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NEUTRON SCATTERING IN DISORDERED ALLOYS: COHERENT AND INCOHERENT INTENSITIES *

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ABSTRACT

A priori it is not clear how to split the total intensity of thermal neutron scattering from disordered alloys into a coherent and an incoherent part. We present here a formalism to do this. The formalism is based on the augmented space technique introduced earlier by one of the authors. It includes disorder in mass, force constants and scattering lengths. A self-consistent CCPA which is tractable for realistic calculations is presented for the coherent and incoherent intensities. This is expected to prove useful in theoretically analysis data for alloys (e.g. Ni_xPt_{1-x}, Ni_xPd_{1-x}, Ni_xCr_{1-x}) for which it is necessary to go beyond the usual single site CPAs for reliable accuracy.

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I. INTRODUCTION

The interaction between neutrons and condensed matter has yielded valuable information regarding elementary excitations in solids and liquids. While a detailed and 'rigorous' theory exists in the case of perfect crystals [1)-3)], that for random alloys has achieved only limited success [4),5)]. The problem is two-fold: one of formulation and the other of actual implementation. In a random alloy it is not clear, a priori, how to separate out the total cross-section into a coherent and an incoherent part. Recently, Nowak and Dederichs [5)] have answered this question using the Yonezawa-Matsubara diagrammatic technique. They have correctly argued that the incoherent part is the sum of all irreducible diagrams and contains only short-ranged correlations. The coherent part then may be expressed as a product of the usual configuration averaged Greeen function and the square of an effective scattering length, which is itself given by irreducible diagrams closely related to those for the self-energy. The problem of implementation in realistic situations remains. The above quoted work indicated how to obtain the coherent and incoherent intensities within the single site coherent potential approximation (CPA). However, in many real situations (e.g. Ni_xPt_{1-x}, Ni_xPd_{1-x}, Ni_xCr_{1-x}) [6)] the CPA fails to handle random masses, force constants and scattering lengths accurately at the same time. An additional difficulty is the incorporation of the force constant sum rule, except in an average sense. The simple relation $\phi_{AA} + \phi_{BB} - 2\phi_{AB} = 0$ used by most authors [7)] to simplify the CPA equations, is hardly applicable in any real alloy. Again, having formulated a diagrammatic technique in principle, it must be recognized that the formalism becomes cumbersome and virtually intractable as to generalize to, say, a nearest neighbour cluster coherent potential approximation (CCPA) (9 sites on a bcc, 13 on a fcc lattice). Even for the 2CPA, the diagram summation is formidable and any mishandling of the diagrams or further approximations leads to serious analytic difficulties [8)].

The success in handling some of the above difficulties within the 'augmented space' technique [9)-11)] encourages us to attempt to formulate the problem in that language. Earlier [12)], the author has shown that diagrams equivalent to the Yonezawa-Matsubara diagrams may be generated in augmented space and has established the relation between diagrams and 'walks' on the augmented 'space lattice'. We shall develop a formulation for splitting the total intensity into coherent and incoherent parts, and show that our result is identical to that of Nowak and Dederichs. But more, we indicate that a CCPA using our method is no more difficult to implement than the actual applications already made by us in other contexts [6),10)]. This is the major point of this work.

II. FORMALISM

Let us begin by writing down a formal expression for the inelastic cross-section for the scattering of a thermal neutron from a state $\vec{k}$ to a state $\vec{k}'$ with a change in energy $E = \hbar\omega = \frac{\hbar^2}{2M_n}(k^2 - k'^2)$ and change in wave-vector $\vec{q} = \vec{k} - \vec{k}' + \vec{Q}$, $\vec{Q}$ being a reciprocal lattice vector

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{2\pi\hbar}\frac{k'}{k}\sum_{i}\sum_{j}\sum_{\mu}\sum_{\nu} b_i b_j\, q^\mu q^\nu\, e^{i\underline{q}\cdot(\underline{r}_i - \underline{r}_j)}\, \mathrm{Im}\, G_{ij}^{\mu\nu}(\omega)\, n(\omega) \qquad (1)$$

where

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

w_j is the scattering length of the j^{th} nucleus (for simplicity we assume one atom per unit cell);
$\vec{r}_j$ is the equilibrium position of the j^{th} atom;
$\vec{x}_j = \vec{r}_j + \vec{u}_j(t)$ is the actual position of the j^{th} atom at time 't';
$G_{ij}^{\mu\nu}(\omega) = \int dt\, e^{i\omega t}\, i\theta(t) \langle [u_i^\mu(t)\, u_j^\nu(0)] \rangle_{th}$ is the Green function which satisfies

$$\sum_{s}\sum_{\nu}(m_i\omega^2\delta_{is}\delta_{\mu\nu} - \phi_{is}^{\mu\nu})\, G_{sj}^{\nu\xi}(\omega) = \delta_{ij}\,\delta_{\mu\xi} \qquad (2)$$

$$n(\omega) = (e^{\beta\omega} - 1)^{-1}$$

In a random alloy, w_j, the Debye-Waller factor, the atomic mass m_i and the force constant matrices $\phi_{ij}^{\mu\nu}$ are random-variables all dependent on one another via the random occupation variable of the sites. We have to carry out averaging over nuclear spins as well as random configurations

$$\left\langle \frac{d^2\sigma}{d\Omega dE} \right\rangle = \frac{1}{2\pi\hbar}\frac{k'}{k}\sum_{i}\sum_{j}\sum_{\mu}\sum_{\nu} q^\mu q^\nu\, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}\, n(\omega)\, \mathrm{Im}\langle \overline{b_i b_j} G_{ij}\rangle \qquad (3)$$

where $\overline{b_i b_j}$ denotes averaging over nuclear spins and $\langle\ldots\rangle$ configuration averaging.

The various random variables may now be expressed in terms of

$$n_i = \begin{cases} 1 & \text{if site labelled } i \text{ is occupied by an A-type atom} \\ 0 & \text{if " " " " " by a B-type atom} \end{cases} . \qquad (4)$$

This occupation is suitable for a binary alloy. In the case of completely random alloy A_cB_{1-c}, the probability density of n_i is given by

$$P(n_i) = c\,\delta(n_i - 1) + (1 - c)\,\delta(n_i) . \qquad (5)$$

Then

$$m_i = m_B + (m_A - m_B)n_i$$

and for $i \neq j$

$$\phi_{ij} = \phi_{ij}^{BB} + \phi_{ij}^{(1)} n_i n_j + \phi_{ij}^{(2)}(n_i + n_j)$$

with

$$\phi_{ij}^{(1)} = \phi_{ij}^{BB} + \phi_{ij}^{AA} - 2\phi_{ij}^{AB} \qquad \text{which is not zero in general}$$

and

$$\phi_{ij}^{(2)} = \phi_{ij}^{AB} - \phi_{ij}^{BB} \qquad (6)$$

The implicit assumption in earlier works [5),7)] that $\phi_{ij}^{(1)} = 0$ omits interesting off-diagonal disorder effects and reduces the random part of the dynamical matrix into one depending on single site occupation variables.

One also has the sum rule

$$\sum_j \phi_{ij} = 0 \quad \Rightarrow \quad \phi_{ii} = -\sum_{j\neq i}\phi_{ij} \qquad (7)$$

If we introduce projection and transfer operators $\underline{P}_i = |\vec{r}_i\rangle\langle\vec{r}_j|$ and $\underline{T}_{ij} = |\vec{r}_i\rangle\langle\vec{r}_j|$ we may rewrite (2) as

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

with

$$\underline{K} = \underline{K}_B + \sum_i \Big[(m_A - m_B)\omega^2 n_i \underline{P}_i \underline{I} - \sum_{s\neq i} \Big\{ \underline{\phi}^{(2)}_{is}(n_i + n_s) + \underline{\phi}^{(1)}_{is} n_i n_s \Big\} \Big]$$

$$+ \sum_{i\neq j} \sum \Big\{ \underline{\phi}^{(2)}_{ij} (n_i + n_j) + \underline{\phi}^{(1)}_{ij} n_i n_j \Big\} \underline{T}_{ij} \qquad (8)$$

$\underline{K}_B$ is the dynamical matrix of the 'solvent' B.

The augmented space development of (8) has now been discussed in great detail in several papers [10),11),1.)] and the reader is referred to these earlier works for the details. We note here the main steps.

In the absence of short-ranged order, we may write

$$P(n_i) = -\frac{1}{\pi} \operatorname{Im} \langle \gamma_0^{(i)} | [(n_i + i0^+)\underline{I} - \underline{M}_i]^{-1} | \gamma_0^{(i)} \rangle \qquad (9a)$$

where $\underline{M}_i \in \psi^{(i)}$ of rank two, spanned by $\gamma_0^{(i)}$ and $\gamma_1^{(1)}$. It has a representation

$$\underline{M}_i = \begin{vmatrix} 0 & \sqrt{c(1-c)} \\ \sqrt{c(1-c)} & 1-c \end{vmatrix} \qquad (9b)$$

Again

$$b_i = b_i(B) + \delta b_i \, n_i$$
$$\delta b_i = b_i(A) - b_i(B)$$

Then

$$\langle \overline{b_i b_j} G_{ij} \rangle = \overline{b_i(B) b_j(B)} \langle G_{ij} \rangle + \overline{b_i(B)\, \delta b_j} \langle n_i G_{ij} \rangle$$

$$+ \overline{\delta b_i b_j(B)} \langle G_{ij} n_j \rangle + \overline{\delta b_i \delta b_j} \langle n_i G_{ij} n_j \rangle \qquad (10)$$

Within the augmented space formalism, it was shown [9)] that

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

$$|\gamma_0\rangle = \prod_i^{\otimes} |\gamma_0^{(i)}\rangle \qquad \Psi = \prod^{\otimes} \psi^{(i)} \qquad (11a)$$

$$\underline{\tilde{K}} = \underline{K}_B \otimes \underline{I} + \sum_i (m_A - m_B) w^2 \underline{P}_i \otimes \underline{M}^{(i)} - \sum_i \sum_{s\neq i} \Big\{ \underline{\phi}^{(2)}_{is} \underline{P}_i \otimes (\underline{M}^{(i)} + \underline{M}^{(s)}) + \underline{\phi}^{(1)}_{is} \underline{P}_i \otimes \underline{M}^{(is)} \Big\} + \sum_{j\neq i} \sum \Big\{ \underline{\phi}^{(2)}_{ij} \underline{T}_{ij} \otimes (\underline{M}^{(i)} + \underline{M}^{(j)}) + \underline{\phi}^{(1)}_{ij} \underline{T}_{ij} \otimes \underline{M}^{(ij)} \Big\} \qquad (11b)$$

$$\left.\begin{aligned} \underline{M}^{(i)} &= I \otimes \cdots \otimes \underline{M}_i \otimes \cdots I \\ \underline{M}^{(ij)} &= \underline{I} \otimes \cdots \otimes \underline{M}_i \otimes \cdots M_j \otimes \cdots I \end{aligned}\right\} \quad \text{are operators on } \underline{\Psi} \qquad (11c)$$

and $\underline{\tilde{G}} \in \mathcal{H} \otimes \underline{\Psi}$, where $\mathcal{H}$ is the Hilbert space spanned by $\{|\vec{r}_i\rangle\}$. Further

$$\langle n_i G_{ij} \rangle = \langle \vec{r}_i \otimes \gamma_0 | \underline{M}^{(i)} \otimes \underline{\tilde{G}}(w) | \vec{r}_j \times \gamma_0 \rangle$$

$$\langle G_{ij} n_j \rangle = \langle \vec{r}_i \otimes \gamma_0 | \underline{\tilde{G}}(w) \otimes \underline{M}^{(j)} | \vec{r}_j \otimes \gamma_0 \rangle$$

$$\langle n_i G_{ij} n_j \rangle = \langle \vec{r}_i \otimes \gamma_0 | \underline{M}^{(i)} \otimes \underline{\tilde{G}}(w) \otimes \underline{M}^{(j)} | \vec{r}_j \otimes \gamma_0 \rangle \qquad (11d)$$

III. THE SCATTERING DIAGRAMS: COHERENT AND INCOHERENT INTENSITIES

In order to obtain scattering diagrams, let us again refer to the methodology described in detail in earlier works [12)]. In the interaction picture

$$\tilde{K}_0 = -\sum_i \sum_{a\neq i} \langle \phi_{ia} \rangle \; a^\dagger(x_i)a(x_i) + \sum_{i\neq j}\sum \langle \phi_{ij} \rangle \; a^\dagger(x_i)a(x_j)$$

$$\tilde{K}_1(t) = \sum_{\underline{x}} \int dy \sum_{\lambda\neq\lambda'} a^\dagger(x)a(x)U_1(x;y)\; B^\dagger_\lambda(y)\; B_{\lambda'}(y)$$

$$+\sum_{\underline{xy}}\sum \int dz \int du \sum_{\lambda\neq\lambda'} \sum a^\dagger(x)a(y)U_2(xy;zu)\left[\; B^\dagger_\lambda(z)B_{\lambda'}(z)+B^\dagger_\lambda(u)B_{\lambda'}(u)\right]$$

$$+\sum_{\underline{xy}}\sum \int dz \int du \sum_{\lambda_1\neq\lambda_2}\sum_{\lambda_3\neq\lambda_4}\sum\sum a^\dagger(x)a\;(y)U_3(xy;zu)\; B^\dagger_{\lambda_1}(z)B_{\lambda_2}(z)B^\dagger_{\lambda_3}(u)B_{\lambda_4}(u)$$

$$-\sum_{\underline{x}} \int dz \int du \sum_{\lambda_1\neq\lambda_2}\sum_{\lambda_3\neq\lambda_4}\sum\sum a^\dagger(x)a(x)\; U_3(xy;zu)\; B^\dagger_{\lambda_1}(z)B_{\lambda_2}(z)B^\dagger_{\lambda_3}(u)B_{\lambda_4}(u) \qquad (12)$$

where $x = (\underline{x},t_x)$; $\int dy = \sum_{\underline{y}} \int dt_y$; $\lambda : \uparrow$ or $\downarrow$;

a^+,a are particle creation/destruction operators (phonons);

$B^+_\uparrow = c^{1/2}b^+_\uparrow$, $B^+_\downarrow = (1-c)^{1/2}\, b^+_\downarrow$ are the creation operators for pseudo-fermions associated with local configurations

and the vertices

$$U_1(x;y) = (m_A-m_B)\; w^2\delta(x-y) \; - 2\sum_{\underline{y}} \phi^{(2)}(\underline{x}-\underline{y})\; \delta(t_x-t_y)$$

$$U_2(xy;zu) = \phi^{(2)}(\underline{x}-\underline{y})\; \delta(t_x-t_y)\; \delta(z-u)\; \{\; \delta(z-x) + \delta(u-y)\}$$

$$U_3(xy;zu) = \phi^{(1)}(\underline{x}-\underline{y})\; \delta(t_x-t_y)\; \delta(z-x)\; \delta(u-y) \qquad (13)$$

We have represented interaction vertices, in general, as full four-centre vertices, but (13) indicates that in particular cases they may be completely diagonal (as in the original Yonezawa-Matsubara work with diagonal disorder) or two centre vertices. We may represent these vertices $\square$ as in earlier works [12]

$$\langle \overline{b_i b_j} G_{ij} \rangle = \left\{ \overline{b(B)}^2 + 2c\; \overline{b(B)}\; \overline{\delta b} \; + c^2\overline{\delta b}^2 \right\} \phi^{(1)}_{ij}$$

$$+ \left\{ \overline{b(B)}\; \overline{\delta b} + c\; \overline{\delta b}^2 \right\} (\phi^{(2)}_{ij} + \phi^{(3)}_{ij}) \; + \overline{\delta b}^2\; \phi^{(4)}_{ij}$$

$$+ \Big[\left\{ \overline{(b(B)^2} - \overline{b(B)}^2) + 2c(\overline{b(B)\delta b} - \overline{b(B)}\; \overline{\delta b}) + c^2(\overline{\delta b^2} - \overline{\delta b}^2) \right\} \phi^{(1)}_{ii}$$

$$+ \left\{ \overline{(b(B)-\overline{b(B)})(\delta b - \overline{\delta b})} + c\overline{(\delta b - \overline{\delta b})^2} \right\} (\phi^{(2)}_{ii} + \phi^{(3)}_{ii})$$

$$+ \overline{(\delta b - \overline{\delta b})^2}\; \phi^{(4)}_{ii} \Big] \delta_{ij} \qquad (14)$$

where, as described in [12] we have, $x = (\underline{x},t_x)$, $y = (\underline{y},t_y)$

$$\phi^{(1)}_{ij} = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1..dt_n \langle 0 |\; T\tilde{K}_1(t_1)..\tilde{K}_1(t_n)a(x)a^\dagger(y)\; | 0\rangle_{conn} \qquad (15a)$$

$$\phi^{(2)}_{ij} = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1..dt_n \langle 0 |\; TB^\dagger_\uparrow(x)B_\downarrow(x)\tilde{K}_1(t_1)..\tilde{K}_1(t_n)a(x)a^\dagger(y)\; | 0\rangle_{conn} \qquad (15b)$$

$$\phi^{(3)}_{ij} = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1..dt_n \langle 0 |\; T\tilde{K}_1(t_1)..\tilde{K}_n(t_n)a(x)a^\dagger(y)B^\dagger_\downarrow(y)B_\uparrow(y)\; | 0\rangle_{conn} \qquad (15c)$$

$$\phi^{(4)}_{ij} \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1..dt_n \langle 0 | TB_\uparrow(x)B_\downarrow(x)\tilde{K}_1(t_1)..\tilde{K}_1(t_n)a(x)a^\dagger(y)B^\dagger_\downarrow(y)B_\uparrow(y)\; | 0\rangle_{conn} \qquad (15d)$$

Note that the 'disorder' propagators

$$g_{\uparrow\uparrow}(x,y) = -\,i\,c\;\Theta(t_x-t_y)\;\delta(\underline{x}-\underline{y})$$

$$g_{\downarrow\downarrow}(x,y) = -i(1-c)\;\Theta(t_y-t_x)\;\delta(\underline{x}-\underline{y}) \qquad (16)$$

are both site diagonal, reflecting the fact that the basic random variable n_i is itself site diagonal. The 'vacuum' configuration is one with $\uparrow$ at all sites.

Let us now examine the various terms in (14). The coefficient of the first term may be written as $\langle \bar{b} \rangle^2$ with $\langle \bar{b} \rangle = \overline{b(B)}(1-c) + \overline{b(A)}\, c$, so that it is clear that it contributes only to coherent scattering with an average scattering length $\langle \bar{b} \rangle = b_{coh}^{av}$. As $c = 0$ or 1 it reduces to the coherent scattering length of the pure species. To obtain scattering diagrams, let us represent the diagonal vertices $\overline{b(B)}$ by ◍ and $\overline{\delta b}$ as ▧. The three terms associated with the first expression are shown in Fig.1(a) and Fig.1(b).

Coming now to the second set of expressions in (14), we may generate the diagrams using (15b) and (15c). These are shown in Fig.1(c). Examination shows that all such diagrams are reducible, and as such using the ideas set forth in Ref.7 contribute to the coherent intensity.

The third set of expressions in (14), in conjuction with (15d) yield two types of diagrams as shown in Fig.1(d). A reducible set [1(d)(i)] which contribute to the coherent scattering, and an irreducible set [1(d)(ii)] which by the arguments of Nowak and Dederichs, are short-ranged and contribute to the incoherent scattering intensity.

The remaining expressions in (14) are all short-ranged. The contributions are identical to Figs.1(a),(c),(di) and (dii) with ◍ and ▨ replaced by ● and ■ which have appropriate contributions as indicated from the last three diagonal terms in (14). Coming back, collecting together diagrams in Figs.1(a), (c) and (dii) we note that the coherent intensity may be written in terms of $\sum_m \sum_n \underline{b}_{im}^{eff} \langle \underline{G}_{mn} \rangle \underline{b}_{nj}^{eff}$, where the diagrams for $\underline{b}^{eff}(\omega)$ are shown in Fig.2(a). Comparing them with the diagrams for the self-energy $\underline{\Sigma}$ as shown in Fig.2(b), we note that they are identical with only the first vertex ▨ instead of □. Thus $\underline{b}^{eff}$ is both ω and $\vec{k}$ dependent (except in the case of a 1CPA, where it is site diagonal and so $\vec{k}$ independent). In any CCPA, the same kind of approximations used for $\underline{\Sigma}$ should be also used for $\underline{b}^{eff}$. Any method that yields incorrect analytic properties for $\underline{\Sigma}$ will also fail for $\underline{b}^{eff}$.

The irreducible diagram contribution to the incoherent scattering also is closely related to the diagrams for $\underline{\Sigma}$. Both the initial and final vertices are ▨ (■) instead of □ and the first order diagram (which is a function of 'c' alone) is missing. We shall indicate this contribution as $\Gamma^{\mu\nu}(\omega)$.

IV. CCPA CALCULATIONS FOR $\underline{\Sigma}$, $\underline{b}^{eff}$ AND $\underline{\Gamma}$

The details of the calculation of $\underline{\Sigma}$ in cluster CP approximations have been given earlier [10),11)]. However, it is relevant here to recall the principal ideas behind the method of 'walks" on the augmented space lattice.

The lattice is generated by associating a 'vertex' with each member of the basis $\{|\vec{r}_i \otimes \gamma\rangle\}$ in augmented space $\mathcal{H} \otimes \Psi$. The 'walks' or 'paths' then are generated by 'linking' these vertices whenever the matrix elements of $\hat{\underline{K}}$ between them is non-zero.

The Green function $\langle G_{ij} \rangle = \sum_{n=0}^{\infty} \sum_{\mathcal{P}_n} \kappa(\mathcal{P}_n^{ij})$, where $\mathcal{P}_n^{ij}$ are all non-intersecting paths from $\vec{r}_i \otimes \gamma$ to $\vec{r}_j \otimes \gamma$ of length 'n', $\mathcal{P}_n$ is the set of all such paths of length 'n' and κ is the contribution of one such a path. The expression for the contribution follows from the Feenberg renormalized perturbation expansion.

The CCPA involved delinking all walks that connect points within a cluster and without and which does not lie entirely in $\mathcal{H}$.

Proof and justification of the above statements have already been published [10)-12)] and we shall only recall them for our use.

Calculation of $\underline{\Sigma}$ on the delinked graph is closely related to the usual CCPA ideas. The 'exact' cluster of a particular configuration is immersed in a medium whose 'effective' dynamical matrix $\underline{K}_{eff}(\omega)$ is to be determined self-consistently via

$$\langle \underline{G}(\underline{K}_{cl};\underline{K}_{eff}) \rangle_{cl} = \underline{G}(\underline{K}_{eff}) \qquad (17)$$

The self-energy is $\underline{K}_{eff} = \underline{K}_B + \underline{\Sigma}$. Schematically,

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

Randomness exists only in the cluster subspace. Going over to augmented space then, the configuration span Ψ_{cl} is of rank 2^N, N being the cluster size

The $\underline{\Gamma}$ is short-ranged with non-zero matrix elements only between sites within one cluster.

This completes the self-consistent calculation for $\underline{\Sigma}$, $\underline{b}^{eff}$ and $\underline{\Gamma}$. Once this is done

$$\left\langle \frac{d^2\sigma}{d\Omega dE} \right\rangle_{coh} = \frac{1}{2\pi\hbar} \frac{k'}{k} \sum_{\mu} \sum_{\nu} q^{\mu} q^{\nu} \, \mathrm{Im} \left\{ \underline{b}_{eff}(q,w) \;\; \underline{G}(q,w) \;\; \underline{b}_{eff}(q,w) \right\}^{\mu\nu}$$

$$\left\langle \frac{d^2\sigma}{d\Omega dE} \right\rangle_{inc} = \frac{N}{2\pi\hbar} \frac{k'}{k} \sum_{\underline{r}} \sum_{\mu\nu} q^{\mu} q^{\nu} \, \mathrm{Im} \left\{ \underline{\Gamma}(\underline{r},w) \right\}^{\mu\nu} \qquad (23)$$

$\vec{r} = \vec{r}_i - \vec{r}_j$, where $\vec{r}_i$, $\vec{r}_j$ belong to the same cluster. $\vec{r}$ takes n_{cl} values where n is the cluster size.

V. SUMMARY

We have described how to obtain an explicit splitting of the total intensity in a thermal neutron scattering from disordered alloys into a coherent and an incoherent part. The formalism is within the augmented space method introduced by one of us. In essence the splitting is identical to that introduced by Nowak and Dederichs [5] within a Yonezawa-Matsubara diagram technique. Whereas the diagram technique is exceedingly difficult to generalize into cluster-CPA, indeed may become intractable for large clusters, the walk-contribution formalism on the augmented space has, for the case of density of states, proved to be practicable with modern computers [10]. We indicate how to calculate the coherent and incoherent intensities with a walk-contribution technique. Except for the restrictions of the Fermi pseudopotential and the Born approximation inherent in the formulation of the scattering cross-section, our formalism has no other restrictions on concentration values, arbitrary changes in force constants, etc. The force constant sum rule is incorporated before averaging. The CCPA yields herglotz results. These are several examples of alloys, where there are large differences in constituent masses and force constants which necessitate going beyond the single particle CPAs. One such class of alloys is Ni_xPt_{1-x}, Ni_xPd_{1-x} and Ni_xCr_{1-x} [6]. Detailed neutron scattering results are available on these alloys. The present formalism should prove useful in theoretical analysis of the data.

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TABLE

DICTIONARY FOR FIG.3

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

$$\underline{A}_2 = \underline{\phi}_{01}^{BB} + \underline{\phi}_{01}^{(1)} + c(1-c)\,\underline{\phi}_{01}^{(2)} + \underline{\sigma}_1$$

$$\underline{A}_3 = \underline{\phi}_{01}^{BB} + (1-c)\,\underline{\phi}_{01}^{(1)} + (1-c)\,\underline{\phi}_{01}^{(2)} + \underline{\sigma}_1$$

$$\underline{A}_4 = \sqrt{c(1-c)}\,(\underline{\phi}_{01}^{(1)} + c\,\underline{\phi}_{01}^{(2)}) \qquad \underline{A}_5 = \sqrt{c(1-c)}\,(\underline{\phi}_{01}^{(1)} + (1-c)\underline{\phi}_{01}^{(2)})$$

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

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

$$\underline{B}_2 = \sqrt{c(1-c)}\left[m_B w^2 \underline{I} + \underline{\phi}_{00}^{(1)} + (1-c)\underline{\phi}_{00}^{(2)}\right] \qquad \underline{B}_2' = \overline{\delta b}\ \underline{I} \qquad B_2'' = (\overline{\delta b^2})^{1/2}\ \underline{I}$$

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

$$\underline{B}_4 = \sqrt{c(1-c)}\left[\underline{\phi}_{00}^{(1)} + c\,\underline{\phi}_{00}^{(2)}\right] \qquad \underline{B}_5 = \sqrt{c(1-c)}\,\underline{I}\,\underline{\phi}_{00}^{(1)} + (1-c)\,\underline{\phi}_{00}^{(2)}\right]$$

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

$$\underline{D}_1' = \overline{b(B)}\ \underline{I} \qquad \underline{D}_1'' = \left[\left\{\overline{\langle b(B)\rangle^2} - \langle\overline{b(B)}^2\rangle\right\}^{1/2} + b_{inc}\right] \underline{I}$$

$$\underline{D}_2 = m_B w^2 \underline{I} + \underline{\phi}_{00}^{BB} + (1-c)\left[\delta m\, w^2 \underline{I} + c\,\underline{\phi}_{00}^{(2)}\right] + \underline{\phi}_{00}^{(1)} + \underline{\sigma}_0$$

$$\underline{D}_3 = m_B w^2 \underline{I} + \underline{\phi}_{00}^{BB} + (1-c)\left[\delta m\, w^2 \underline{I} + 2\,\underline{\phi}_{00}^{(1)} + (1-c)\,\underline{\phi}_{00}^{(2)}\right] + \underline{\sigma}_0$$

$$\underline{D}_4 = m_B w^2 \underline{I} + \underline{\phi}_{00}^{BB} + c\left[\delta m\, w^2 \underline{I} + (1-c)\,\underline{\phi}_{00}^{(1)}\right] + \underline{\phi}_{00}^{(2)} + \underline{\sigma}_0$$

$$\underline{\sigma} = \underline{K}_{eff}^{(1)}\ \underline{\Omega}\ \underline{K}_{eff}^{(1)}$$

FIGURE CAPTIONS

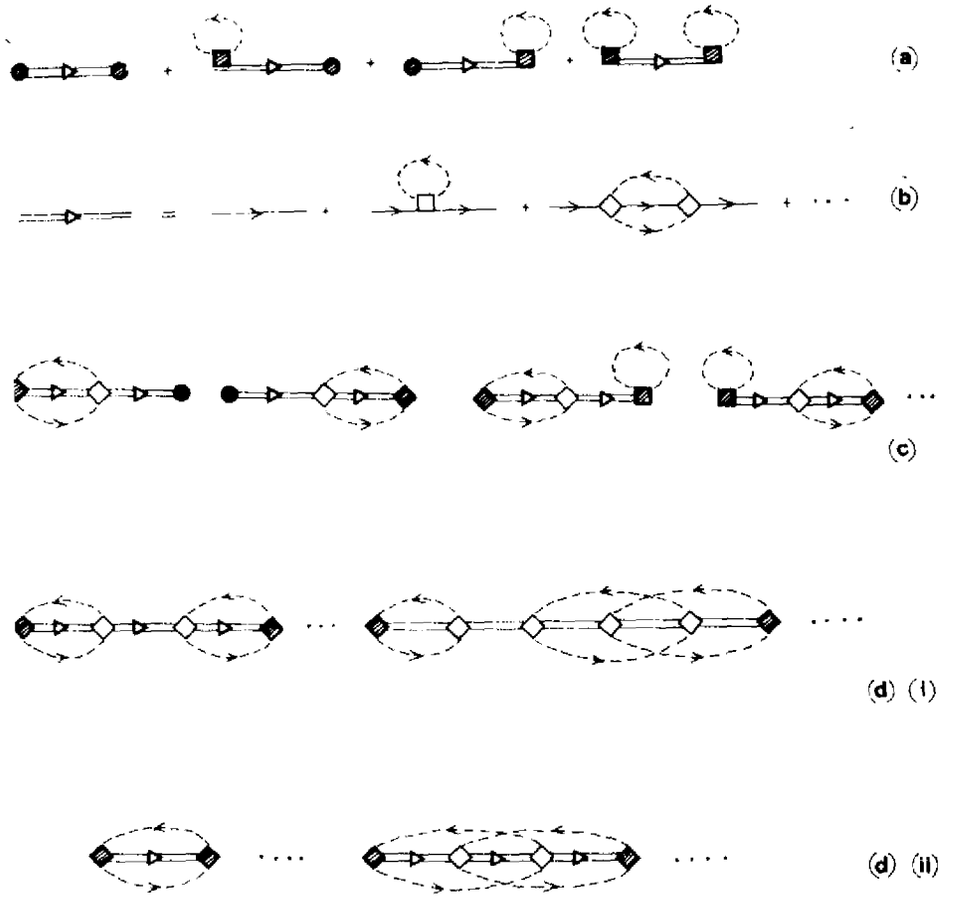
Figs.1 - Scattering diagrams in augmented space for the set of the first three terms in Eq.(14b).

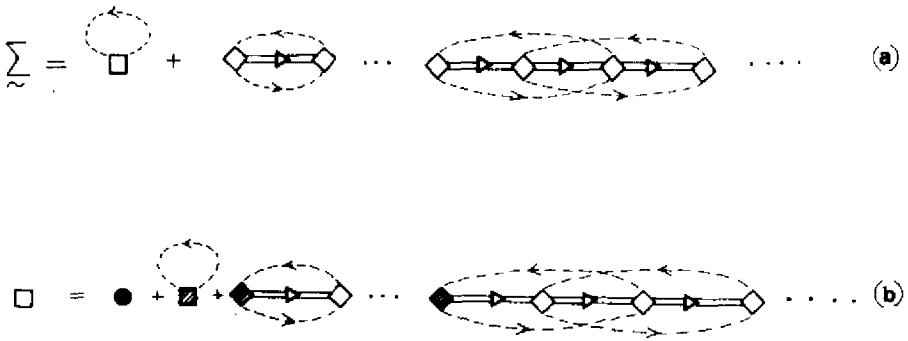
Figs.2 - The scattering diagrams for $\underline{\Sigma}$ and $\underline{b}^{eff}$.

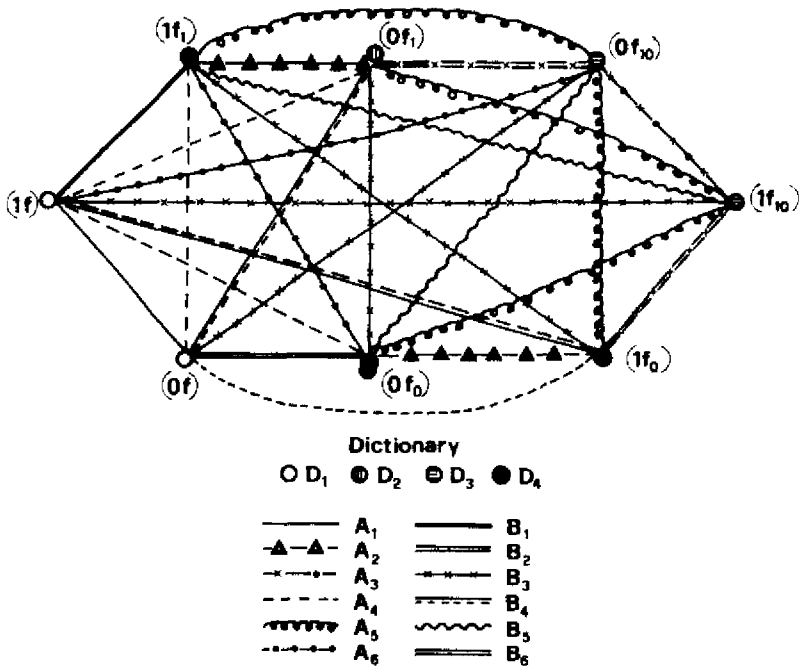
Fig.3(a) - The graph for $\underline{\Sigma}$ in augmented space.

(b) - The graph for $\underline{b}^{eff}$ in augmented space.

(c) - The graph for the incoherent intensity in augmented space.




(a)
(b)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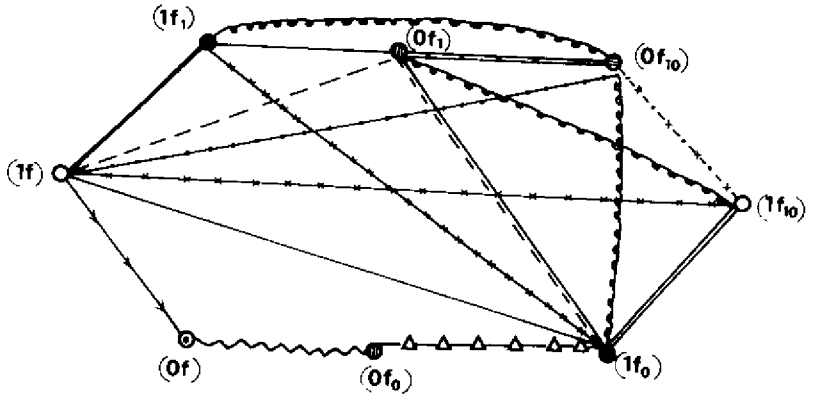
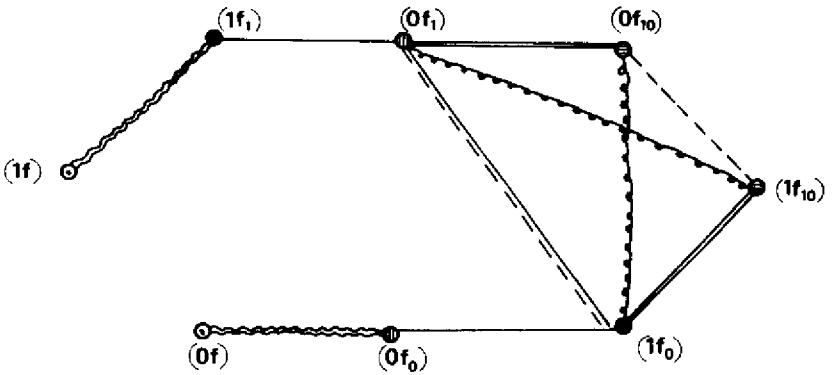
Dictionary
O D1 D2 D3 D4
A1 B1
A2 B2
A3 B3
A4 B4
A5 B5
A6 B6



Dictionary

B_2' ⊙ D_1'



Dictionary

B_2'' ⊙ D_2''