_{ij} + \sum_{i \neq j} \underline{\phi}_{ij}^{(1)} n_i n_j\, \underline{T}_{ij} \end{aligned} \tag{18a}$$

where

$$\underline{K}_B = -\sum_{i,m \neq i} \underline{\phi}_{im}^{BB} \underline{P}_i + \sum_{i,j} \underline{\phi}_{ij}^{BB} \underline{T}_{ij} \tag{18b}$$

is the dynamical matrix of the solvent B.

The random dynamical matrix is now in a form to be used in the augmented space formalism of Mookerjee [9)]. In the absence of short range order, $p(n_i) = c\,\delta(n_i - 1) + (1-c)\delta(n_i)$ and one can have a two-dimensional space with an operator n^i such that

$$p(n_i) = -\frac{1}{\pi} \operatorname{Im} \langle \gamma_0^{(i)} | [n_i + i\sigma)\underline{I} - \underline{M}^i] | \gamma_0^{(i)} \rangle \tag{19a}$$

where n^i has the representation [9)]

$$\underline{\underline{M}}^{1} = \begin{bmatrix} c & c(1-c) \\ c(1-c) & 1-c \end{bmatrix} \qquad (19b)$$

The augmented space is the direct product of the actual space spanned by $|\vec{r}_i\rangle$ and the mathematical space spanned by $|r_0^i\rangle$ at each site. Thus the vector of the augmented space may be written as

$$|r_i, \gamma_0\rangle = |\underline{r}_i\rangle \otimes |\gamma_0\rangle \qquad (19c)$$

where

$$\gamma_0 = \prod_i \otimes \gamma_0^{(i)} \qquad (19d)$$

The operator in the augmented space are directed products of operators in actual space (like D) and operators for randomness given by n^i. Thus the augmented space dynamical matrix is given by

$$\tilde{\underline{\underline{K}}} = \tilde{\underline{\underline{K}}}_B \otimes \underline{\underline{I}} + \sum_i (m_A - m_B) w^2 \underline{\underline{P}}_i \otimes \underline{\underline{M}}^i - \sum_{i,m\neq i} \sum [\phi^{(2)}_{\underline{\underline{im}}} \underline{\underline{P}}_i \otimes (\underline{\underline{M}}^i + \underline{\underline{M}}^m) + \phi^{(1)}_{im} \underline{\underline{P}}_i \otimes \underline{\underline{M}}^i \times \underline{\underline{M}}^m]$$

$$+ \sum_{i,j} \phi^{(1)}_{\underline{\underline{ij}}} \underline{\underline{T}}_{ij} \otimes \underline{\underline{M}}^i \otimes \underline{\underline{M}}^j + \sum_{i,j} \phi^{(2)}_{\underline{\underline{ij}}} \underline{\underline{T}}_{ij} \otimes (\underline{\underline{M}}^i + \underline{\underline{M}}^j) \qquad (20)$$

Finally it can be shown [9] that the configuration average of the Green function is exactly given by

$$\langle \underline{\underline{G}}_{ij}(w) \rangle = \langle \vec{r}_i, \gamma_0 | (m_B w^2 \underline{\underline{I}} - \tilde{\underline{\underline{}}})^{-1} | \vec{r}_j, \gamma_0 \rangle$$

$$= \langle \vec{r}_i, \gamma_0 | \tilde{\underline{\underline{G}}}(w) | \vec{r}_j, \gamma_0 \rangle \qquad (21)$$

Approximate and self-consistent methods corresponding to CPA with different cluster sizes can be done to evaluate $\langle G_{ij} \rangle$. We discuss these in Sec. 4. Note that Eq. (21) is exact and therefore no approximation has been done before the configuration average is taken. This point is crucial for the analiticity (herglotz) properties of the Green function.

3. COHERENT AND INCOHERENT SCATTERING

The scattering cross section in Eq. (12) involves two averaging processes: (a) averages of scattering lengths over nuclear spins and (b) the configuration average of the product of the Green function and scattering lengths over the random distribution of constituent atoms in alloys. It is the first averaging that gives [3] the coherent and incoherent scattering cross sections in the perfect crystals. This is basically the difference between the correlations of nuclear spins at the same site and the uncorrelated nuclear spins at different sites. Thus the $\overline{B^2}$ is the same as $[\overline{B}]^2$ for different sites but at the same site due to correlations of nuclear spins $\overline{B^2}$ is not equal to $[\overline{B}]^2$. One can write

$$\overline{B_i B_j} = [\overline{B}]^2 + \delta_{ij}(\overline{B^2} - [\overline{B}]^2) = \overline{B}^2 + \delta_{ij}\overline{(B-\overline{B})^2} \qquad (22)$$

The second term in this decomposition gives the incoherent scattering in perfect crystals. In alloys, this is also present but the dominant feature is the configuration average over random distributions. This average is not as easy to perform as the process. Here we employ the augmented space method to do this average. Obviously the randomness of composition will in general give rise to incoherent scattering which for large concentration may be much stronger than that due to correlations of nuclear spins at the same site. No previous work has correctly treated these two averages which we describe below.

We first perform the configuration averaging. The scattering lengths at each site are random in two ways. First, it contributes to the diagonal disorder like the mass in phonon calculations [8]. But from Eq. (11), we note that B_j has a Debye-Waller factor which includes the effects of off-diagonal disorder. Therefore there is an off diagonal disorder effect in B_j. However, we neglect this indirect effect in the first approximation. Then we write

$$B_j = B_j(B) + \delta B_j \, n_j \tag{23}$$

where

$$\delta B_j = B_j(A) - B_j(B)$$

Then,

$$\langle \overline{B_i B_j} G_{ij} \rangle = \overline{B_i(B) B_j(B)} \langle G_{ij} \rangle + \overline{B_i(B) \delta B_j} \langle n_j G_{ij} \rangle + \overline{\delta B_i B_j(B)} \langle n_i G_{ij} \rangle + \overline{\delta B_i \delta B_j} \langle n_i G_{ij} n_j \rangle \tag{24}$$

The quantities $\langle n_i G_{ij} \rangle$ etc. have been used in the phonon problem [8]. They may be written, using Eq. (21), as

$$\langle G_{ij} \rangle = \langle \vec{r}_i, \gamma_0 | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle \tag{25a}$$

$$\langle n_i G_{ij} \rangle = c \langle \vec{r}_i, \gamma_0 | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle + \sqrt{c(1-c)} \langle \vec{r}_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle \tag{25b}$$

and

$$\langle n_i G_{ij} n_j \rangle = c^2 \langle \vec{r}_i, \gamma_0 | \tilde{\underline{G}} | r_j, \gamma_0 \rangle + 2c \sqrt{c(1-c)} \langle r_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle + c(1-c) \langle \vec{r}_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_j, \gamma_0^j \rangle \tag{25c}$$

We substitute these expressions in Eq. (24) and use Eq. (22) to obtain the various terms given below.

$$\begin{aligned}
\overline{B_i B_j} G_{ij} = {} & \left[\overline{(B(B)-\overline{B(B)})^2} + 2c \, \overline{(B(B)-\overline{B(B)})(\delta B - \overline{\delta B})} + c^2 \overline{(\delta B - \overline{\delta B})^2} \right] \langle \vec{r}_i, \gamma_0 | \tilde{\underline{G}} | r_i, \gamma_0 \rangle \\
& + 2\sqrt{c(1-c)} \left[\overline{(B(B)-\overline{B(B)})(\delta B - \overline{\delta B})} + c \, \overline{(\delta B - \overline{\delta B})^2} \right] \langle r_i, \gamma_0^i \tilde{\underline{G}} | r_j, \gamma_0 \rangle \\
& + c(1-c) \left[\overline{(\delta B - \overline{\delta B})^2} \right] \langle r_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_i, \gamma_0^j \rangle \\
& + \left[\overline{B(B)}^2 + 2c \, \overline{B(B)} \, \overline{\delta B} + c \, (\overline{\delta B})^2 \right] \langle r_i, \gamma_0 | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle \\
& + 2\sqrt{c(1-c)} \left[\overline{B(B)} \, \overline{\delta B} + c \, (\overline{\delta B})^2 \right] \langle r_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_j, \gamma_0 \rangle \\
& + c(1-c) \, (\overline{\delta B})^2 \langle \vec{r}_i, \gamma_0^i | \tilde{\underline{G}} | \vec{r}_j, \gamma_0^j \rangle
\end{aligned} \tag{26}$$

The first three terms here refer to the same site in actual space and therefore contribute to incoherent scattering. There are three types of these terms. The last three terms of Eq. (26) represent contributions to the coherent scattering. These are very general expressions. The diagrammatic analysis [5] does not yield so many terms. It essentially gives the first and the fourth terms which are nevertheless important terms. In the limit of $c = 0$, i.e. perfect B lattice, these two terms survive in the correct form whereas other terms vanish. Thus

$$\lim_{c\to 0} \langle B_i B_j G_{ij} \rangle = \overline{(B(B)-\overline{B(B)})^2} \langle \vec{r}_i, \gamma_0 | \tilde{\underline{G}} | \vec{r}_i, \gamma_0 \rangle + (\overline{B(B)})^2 \langle \vec{r}_i, \gamma_0 \tilde{\underline{G}} \vec{r}_j, \gamma_0 \rangle \quad (27)$$

Similarly it is easy to check that in the limit of $c = 1$, one gets the scattering from the perfect A lattice and in Eq. (27), all the $B(B)$ get replaced by $B(A)$. In the limit of very small c, two additional terms proportional to c appear in Eq. (27). It is important to remember that the effects of mass and force constant changes are present in the different averages of the Green function appearing in equation (26). These averages can be evaluated by systematic approximations as discussed in the following section.

We conclude this section by writing down the epressions for the cross sections. When Eq. (26) is used in Eq. (12), we obtain,

$$\left\langle \frac{d^2\sigma}{d\Omega dE} \right\rangle = \frac{d^2\sigma_{inc}}{d\Omega dE} + \frac{d^2\sigma_{coh}}{d\Omega dE} \quad (28)$$

Here the incoherent cross-section is given by

$$\frac{d^2\sigma_{inc}}{d\Omega dE} = \frac{1}{2\pi\hbar} \frac{k'}{k} \sum_{i,\mu,\nu} \sum q^\mu q^\nu \, \mathrm{Im} \left[B^2_{inc}(1) \langle \vec{r}_i, \gamma_0 | \tilde{G}^{\mu\nu} | \vec{r}_i, \gamma_0 \rangle \right.$$

$$\left. + B^2_{inc}(2) \langle \vec{r}_i, \gamma_0^i | \tilde{G}^{\mu\nu} | \vec{r}_i, \gamma_0 \rangle + B^2_{inc}(3) \langle \vec{r}_i, \gamma_0^i | \tilde{G}^{\mu\nu} | \vec{r}_i, \gamma_0^j \rangle \right] \quad (29)$$

where

$$B^2_{inc}(1) = \overline{B^2(B)} - \overline{B(B)}^2 + 2c(\overline{B(B)\delta B} - \overline{B(B)}\,\overline{\delta B}) + c\,(\overline{\delta B^2} - \overline{\delta B}^2) \quad (30a)$$

$$B^2_{inc}(2) = 2\sqrt{c(1-c)}\,[\overline{B(B)\delta B} - \overline{B(B)}\,\overline{\delta B} + c(\overline{\delta B^2} - \overline{\delta B}^2)] \quad (30b)$$

$$B^2_{inc}(3) = c(1-c)\,[\overline{\delta B^2} - \overline{\delta B}^2] \quad (30c)$$

All the contributions to the incoherent cross-section in Eq. (29) refer to the same site i in actual space. Thus they show the effect of short range correlations between nuclear spins with random distribution of the constituent atoms.

The coherent scattering cross-section on the other hand incorporates long range correlations. The formula analogous to Eq. (29) for the coherent cross-section may be written down as

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar} \frac{k'}{k} \sum_{i,j,\mu,\nu} \sum \sum e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \, q^\mu q^\nu \, \mathrm{Im} \left[B^2_{coh}(1) \langle \vec{r}_i, \gamma_0 | \tilde{G}^{\mu\nu} | \vec{r}_j, \gamma_0 \rangle \right.$$

$$+ B^2_{coh}(2) \langle \vec{r}_i, \gamma_0^i | \tilde{G}^{\mu\nu} | \vec{r}_j, \gamma_0 \rangle$$

$$\left. + B^2_{coh}(3) \langle \vec{r}_i, \gamma_0^i | \tilde{G}^{\mu\nu} | \vec{r}_j, \gamma_0^j \rangle \right] \quad (31)$$

where

$$B^2_{coh}(1) = \overline{B(B)}^2 + 2c\,\overline{B(B)}\,\overline{\delta B} + c^2\overline{\delta B}^2 \quad (32a)$$

$$B^2_{coh}(2) = 2\sqrt{c(1-c)}\,[\overline{B(B)}\,\overline{\delta B} + c\,\overline{\delta B}^2] \quad (32b)$$

$$B^2_{coh}(3) = c(1-c)\,\overline{\delta B}^{\,2} \qquad (32c)$$

It is very clear from these expressions that even the diagrammatic analysis [5] does not fully reveal the true features of thermal neutron scattering in disordered alloys. For example, the result of Nowak and Diedericks [5] that one can write $\frac{d^2\sigma\ coh}{d\Omega\, dE}$ as proportional to $B_{eff}(\omega) \langle G(\omega) \rangle B'_{eff}(\omega)$ is an approximation of the terms containing $B^2_{coh}(1)$. The other two terms do not appear in their analysis. The need for augmented space formulation is amply justified by the presence of all terms in Eqs. (29) and (31).

4. SELF-CONSISTENT CALCULATION OF SELF-ENERGIES IN DIFFERENT CLUSTER APPROXIMATIONS

To evaluate the scattering cross-sections, one must calculate $\langle \vec{r}_i, r_0 |\tilde{G}| \vec{r}_j, \gamma_0 \rangle$, $\langle \vec{r}_i, \gamma_0^i |\tilde{G}| \vec{r}_j, \gamma_0 \rangle$, and $\langle \vec{r}_i, \gamma_0^i |\tilde{G}| \vec{r}_j, \gamma_0^j \rangle$. It was the calculation of these quantities where all the previous work had had difficulties. Drastic assumptions of single site CPA and linear super imposition of force constants were needed to derive some results. The formalism presented here has no such restrictions. Force constant sum rule has been used already so that it is builts into the formalism . Herglotz properties of Green functions have been preserved. We now show that it is possible to perform self-consistent calculations within a systematic approximation scheme that is in correspondence with the various cluster CPA calculations.

In a strict sense, it is inconsistent to use one site CPA when the force constant changes affect at least two sites (nearest neighbours). It

has been used in the past when nothing better could be done. Here we use the two site cluster CPA approximation in the augmented space. Although the approximation scheme has been discussed in detail in earlier publications [8),11)-14)] it is relevant to recall some of the principal ideas behind them. The cluster CPA is generated in a way identical to the usual CCPA ideas [4)]. An "exact" cluster of a particular configuration is immersed in a medium whose 'effective' dynamical matrix $\underset{\sim}{K}_{eff}(\omega)$ is to be determined self-consistently via

$$\left\langle \underline{\underline{G}}[\underline{\underline{K}}_{cl}; \underline{\underline{K}}_{eff}] \right\rangle_{\substack{\text{cluster} \\ \text{configurations}}} = \underline{\underline{G}}[\underline{\underline{K}}eff] \qquad (33a)$$

The dynamical matrix of the above situation may be schematically written as

$$\underline{\underline{K}} = \begin{bmatrix} \underline{\underline{K}}_{cl} & \underline{\underline{K}}^{(1)}_{eff} \\ \underline{\underline{K}}^{(1)}_{eff} & \underline{\underline{K}}^{(2)}_{eff} \end{bmatrix} \qquad \underline{\underline{K}}, \underline{\underline{K}}_{eff} \in \mathcal{H}$$

Randomness exists only in the cluster subspace. Going over the augmented space then, the configuration space Φ is of rank 2^N, N being the cluster size.

$$\tilde{\underline{\underline{K}}} = \begin{bmatrix} \tilde{\underline{\underline{K}}}_{cl} & \tilde{\underline{\underline{K}}}^{(1)}_{eff} \\ \tilde{\underline{\underline{K}}}^{(1)}_{eff} & \tilde{\underline{\underline{K}}}^{(2)}_{eff} \end{bmatrix}$$

here no element is random and $\tilde{\underline{\underline{K}}} \in \mathcal{H} \otimes \Phi$.

(33b)

In the 2CPA , e.g. $\tilde{K}_{cl}$ of rank is $3 \times 2 \times 2^2 = 24$, (polarizations x cluster size x cluster configurations) and its graphical representation is shown in Fig. 1(a), the averaging theorem on augmented space [9)] states that

$$\langle \tilde{\underline{\underline{G}}}[\tilde{\underline{\underline{K}}}_{cl}, \tilde{\underline{\underline{K}}}_{eff}] \rangle_{cl} = \langle \gamma_0 | \tilde{\underline{\underline{G}}}[\tilde{\underline{\underline{K}}}_{cl}, \tilde{\underline{\underline{K}}}_{eff}] | \gamma_0 \rangle \qquad (33c)$$

or the averaging is reduced to taking a particular matrix element.

Let us illustrate the setting up of the self-consistent equations for a 2 CPA. Here $\underline{K}_{eff} = \underline{K}_B + \underline{\Sigma}$ and the self energy $\underline{\Sigma}$ has two distinct matrix elements $\underline{\Sigma}_0^{\mu\nu} = \underline{\Sigma}^{\mu\nu}(\vec{r}_i, \vec{r}_j)$ and $\underline{\Sigma}_1^{\mu\nu} = \underline{\Sigma}^{\mu\nu}(\vec{r}_i, \vec{r}_j)$ between nearest neighbours. We shall also use the matrix partitions theorem which states that if we partition a matrix $\underline{A}$ as $\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$ and $\underline{X}^{-Py}$ denotes inverse of $\underline{X}$ in subspace y, then

$$\underline{G} = (w^2\underline{I} - \underline{A})^{-P_1} = (w^2\underline{I} - \underline{A}_{11} - \underline{A}_{12}\underline{G}_2(w)\underline{A}_{21})^{-P_1} \; ; \; \underline{G}_2(w) = (w^2\underline{I} - \underline{A}_{22})^{-P_2}$$

so that instead of working with the full A, we may work with an effective $\underline{A}_{eff}(\omega) = \underline{A}_{11} + \underline{A}_{12}\, G_2(\;)\, \underline{A}_{21}$ in the subspace '1'.

To satisfy both 33(a) and 33(b), we have to construct out of $\tilde{\underline{\underline{K}}}$ and effective $\underline{\underline{K}}_{eff}$ in the subspace of the augmented space spanned by $\{ | \vec{r}_i \otimes \gamma_0 \rangle \}$ using the matrix partition theorem. This is done in two steps: the first partition is that shown in (33b), which reduces $\tilde{\underline{\underline{K}}}[\underline{\Sigma}]$ to a $\tilde{\underline{\underline{K}}}^{eff}_{cl}[\underline{\Sigma}]$ which is a 24 x 24 matrix as shown in Fig. 1(b).

$$\tilde{\underline{\underline{K}}}^{eff}_{cl}[\underline{\Sigma}] = \tilde{\underline{\underline{K}}}_{cl} + \tilde{\underline{\underline{K}}}^{(1)}_{eff}[\underline{\Sigma}]\, \underline{\underline{g}}[\underline{\Sigma}]\, \tilde{\underline{\underline{K}}}^{(1)}_{eff}[\underline{\Sigma}] \qquad (34a)$$

with $\underline{\underline{G}}[\underline{\Sigma}] = (w^2\underline{\underline{I}} - \tilde{\underline{\underline{K}}}^{(2)}_{eff})^{-P_2}$

To obtain $\underline{\Sigma}$, we next partition the above 3 x N x 2^N rank matrix into a 3N x 3N one on the subspace spanned by $\{ | \vec{r}_i \otimes \gamma_0 \rangle$ (ab x b for the 2 CPA) and the rest. The theorem then yields a $\underline{K}_{eff}$ which may be written as

$$\hat{\underline{\underline{K}}}_{eff} = \underline{\underline{K}}_B + \underline{\underline{K}}_{BM}\underline{\underline{G}}_M\underline{\underline{K}}_{MB} \qquad (34b)$$

These constitute the self-consistent equations for $\underline{\Sigma}$. For example, starting from, say, $\underline{\Sigma} = \underline{\Sigma}_{1CPA}$, we generate $\mathcal{T}[\underline{\Sigma}_{1CPA}]$ from (34a) and then use (34b) to generate the next better $\underline{\Sigma}[\mathcal{T}]$ and iterate till convergence is achieved.

To obtain the elements of the Green function off-diagonal in augmented space, let us illustrate for the 2CPA. Having obtained $\underline{\mathcal{T}}$, and $\underline{\Sigma}$ from the above procedure, we now partition the N x 2^N rank matrix $\underline{K}^{eff}_{cl}(\underline{\Sigma})$ into one spanned by $\{ | \vec{r}_i, \gamma_0 \rangle , | \vec{r}_i, \gamma_0^i \rangle \}$ (a 4 x 4 the 2CPA and the rest). The partition theorem now yields a (4 x 4) $\hat{\underline{\underline{K}}}_{eff}$ whose graphical representation is shown in Fig. 1(c).

Note first that there is full translation symmetry in the lattice space. This arises out of the underlying translational symemtry in augmented space due to statistical homogeniety, and equivalence of all sites in the 2-cluster. In a larger cluster CPA we would expect cluster translational symmetry, unless the Kaplan-type of prescription is used. This translational symmetry yields

$$\begin{aligned} \langle \vec{r}_i, \gamma_0 | \tilde{\underline{\underline{G}}} | \vec{r}_j, \gamma_0 \rangle &= \mathcal{G}_{11}(r_i - r_j) \\ \langle r_i, \gamma_0^i | \tilde{\underline{\underline{G}}} | \vec{r}_j, \gamma_0 \rangle = \langle \vec{r}_i, \gamma_0 | \tilde{\underline{\underline{G}}} | \vec{r}_j, \gamma_0^j \rangle &= \mathcal{G}_{12}(r_i - r_j) \\ \langle r_i, \gamma_0^i | \tilde{\underline{\underline{G}}} | \vec{r}_j, \gamma_0^j \rangle &= \mathcal{G}_{22}(r_i - r_j) \end{aligned} \qquad (35)$$

The matrix element $\mathcal{G}_{\alpha\beta}(\vec{r}_i, \vec{r}_i)$ may be calculated on the graph of Fig. 1(c) using the recursion method. For the coherent cross-section (35) and (31) gives

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar}\frac{k'}{k} N \sum_{\mu\nu} q^\mu q^\nu \, \mathrm{Im}\, [B^2_{coh}(1)\mathcal{G}^{\mu\nu}_{11}(q,w) + B^2_{coh}(2)\mathcal{G}^{\mu\nu}_{12}(q,w) + B^2_{coh}(3)\mathcal{G}^{\mu\nu}_{22}(q,w)]\, n(\omega) \qquad (36)$$

For the CPA, $\mathcal{G}^{\mu\nu}_{\alpha\beta}(\vec{q}, \omega)$ may be immediately found by inverting the 3Nx3N matrix

$$\underline{\underline{G}}^{\mu\nu}(\vec{q},w) = [\, w^2\underline{\underline{I}} - \underline{\underline{\hat{K}}}^{\mu\nu}_{eff}(\vec{q}) \,]^{-1} \qquad (37)$$

Here $\hat{K}^{\mu\nu}_{eff}(\vec{q},\omega) = \underline{\underline{K}}^{0}_{B} + \underline{\underline{\Sigma}}(\vec{q},\omega)$ are 2x2 matrices, where

$$\underline{\underline{\Sigma}}(\vec{q},w) = \underline{\underline{\Sigma}}_0(w) + \underline{\underline{\Sigma}}_1(w)\, S(\vec{q}) \quad , \quad \underline{\underline{\Sigma}}_0 = \begin{pmatrix} \Sigma_{0f,0f} & \Sigma_{0f,0f_0} \\ \Sigma_{0f_0,0f} & \Sigma_{0f_0,0f_0} \end{pmatrix}$$

$$\underline{\underline{\Sigma}}_1 = \begin{pmatrix} \Sigma_{0f,1f} & \Sigma_{0f,1f_1} \\ \Sigma_{0f_0,1f} & \Sigma_{0f_0,1f_1} \end{pmatrix}$$

and $S(\vec{q})$ is the structure factor $\sum_{\vec{x}} e^{i\vec{q}\cdot\vec{x}}$

of the lattice with $\vec{x}$ as the nearest neighbour vectors. In terms of the polarization vectors or the eigenvectors of the effective dynamical matrix $e_\mu(\vec{\ },\omega;\lambda) = e^*_\mu(\vec{\ },-\omega;\lambda)$.

$$G^{\mu\nu}_{\alpha\beta}(\vec{q},w) = \sum_\lambda e^\mu(\vec{q},w;\lambda)\, e^*_\nu(\vec{q},w;\lambda)\, [(w^2-w_{o\lambda}^2)\begin{pmatrix}1&0\\0&0\end{pmatrix} - \underline{\underline{\Sigma}}(\vec{q},w;\lambda)\,]^{-1}_{\alpha\beta}$$

Now defining $\mathcal{B}^{(\alpha)}_\lambda(\vec{q},\omega) = \sum_\mu q^\mu e_\mu(\vec{q},\omega;\lambda) B_{coh}(\alpha)$

where λ labels the phonon "branch" and α is 1, 2 or 3, (same labels as in (36)), one gets

$$\frac{d^2\sigma_{coh}}{d\Omega dE} = \frac{1}{2\pi\hbar}\frac{k'}{k}\,\mathrm{Im}\sum_\lambda \left\{ \frac{\mathcal{B}^{(1)}_\lambda(\vec{q},\omega)\;\mathcal{B}^{*(1)}_\lambda(\vec{q},-\omega)}{\omega^2 - \omega_{o\lambda}^2(\vec{q},\omega) - \Sigma_\lambda(\vec{q},\omega) - \xi_\lambda^2/\eta_\lambda} \right.$$

$$- \frac{\mathcal{B}^{(2)}_\lambda(\vec{q},\omega)\;\mathcal{B}^{(2)*}_\lambda(\vec{q},-\omega)}{\xi_\lambda(\vec{q},\omega) + \{\omega^2 - \omega_{o\lambda}^2 - \Sigma_\lambda)(\eta_\lambda/\xi_\lambda)}$$

$$\left. + \frac{\mathcal{B}^{(3)}_\lambda(\vec{q},\omega)\;\mathcal{B}^{(3)*}_\lambda(\vec{q},-\omega)}{\eta_\lambda(\vec{q},\omega) - \dfrac{\xi_\lambda^2(\vec{q},\omega)}{\omega^2 - \omega_{o\lambda}^2 - \Sigma_\lambda(\vec{q},\omega)}} \right\} \qquad (38)$$

Here $\Sigma_\lambda(\vec{k},\omega) = \Sigma^\lambda_{of,of}(\omega) + \Sigma^\lambda_{of,1f}(\omega)\, S(\vec{q})$

$$\xi_\lambda(\vec{k},\omega) = \Sigma^\lambda_{of,of_c}(\omega) + \Sigma^\lambda_{of,1f_1}(\omega)\, S(\vec{q})$$

$$= \Sigma^\lambda_{of_c,of}(\omega) + \Sigma^\lambda_{of_0,1f}(\omega)\, S(\vec{q})$$

this equality holds due to translational invariance in augmented space.

$$\eta_\lambda(\vec{k},\omega) = \Sigma^\lambda_{of_c,of_0}(\omega) + \Sigma^\lambda_{of_c,1f_1}(\omega)\, S(\vec{q}).$$

If we write $\Sigma_\lambda + \xi^2/\eta_\lambda$ as $\Sigma'_\lambda + i\Sigma''_\lambda$ where Σ'_λ and Σ''_λ are <u>real</u> functions herglotz property ensuring Σ''_λ to be strictly of one sign for all $\vec{k}$, ω. Similarly $\xi_\lambda = \xi'_\lambda + i\eta'_\lambda$ and $\eta_\lambda = \eta'_\lambda + i\eta''_\lambda$ and since the coefficients $B^{(\alpha)}_\lambda(\vec{k},\omega)B^{(\alpha)*}_\lambda(\vec{k},-\omega)$ are real, rewriting them as $\eta b^{(\alpha)}_\lambda(\vec{k},\omega)$

$$\frac{d^2\sigma_{coh}}{d\Omega\, dE} = \frac{1}{2\pi\hbar}\frac{k'}{k}\,\mathrm{Im}\sum_\lambda \left\{ \eta b^{(1)}_\lambda(\vec{q},\omega)\, \frac{\Sigma''_\lambda}{(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)^2+\Sigma''^2_\lambda} \right.$$

$$+ \eta b^{(3)}_\lambda(\vec{q},\omega)\, \frac{\Sigma''_\lambda\{\eta'_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)+\eta''_\lambda\Sigma''_\lambda-\xi'^2_\lambda+\xi''^2_\lambda\} + (\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)\{\eta''_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)-\Sigma''_\lambda\eta'_\lambda\}}{\{\eta'_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)+\eta''_\lambda\Sigma''_\lambda-\xi'^2_\lambda+\xi''^2_\lambda\}^2+\{\eta''_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)-\Sigma''_\lambda\eta'_\lambda\}^2}$$

$$\left. - \eta b^{(2)}_\lambda(\vec{q},\omega)\, \frac{\xi'_\lambda\{2\xi'_\lambda\xi''_\lambda+\eta''_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)-\Sigma''_\lambda\eta''_\lambda\}+\xi''_\lambda\{\xi'^2_\lambda-\xi''^2_\lambda+(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)\eta'_\lambda+\Sigma''_\lambda\eta''_\lambda\}}{\{\xi'^2_\lambda-\xi''^2_\lambda+(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)\eta'_\lambda+\Sigma''_\lambda\eta''_\lambda\}^2+\{2\xi'_\lambda\xi''_\lambda+\eta''_\lambda(\omega^2-\omega_{o\lambda}^2-\Sigma'_\lambda)-\Sigma''_\lambda\eta'_\lambda\}^2} \right\}$$

(39)

In addition to the usual Lorentzian phonon line shape given by the first term, the last two terms lead to an asymmetry of the phonon line. These terms would be absent of the scattering lengths did not fluctuate and $\eta b^{(2)} = \eta b^{(3)} = 0$. In any particular situation one has to carefully

evaluate these terms to decide whether or not they are negligible. Note that a direct comparison with Nowak and Dedericks[5] is not possible, as their diagrams are valid only for diagonal disorder (these are the Yonezawa-Matsubara diagrams for diagonal disorder). We have taken a case of coupled diagonal and off-diagonal disorders suitable for an alloy. Since for diagonal disorder Mookerjee[11] has shown that the Yonezawa-Matsubara diagrams are identical to the augmented space diagrams, it is logical to argue that for diagonal disorder only Eq.(38) reduces to Eq.(2.11) of Nowak and Dederick[5] - both reducing to asymmetric line shapes.

5. SUMMARY

Here we have described a new comprehensive theory of thermal neutron scattering from disordered systems. The details of the formalism for random binary alloys described above can be very easily generalized to more general cases. Except the restrictions of Fermi pseudopotential and Born approximation which describe thermal neutron scattering in perfect crystals quite well, our formalism has no restrictions on the concentration values, changes in force constants etc. In addition to these, we have for the first time taken the force constant sum rule into account and described an averaging procedure which preserves analytic properties of the Green function also within the framework of a self-consistent calculation.

Our main new results are the expressions for the coherent (Eq.(31)) and incoherent (Eq.(29)) differential scattering cross-sections for random binary alloys. They explicitly show how the averages of scattering lengths over nuclear spins and also the random configurations of the constituents together produce the coherent and incoherent inelastic scattering in disordered systems. We get new terms in the scattering cross-sections which depend upon concentration c and the difference $\delta B = B(A) - B(B)$ of scattering lengths. The random changes in masses and force constants in the alloy enter the evaluation of the different types of augmented space averages discussed in the last section.

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FIGURES CAPTIONS

Figs. 1(a) The graph for the $\tilde{K}_{Cl}$ and its dictionary.

(b) The matrix for $\tilde{K}^{eff}_{Cl}$ and its dictionary.

(c) The graphical representation of $\hat{K}_{eff}$ and its dictionary

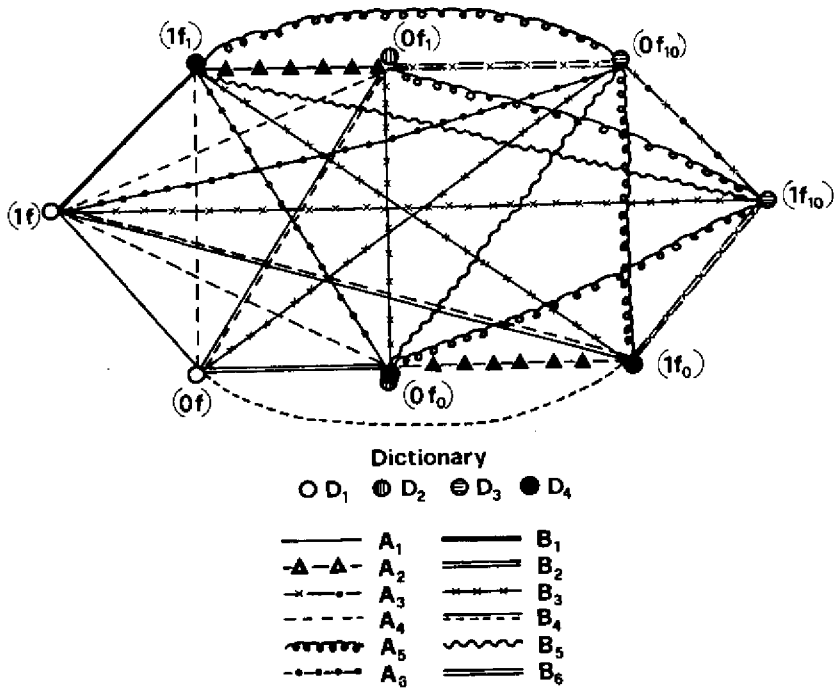

Fig. 1 a

$$
\begin{bmatrix}
D_1 & A_1 & A_4 & B_4 & B_3 & A_6 & A_4 & B_1 \\
A_1 & D_1 & B_1 & A_4 & A_6 & B_3 & B_4 & A_4 \\
A_4 & B_1 & D_3+\sigma_1 & A_2+\sigma_1 & A_5 & B_5 & B_3 & A_6 \\
B_4 & A_4 & A_2+\sigma_1 & D_2+\sigma_0 & B_2 & A_5 & A_6 & B_3 \\
B_3 & A_6 & A_5 & B_2 & D_4+\sigma_0 & A_3+\sigma_1 & A_5 & B_5 \\
A_6 & B_3 & B_5 & A_5 & A_3+\sigma_1 & D_4+\sigma_0 & B_2 & A_5 \\
A_4 & B_4 & B_3 & A_6 & A_5 & B_2 & D_2+\sigma_0 & A_2+\sigma_1 \\
B_1 & A_4 & A_6 & B_3 & B_5 & A_5 & A_2+\sigma_1 & D_3+\sigma_0
\end{bmatrix}
= \underline{\underline{K}}_{eff}
$$

Dictionary

$$\underline{\underline{A}}_1 = \underline{\underline{\phi}}^{BB}_{01} + 2c\,\underline{\underline{\phi}}^{(1)}_{01} + c^2\,\underline{\underline{\phi}}^{(2)}_{01}$$

$$\underline{\underline{A}}_2 = \underline{\underline{\phi}}^{BB}_{01} + \underline{\underline{\phi}}^{(1)}_{01} + c(1-c)\underline{\underline{\phi}}^{(2)}_{01}$$

$$\underline{\underline{A}}_3 = \underline{\underline{\phi}}^{BB}_{01} + 2(1-c)\underline{\underline{\phi}}^{(1)}_{01} + (1-c)^2\underline{\underline{\phi}}^{(2)}_{01}$$

$$\underline{\underline{A}}_4 = \sqrt{c(1-c)}(\underline{\underline{\phi}}^{(1)}_{01} + c\,\underline{\underline{\phi}}^{(2)}_{01})$$

$$\underline{\underline{A}}_5 = \sqrt{c(1-c)}[\underline{\underline{\phi}}^{(1)}_{01} + (1-c)\underline{\underline{\phi}}^{(2)}_{01}]$$

$$\underline{\underline{A}}_6 = c(1-c)[\underline{\underline{\phi}}^{BB}_{01} + \underline{\underline{\phi}}^{(1)}_{01} + c(1-c)\underline{\underline{\phi}}^{(2)}_{01}]$$

$$\underline{\underline{B}}_1 = \sqrt{c(1-c)}[\underline{\underline{\delta m}}\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{(1)}_{00} + c\,\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{B}}_2 = \sqrt{c(1-c)}[m_B\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{(1)}_{00} + (1-c)\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{B}}_3 = c(1-c)[\underline{\underline{\phi}}^{BB}_{00} + \underline{\underline{\phi}}^{(1)}_{00} + c(1-c)\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{B}}_4 = \sqrt{c(1-c)}[\underline{\underline{\phi}}^{(1)}_{00} + c\,\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{B}}_5 = \sqrt{c(1-c)}[\underline{\underline{\phi}}^{(1)}_{00} + (1-c)\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{D}}_1 = m_B\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{BB}_{00} + c[\underline{\underline{\delta m}}\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{(1)}_{00} + c\,\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{D}}_2 = m_B\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{BB}_{00} + (1-c)[\underline{\underline{\delta m}}\omega^2\underline{\underline{I}} + c\,\underline{\underline{\phi}}^{(2)}_{00}] + \underline{\underline{\phi}}^{(1)}_{00}$$

$$\underline{\underline{D}}_3 = m_B\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{BB}_{00} + (1-c)[\underline{\underline{\delta m}}\omega^2\underline{\underline{I}} + 2\underline{\underline{\phi}}^{(1)}_{00} + (1-c)\underline{\underline{\phi}}^{(2)}_{00}]$$

$$\underline{\underline{D}}_4 = m_B\omega^2\underline{\underline{I}} + \underline{\underline{\phi}}^{BB}_{00} + c[\underline{\underline{\delta m}}\omega^2\underline{\underline{I}} + (1-c)\underline{\underline{\phi}}^{(2)}_{00}] + \underline{\underline{\phi}}^{(1)}_{00}$$

$$\underline{\underline{g}} = \underline{\underline{K}}^{(1)}_{eff}\,\underline{\underline{G}}\,\underline{\underline{K}}^{(1)}_{eff}$$

Fig.1(b)

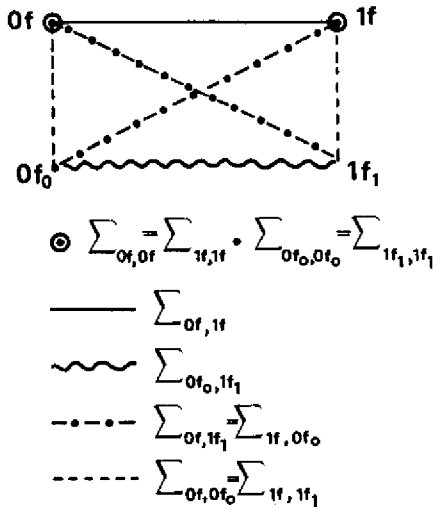
0f
1f
$0f_0$
$1f_1$
$\sum_{0f,0f} = \sum_{1f,1f}$ • $\sum_{0f_0,0f_0} = \sum_{1f_1,1f_1}$
$\sum_{0f,1f}$
$\sum_{0f_0,1f_1}$
$\sum_{0f,1f_1} = \sum_{1f,0f_0}$
$\sum_{0f,0f_0} = \sum_{1f,1f_1}$

Fig.1 c