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Status Report on the B1T Program, -
Provides Thermal-Neutron Flux and Current Spectra,
Isotropic and Anisotropic Group Cross Sections

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Status Report on the BLT Program,
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I. INTRODUCTION

WANL broad group cross sections are obtained using an iterative procedure. The GAM⁽¹⁾, QUERY⁽²⁾, and TNS⁽³⁾ slowing down programs are used to calculate fine group fluxes and currents and subsequently to obtain multigroup cross sections. Using these cross sections, more realistic fluxes and currents are then obtained for any particular physical situation from a multigroup transport calculation. These better flux and current distributions are used by the GAM and TNS codes along with the GAM and TNS cross section libraries to obtain final broad group cross sections. The fluxes and currents that are obtained from the transport calculation are "broad-group" quantities and some interpolation scheme must be used to obtain the fine group fluxes and currents that are required as input to GAM and TNS. The GAM-QUERY programs are used for the energy range above thermal up to 10 Mev and TNS is used for the "thermal" energy range, usually from 0 - 1.86 ev, however, it may be used up to 2.38 ev. GAM provides initial fluxes and currents for cross section averaging through the solution of the time independent Boltzmann equation in the P(1) or B(1) approximation when a buckling term is input. Resonance absorption including the effects of Doppler Broadening is treated with the QUERY program; a temperature must be specified and resonance parameters are needed in the cross section library. TNS is used to calculate the thermal neutron flux for an

infinite homogenous isotropic medium, i.e. spatial and angular dependencies are ignored⁽⁴⁾. "Up-scattering" is included, of course, in the TNS calculation, but is unimportant in the GAM energy range and is ignored in GAM calculations. The source of neutrons in the thermal range arises from "down-scattering" from the GAM energy range; whereas neutrons are born in the GAM energy range as a result of the fission process. Cross sections in the TNS library are input pointwise, i.e. there is a cross section value input for each microscopic energy group, and no use is made of resonance parameters. In order to account for temperature effects in the TNS calculation the cross sections must be calculated externally and input into the library for every temperature that is to be considered.

In this status report a new program, BLT, is described. A set of equations that provide for the calculation of the thermal neutron spectrum (fluxes and currents) in the P(1) or B(1) approximation consistent with the GAM type of calculation are presented along with the method of solution. Since we wish to retain the same energy mesh that exists in the TNS library there are 99 energy points over the thermal range. Hence a set of $2 \times 99 = 198$ equations must be solved for 198 unknowns. However, the fluxes and currents can be separated so that two sets of equations each consisting of 99 equations and 99 unknowns must be solved. The Westinghouse program ISIMEQ⁽⁵⁾ (Gauss elimination method) has been successfully tested for solving such sets of equations, and it is used in the BLT program. In addition to treating the angular dependence, BLT differs from TNS in that resonance parameters may be

input and the Doppler broadened cross sections calculated when the temperature is specified. Doppler broadened cross sections are calculated using EXT⁽⁶⁾ which has been in operation at WANL. Furthermore, all nuclei are treated the same in the BlT program unlike the TNS program where nuclei are classified as moderators or absorbers and where the cross sections required in the library differ depending on the classification. The following paragraphs explain the need for this more accurate thermal cross section calculation.

For low neutron energies crystalline binding effects are important and scattering cross sections can be quite anisotropic. For example, there are discontinuous increases in the coherent elastic scattering cross section at certain neutron energies in polycrystalline materials. This increase occurs when a new set of lattice planes can contribute to the scattering and is, therefore, extremely anisotropic. Whether the crystalline binding effects are important or not depends on the physical situation. For example, in a NERVA type reactor there is an annular Be reflector, which is cooled by liquid H₂, surrounding the core. If the neutron flux is characterized by the core temperature ($\sim 2000^{\circ}\text{C}$) binding effects are probably not important, however if the neutron flux is characterized by the temperature of liquid H₂ ($\sim -253^{\circ}\text{C}$) binding effects are extremely important. Aside from crystalline effects anisotropic scattering can also be important for nuclei having a small mass number (e.g. hydrogen).

Also, at the extremely high temperatures at which the NERVA reactor core operates the resonance absorption cross sections will be affected by the Doppler effect even in the thermal range.

The crystalline neutron scattering cross sections required for input to BLT will be obtained from HEXSCAT⁽⁷⁾, SUMMIT⁽⁸⁾, and FLANGE⁽⁹⁾. The program HEXSCAT which is in operation at WANL provides the P(0) and P(1) transfer matrices for polycrystalline coherent elastic scattering. The program in operation at WANL at present for providing the crystalline inelastic scattering cross section (SUMMIT-incoherent approximation) does not calculate the P(1) transfer matrix. However, evaluated inelastic scattering law $S(\alpha, \beta)$ decks (obtained from the GASKET⁽⁹⁾ program) are available in the ENDF at Brookhaven, and the FLANGE program which is in operation at WANL can be used to obtain the P(0) and P(1) transfer matrices from these decks. In addition, A. S. Johnston at this lab is working on crystalline scattering⁽¹⁰⁾ cross sections based on a coherent theory.

An option will also provide for generating the P(0) and P(1) scattering kernels from a free-gas scattering model. This will be done by a modification of WANL's SIGGAS⁽¹¹⁾ program.

At present there are no plans for calculating and printing out the transport approximation cross sections, only the group cross sections required for an explicit P(1) calculation will be made available.

A report will be issued giving the program listing, input quantities, etc. after it has been adequately debugged, and after a reasonable cross section library is available. Any suggested changes in the printout quantities, etc. as described in this status report may be incorporated into the program.

II. EQUATIONS FOR FLUXES AND CURRENTS AND METHOD OF SOLUTION

A. Equations

The time independent Boltzmann equation with out sources (no fission neutrons are born in the thermal range) is

$$\vec{\nabla} \cdot \vec{F}(\vec{r}, E, \hat{\Omega}) + \Sigma_T(E) F(\vec{r}, E, \hat{\Omega}) = \iint \Sigma_S(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) F(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}' \quad (1)$$

where $\vec{F}(\vec{r}, E, \hat{\Omega}) = F(\vec{r}, E, \hat{\Omega}) \hat{\Omega}$ is the vector flux, - a vector whose magnitude equals the number of neutrons traveling in a direction $\hat{\Omega}$ (a unit vector) that cross a unit area normal to $\hat{\Omega}$ in unit time. Hence

$$F(\vec{r}, E, \hat{\Omega}) = n(\vec{r}, E, \hat{\Omega}) v,$$

$\vec{r}$ defines a point in space, E is the neutron energy, and v is the neutron velocity.

$\Sigma_S(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$ is the composite (summed over all isotopes) macroscopic cross section for a scattering event that results in the neutron energy in the Laboratory coordinate system changing from E' to E and the direction of the neutron's velocity from $\hat{\Omega}'$ to $\hat{\Omega}$, i.e. $\Sigma_S(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \sum_i \rho^i \sigma_S^i(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$ where ρ^i is the number density of the i^{th} isotope and σ_S^i is the microscopic neutron scattering cross section of the i^{th} isotope. Finally,

$$\Sigma_T(E) = \Sigma_a + \iint \Sigma(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') dE' d\hat{\Omega}' = \Sigma_a(E) + \Sigma_S(E) \quad (2)$$

where $\sum_a$ is the composite macroscopic absorption cross section. Making $\sum_T$ independent of $\vec{r}$ implies a uniform homogenous medium. Making $\sum_T$ independent of $\hat{\Omega}$ assumes an isotropic medium; in the case of crystalline scattering it implies using a cross section averaged over the initial directions of the neutron. This is an adequate approximation for a polycrystalline material.

In appendix I the following equations (B-1 approximation) for the fluxes, ϕ_k , and the currents, j_k , are derived from the Boltzmann equation (in a manner similar to the GAM⁽¹⁾ program) by expanding the scattering cross section in Legendre polynomials; representing the flux by its Fourier Transform, and then expanding the transform in Legendre polynomials and retaining terms out to the first order.

$$-B\phi_k + 3\gamma_k \sum_{T_k} j_k - \sum_{l=1}^{99} \sum_{l,k}^I j_l \Delta_l = S_k^I \quad k=1,2,3\dots I \quad (3)$$

and $I = 99$.

$$B j_k + \sum_{T_k} \phi_k - \sum_{l=1}^{99} \sum_{l,k}^0 \phi_l \Delta_l = S_k^0 \quad (4)$$

where k is the index for the fine energy group, B^2 is the Buckling,

$$\gamma_k = \frac{1}{3} \left(\frac{B}{\sum_{T_k}} \right)^2 \tan^{-1} \frac{B}{\sum_{T_k}} / \left(\frac{B}{\sum_{T_k}} - \tan^{-1} \frac{B}{\sum_{T_k}} \right), \quad (5)$$

$$\sum_{T_R} = \sum_i \sum_{T_R}^i = \sum_{a,k}^i + \sum_{l=1}^{99} \sum_{k,l}^{oi} \Delta_l \quad i \text{ identifies an isotope, } (6)$$

$$\sum_{\ell,k}^{oi} = \rho^i S_o^i(E_\ell \rightarrow E_k) \quad \text{and} \quad \sum_{\ell,k}^{ii} = \rho^i S_i^i(E_\ell \rightarrow E_k) \quad (7)$$

where

$$\sigma_S^i(E_\ell \rightarrow E_k, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{1}{4\pi} \sum_m S_m^i(E_\ell \rightarrow E_k) P_m(\mu_S) \quad (8)$$

and $\mu_S = \hat{\Omega}' \cdot \hat{\Omega}$.

$$S_k^o = \sum_i \frac{\sum_s^i}{1 - \alpha^i} \left(\frac{1}{E_c} - \frac{\alpha^i}{E_k} \right) \quad \alpha E_c \leq E_k \leq E_c \quad (9)$$

$$S_k^o = 0 \quad E_k \leq \alpha E_c$$

$$\alpha^i = \left(\frac{A^i - 1}{A^i + 1} \right)^2 \quad (10)$$

A^i is the mass number of isotope i ,

E_c is the upper cutoff energy of the thermal range,

$\sum_S^i$ is the scattering cross section (treated as a constant) at energies greater than E_c ,

$$S_k^i = \sum_i D^i B^3 \sum_S^i \frac{(A^i - 1)(A^i + 1)^2}{4A^i} \frac{1}{E_c} \left\{ \frac{1}{3\alpha^i} \left[\sqrt{\frac{E}{E_c}} - (\alpha^i)^{3/2} \frac{E_c}{E} \right] + \sqrt{\alpha^i} \left(\frac{E_c}{E} \right) - \sqrt{\frac{E_c}{E}} \right\} \quad \alpha^i E_c \leq E \leq E_c \quad (11)$$

$$S_k^i = 0 \quad E \leq \alpha^i E_c,$$

D^i = diffusion coefficient,

Δ_l = energy increment of the l^{th} fine group,

i.e.

$$\Delta_l = \frac{E_{l+1} - E_{l-1}}{2} \quad l=2, \dots, I-1$$

$$\Delta_I = \frac{E_I - E_{I-1}}{2} \quad l=I; E_I = E_c \quad (12)$$

$$\Delta_1 = \frac{E_2}{2} + \frac{E_1}{2} \quad l=1$$

$$\sum_l \Delta_l = E_I$$

From equations 3 and 4 the equations which must be solved for the flux are found to be given in matrix form (see Appendix II) as

$$\underline{\underline{S}} \underline{\underline{\phi}} = \underline{\underline{\eta}} \quad (13)$$

where $\underline{\underline{S}}$ is a 99 x 99 element matrix, and $\underline{\underline{\phi}}$ and $\underline{\underline{\eta}}$ are 99 component vectors.

$$\xi_{kl} = \sum_j \beta_{kj} \alpha_{jl} \quad k \neq l, \quad \xi_{kl} = \sum_j \beta_{kj} \alpha_{jl} + B^2 \quad k=l \quad (14)$$

$$\alpha_{kl} = - \sum_i \sum_{lk}^{oi} \Delta_l \quad k \neq l, \quad \alpha_{kl} = \sum_i \left[\sum_{TR}^i - \sum_{lk}^{oi} \Delta_l \right] \quad k=l \quad (15)$$

$$\beta_{kl} = - \sum_i \sum_{lk}^i \Delta_l \quad k \neq l, \quad \beta_{kl} = 3 \sum_i \left[\gamma_k^i \sum_{lk}^i - \sum_{lk}^i \Delta_l \right] \quad k=l \quad (16)$$

$$\underline{\eta} = \underline{\beta} \underline{S}^o - \underline{B} \underline{S}'$$

or

$$\eta_k = \sum_j \beta_{kj} S_j^o - B S'_k \quad (17)$$

$$S_k^o = \frac{ev}{cm^2 sec} \sum_i \frac{\sum_s^i}{1 - \alpha^i} \left[\frac{1}{E_c} - \frac{\alpha^i}{E_k} \right] \quad \alpha E_c \leq E_k \leq E_c$$

$$S_k^o = 0 \quad E_k < \alpha E_c \quad (18)$$

$$S'_k = \sum_i D^i B 3 \sum_s^i \frac{(A^i - 1)(A^i + 1)^2}{4 A^i} \frac{1}{E_c} \left\{ \frac{1}{3 \alpha^i} \left[\sqrt{\frac{E_k}{E_c}} - (\alpha^i)^{3/2} \frac{E_c}{E_k} \right] \right. \\ \left. + \sqrt{\alpha^i} \left(\frac{E_c}{E_k} \right) - \sqrt{\frac{E_c}{E_k}} \right\} \frac{ev}{cm^2 sec} \quad \alpha E_c \leq E_k \leq E_c$$

$$S'_k = 0 \quad E_k < \alpha E_c \quad (19)$$

After solving the matrix equation (13) for the flux using ISIMEQ⁽⁵⁾, the current can be obtained directly from the matrix equation:

$$\underline{j} = \frac{1}{B} \underline{S}^o - \frac{1}{B} \underline{\alpha} \underline{\phi} \quad (20)$$

Equations 3 and 4 represent the B(1) approximate equations derived from the Boltzmann equation. Setting $\gamma_k = 1$ in equations 3 and 4 corresponds to the P(1) approximation. See Appendix I.

B. Method of Solution

There are two general methods of solving a system of simultaneous linear algebraic equations (equations (13) of Section II A are of this type). These are the direct and the iterative methods. It was decided after considering computer time and desired accuracy that the direct was better for obtaining a solution to equations (13).

ISIMEQ⁽⁵⁾ is a digital computer program that was designed to find a solution to a system of non-homogeneous equations with a non-singular coefficient matrix. This routine does a Gauss elimination on the largest (absolute value) elements of the columns. Using the elimination method places ISIMEQ in the direct-method category. ISIMEQ has been tested for accuracy by using it to obtain a solution to a problem (for which the solution was known) of order 100. In this way it was possible to measure the accuracy of ISIMEQ's results for this problem. This same problem was solved using DSIMEQ* and its results were compared with those of ISIMEQ. Also ISIMEQ was used in conjunction with a method, outlined by Hanming⁽¹³⁾, for increasing the accuracy of a solution. There is a computer code called ISUDS⁽¹⁴⁾ that will perform this third type of computation. The results of these computer runs are presented in Table I.

ISUDS will be used for the solution of equation (13) for two distinct reasons.

1. One can control the amount of accuracy desired using ISUDS.
2. The storage of the large coefficient matrix (99 x 99) need only be a single precision matrix. If DSIMEQ is used it would require 2(99 x 99) locations.

*Double precision ISIMEQ.

TABLE I

Method No.	Program	Remarks	Time	Accuracy of Unknowns on 100th Order System
1	ISIMEQ	one-shot, direct	7 sec.	3 digits
2	DSIMEQ	one-shot, direct	10 sec.	10 digits
3	ISUDS	1 improvement iteration	14 sec.	8 digits
		2 improvement iterations	21 sec.	10 digits

C. Input Quantities

In order to solve the equations for the fluxes and currents the following cross sections are required in the library for each isotope:

1. the scattering matrices $\sum_{l,k}^{\circ}$, and $\sum_{l,k}'$ for any temperatures that are to be investigated,
2. the capture cross section $\sigma_{\gamma i}$, and
3. the fission cross section $\sigma_{f,i}$.

If there are no crystalline scattering matrices in the library for a particular nucleus then by specifying the temperature, T , the mass number, A , and the free scattering cross section, σ_s^f , a free-gas scattering kernel can be generated from a subroutine which is a modified version of SIGGAS⁽¹¹⁾.

In addition to smooth (temperature independent) fission and capture cross sections, resonance parameters can be input and the resonance cross section will be calculated for any temperature, T , by the subroutine EXT⁽⁶⁾.

For each problem the elements must be identified, I.D. number, and their number density, ρ^i , must be input, as well as their mass number, A^i . The temperature, T , the buckling, B^2 , and the cutoff energy, E_c , for the thermal range must also be input.

Single values for the scattering cross section and diffusion coefficient for the energy range above thermal are input quantities that are required for calculating the source terms. ν , the average number of fast neutrons released per fission is a useful input quantity so that flux averaged values of $\nu \sigma_f$ may be printed out.

III. FLUX CURRENT AVERAGING OF CROSS SECTIONS AND PRINTOUT QUANTITIES

Broad group cross sections which are required for diffusion or transport calculations can be obtained by flux and current averaging of the cross sections in the BlT library using

- a) fluxes and currents that are calculated as described in Section II, or
- b) fluxes and currents that are input, or
- c) fluxes and currents based on a Maxwellian distribution at some temperature, T.

The Maxwellian flux is given by $\phi(E) \sim E e^{-E/kT}$ and the current may be obtained from $j_k = B D_k \phi_k$ where the constant B is input and D_k is obtained from the cross section library, i.e.

$$D_k = \frac{1}{3 \sum_{T_k} (1 - \bar{\mu}_k) \left(1 - \frac{4}{5} \frac{\sum a_k}{\sum I_k} + \frac{\sum a_k}{\sum T_k} \frac{\bar{\mu}_k}{1 - \bar{\mu}_k} \right)} \quad (21)$$

and

$$\bar{\mu}_k = \frac{1}{3} \frac{\sum_l \sum' S_{kl} \Delta l}{\sum_l \sum^o S_{kl} \Delta l} \quad (22)$$

The average macroscopic cross section, $\langle \Sigma_x^i \rangle_g$ for isotope i and for broad group g (where $x = f$ for fission, $x = c$ for capture) is obtained from

$$\langle \Sigma_x^i \rangle_g = \frac{\int_{E_{Lg}}^{E_{ug}} \Sigma_x^i(E) \phi(E) dE}{\int_{E_{Lg}}^{E_{ug}} \phi(E) dE} = \frac{\sum_{k=k_{Lg}}^{k_{ug}} \Sigma_{xk}^i \phi_k \Delta_k}{\sum_{k=k_{Lg}}^{k_{ug}} \phi_k \Delta_k} \quad (23)$$

where E_{Lg} and E_{ug} are the lower and upper energy bounds of group g ; similarly the energy mesh points k_{Lg} and k_{ug} represent the lower and upper bounds of broad group g . The average macroscopic cross section for the composite case is

$$\langle \Sigma_{xg} \rangle = \sum_i \langle \Sigma_{xg}^i \rangle \quad (24)$$

The broad group transfer term $P(0)_{g \rightarrow g'}^i$ for isotope i and from broad group g to g'

$$P(0)_{g \rightarrow g'}^i = \frac{\int_{E_{Lg'}}^{E_{ug'}} dE' \int_{E_{Lg}}^{E_{ug}} \Sigma_{xg'}^i(E \rightarrow E') \phi(E) dE}{\int_{E_{Lg}}^{E_{ug}} \phi(E) dE},$$

or

$$P(0)_{g \rightarrow g'}^i = \frac{\sum_{l=l_{Lg}}^{l_{ug'}} \Delta_l' \sum_{k=k_{Lg}}^{k_{ug}} \sum_{k \rightarrow l}^{oi} \phi_k \Delta_k}{\sum_{k=k_{Lg}}^{k_{ug}} \phi_k \Delta_k} \quad (25)$$

For the composite case

$$P(0)_{g \rightarrow g'} = \sum_i P(0)_{g \rightarrow g'}^i \quad (26)$$

The $P(1)_{g \rightarrow g'}^i$ broad group transfer terms are obtained in the same manner except the current j replaces the flux ϕ and $\sum_{k \rightarrow l}^{i'}$ replaces $\sum_{k \rightarrow l}^{oi}$ in equation 25.

The quantities that will be printed out (in addition to the input quantities) are the:

1. energy mesh, E_k ,
2. fluxes, ϕ_k , for fine groups, and
3. currents, j_k , for fine groups.

There will be options for obtaining the following broad group sections by element or for the composite case or both:

4. $\langle \sum_f \rangle_g$ macroscopic fission cross section for broad group g ,
5. $\nu \langle \sum_f \rangle_g$,
6. $\langle \sum_c \rangle_g$ capture cross section,

7. $\sum_{g'} P(0)_{g \rightarrow g'}$ scattering cross section,
and 8. $\langle \sum_T \rangle_g$ total cross section, i.e.

$$\langle \sum_T \rangle_g = \langle \sum_f \rangle_g + \langle \sum_c \rangle_g + \sum_{g'} P(0)_{g \rightarrow g'}.$$

There will be an option to print out in addition either

9. $\langle \sum_T \rangle_g - P(0)_{g \rightarrow g}$

or

10. $\langle \sum_T \rangle_g - P(0)_{g \rightarrow g} - \frac{1}{3} P(1)_{g \rightarrow g}.$

11. Either the transfer matrix with elements $P(0)_{g \rightarrow g'}$, or there will be an option to print out the transfer matrix with the diagonal terms set equal to zero, i.e. $P(0)_{g \rightarrow g} = 0$.
12. Either the transfer matrix with elements $1/3 P(1)_{g \rightarrow g'}$, or there will also be an option to print out this matrix with the diagonal terms set equal to 0.

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APPENDIX I. DERIVATIONS OF EQUATIONS

The time independent Boltzmann Equation with no sources (no fission neutrons are born in the thermal range) is:

$$\vec{\nabla} \cdot \vec{F}(\vec{r}, E, \hat{\Omega}) + \sum_T (E, \hat{\Omega}) F(\vec{r}, E, \hat{\Omega}) = \iint \sum_S (E' \rightarrow E, \hat{\Omega} \rightarrow \hat{\Omega}') F(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}' \quad (1)$$

where

$$\begin{aligned} \sum_T^i (E, \hat{\Omega}) &= \rho^i \sigma_a^i(E) + \rho^i \sigma_s^i(E, \hat{\Omega}) = \rho^i \sigma_a^i(E) \\ &+ \rho^i \int \int \sigma_s^i(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') dE' d\hat{\Omega}' \end{aligned} \quad (2)$$

and summing over the isotopes

$$\sum_T (E, \hat{\Omega}) = \sum_i \sum_T^i (E, \hat{\Omega});$$

since $\sum_T$ is independent of position, a uniform medium is assumed. The vector flux

$$\vec{F}(\vec{r}, E, \hat{\Omega}) = F(\vec{r}, E, \hat{\Omega}) \hat{\Omega} \quad (3)$$

is a vector whose magnitude is the number of neutrons traveling in a direction $\hat{\Omega}$ (unit vector) that cross a unit area normal to $\hat{\Omega}$ in unit time.

$$F(\vec{r}, E, \hat{\Omega}) = n(\vec{r}, E, \hat{\Omega}) v. \quad (4)$$

Hence, the scalar flux

$$\Phi(\vec{r}) = \iint_{E, \hat{\Omega}} F(\vec{r}, E, \hat{\Omega}) d\hat{\Omega} dE, \quad (5)$$

and the net current density

$$\vec{J}(\vec{r}) = \int_E \int_{\Omega} \hat{\Omega} F(\vec{r}, E, \hat{\Omega}) d\hat{\Omega} dE. \quad (6)$$

Now

$$\vec{\nabla} \cdot \vec{F} = \vec{\nabla} \cdot F \hat{\Omega} = \hat{\Omega} \cdot \vec{\nabla} F.$$

So the Boltzmann equation becomes

$$\hat{\Omega} \cdot \vec{\nabla} F(\vec{r}, E, \hat{\Omega}) + \sum_T(E, \hat{\Omega}) F(\vec{r}, E, \hat{\Omega}) = \iint \sum_S(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \quad (7)$$

$$F(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}'.$$

Assuming an isotropic medium, i.e.

assuming that the scattering cross section does not depend on the direction of the neutron velocity prior to the collision, the scattering cross section can be expanded in Legendre Polynomials as

$$\sigma_S(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{1}{4\pi} \sum_{\ell} S^{\ell}(E' \rightarrow E) P_{\ell}(\mu_S) \quad (8)$$

where $\mu_S = \hat{\Omega}' \cdot \hat{\Omega}$.

The first two expansion coefficients may be obtained in the following way: Multiply Equation 8 by $P^k(\mu_S)$; now integrating over $\int_0^{2\pi} d\phi \int_{-1}^1 d\mu_S$ yields:

$$2\pi(2k+1) \int_{-1}^1 P^k(\mu_S) \sigma_S(E' \rightarrow E, \mu_S) d\mu_S = S^k(E' \rightarrow E) \quad (9)$$

$$\therefore S^0(E' \rightarrow E) = 2\pi \int_{-1}^1 \sigma_S(E' \rightarrow E, \mu_S) d\mu_S = \sigma_S(E' \rightarrow E) \quad (10)$$

and $S^0(E') = \int S^0(E' \rightarrow E) dE = \int \sigma_S(E' \rightarrow E) dE = \sigma_S(E')$ (11)

Also $S'(E' \rightarrow E) = 2\pi(3) \int_{-1}^1 P'(\mu_S) \sigma_S(E' \rightarrow E, \mu_S) d\mu_S$
or $\frac{1}{3} S'(E' \rightarrow E) = 2\pi \int_{-1}^1 \sigma_S(E' \rightarrow E, \mu_S) \mu_S d\mu_S$. (12)

Therefore,

$$\begin{aligned} \frac{1}{3} S'(E') &= \frac{1}{3} \int S'(E' \rightarrow E) dE = 2\pi \int_{-1}^1 \left\{ \int \sigma_S(E' \rightarrow E, \mu_S) dE \right\} \mu_S d\mu_S \\ \text{or } \frac{1}{3} S'(E') &= 2\pi \int_{-1}^1 \sigma_S(E', \mu_S) \mu_S d\mu_S \left(\frac{2\pi \int_{-1}^1 \sigma_S(E', \mu_S) d\mu_S}{2\pi \int_{-1}^1 \sigma_S(E', \mu_S) d\mu_S} \right) \\ \text{so } \frac{1}{3} S'(E') &= \bar{\mu}_S 2\pi \int_{-1}^1 \sigma_S(E', \mu_S) d\mu_S = \bar{\mu}_S S_0(E') = \bar{\mu}_S \sigma_S(E') \end{aligned} \quad (13)$$

Summarizing, we have obtained the well known results

$$S^0(E') = \sigma_S(E') \quad \text{and} \quad \frac{1}{3} S'(E') = \bar{\mu}_S \sigma_S(E').$$

The ℓ^{th} coefficient for the macroscopic scattering cross section of the i^{th} isotope is:

$$\sum_S \ell_i(E' \rightarrow E) = \rho_i S_i^\ell(E' \rightarrow E) \quad \text{and} \quad \sum_S \ell = \sum_i \rho_i S_i^\ell(E' \rightarrow E). \quad (14)$$

Equation 7 becomes

$$\hat{\Omega} \cdot \vec{\nabla} F(\vec{r}, E, \hat{\Omega}) + \sum_T F(\vec{r}, E, \hat{\Omega}) = \frac{1}{4\pi} \sum_{\ell} \iint \sum_S^{\ell} (E' \rightarrow E) P_{\ell}(H_S) F(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}' \quad (15)$$

If we restrict ourselves to 1 dimension, viz. the Z direction,

$$\vec{\nabla} F = \hat{i} \frac{\partial F}{\partial x} + \hat{j} \frac{\partial F}{\partial y} + \hat{k} \frac{\partial F}{\partial z} = \hat{k} \frac{\partial F}{\partial z} \quad \text{so}$$

$$\hat{\Omega} \cdot \vec{\nabla} F = \hat{\Omega} \cdot \hat{k} \frac{\partial F}{\partial z} = \mu \frac{\partial F}{\partial z} \quad (16)$$

and Equation 15 becomes

$$\mu \frac{\partial F(z, E, \mu)}{\partial z} + \sum_T F(z, E, \mu) = \frac{1}{4\pi} \sum_{\ell} \int_0^{2\pi} d\varphi' \int dE' \int_{-1}^1 \sum_S^{\ell} (E' \rightarrow E) P_{\ell}(H_S) F(z, E', \mu') d\mu' \quad (17)$$

where

$$d\hat{\Omega}' = \int_0^{2\pi} \int_0^{\pi} \sin \theta' d\theta' d\varphi' = \int_0^{2\pi} d\varphi' \int_{-1}^1 (-d\mu') = \int_0^{2\pi} d\varphi' \int_{-1}^1 d\mu'$$

From the addition theorem for Legendre polynomials:

$$P_l(\mu_s) = P_l(\mu) P_l(\mu') + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu) P_l^m(\mu') \cos m(\varphi - \varphi') \quad (18)$$

Substituting (18) into (17) gives

$$\begin{aligned} \mu \frac{\partial F(z, E, \mu)}{\partial z} + \sum_T (E, \mu) F(z, E, \mu) = \frac{1}{4\pi} \sum_l \int_0^{2\pi} d\varphi' \int dE' \int_{-1}^1 \sum_s^l (E' \rightarrow E) \\ \left\{ P_l(\mu) P_l(\mu') + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu) P_l^m(\mu') \cos m(\varphi - \varphi') \right\} \\ F(z, E', \mu') d\mu'. \end{aligned} \quad (19)$$

Now integrating with respect to φ' yields

$$\begin{aligned} \mu \frac{\partial F(z, E, \mu)}{\partial z} + \sum_T (E, \mu) F(z, E, \mu) = \frac{1}{2} \sum_l \int dE' \int_{-1}^1 d\mu' \\ \left\{ \sum_s^l (E' \rightarrow E) P_l(\mu) P_l(\mu') F(z, E', \mu') \right\} \end{aligned} \quad (20)$$

Let us now derive the usual P(1) set of equations. Integrating Equation 20 over $d\hat{\Omega}$, i.e. $\int_{-1}^1 d\mu \int_0^{2\pi} d\varphi$, yields

$$\begin{aligned} 2\pi \int_{-1}^1 \mu \frac{\partial F(z, E, \mu)}{\partial z} d\mu + 2\pi \int_{-1}^1 \sum_T (E, \mu) F(z, E, \mu) d\mu = \frac{1}{2} \sum_l \int dE' \int_{-1}^1 d\mu' \\ \left\{ \sum_s^l (E' \rightarrow E) P_l(\mu') F(z, E', \mu') \int_{-1}^1 P_l(\mu) d\mu \right\} 2\pi \end{aligned} \quad (21)$$

Since it has been assumed that the scattering cross section is independent of

$$\hat{\Omega}, \quad 2\pi \int_0^1 \int_{-1}^1 \Sigma_T(E, \mu) d\mu = \Sigma_T(E) \int_0^1 \int_{-1}^1 d\mu, \quad (22)$$

and

$$2\pi \int_{-1}^1 \mu \frac{\partial F(z, E, \mu)}{\partial z} d\mu + \Sigma_T(E) \Phi(z, E) = 2\pi \int dE' \int_{-1}^1 d\mu' \left\{ \Sigma_s^0(E' \rightarrow E) P_0(\mu') F(z, E', \mu') \right\}. \quad (23)$$

Now expand the flux in Legendre polynomials.

$$F(z, E, \mu) = \frac{1}{4\pi} \sum_{\ell} f^{\ell}(z, E) P^{\ell}(\mu). \quad (24)$$

So

$$\int_{-1}^1 F(z, E, \mu) P^k(\mu) d\mu = \frac{1}{4\pi} \int_{-1}^1 \sum_{\ell} f^{\ell}(z, E) P^{\ell}(\mu) P^k(\mu) d\mu,$$

$$\text{or } \int_{-1}^1 F(z, E, \mu) P^k(\mu) d\mu = \frac{1}{4\pi} \left(\frac{2}{2k+1} \right) f^k(z, E). \quad (25)$$

$$f^0(z, E) = 2\pi \int_{-1}^1 F(z, E, \mu) d\mu = \Phi(z, E) \quad (26)$$

which is the scalar flux as defined in Equation 5.

$$f'(z, E) = 2\pi(3) \int_{-1}^1 \mu F(z, E, \mu) d\mu = 3J_z(z, E) \quad (27)$$

which is the net current density as defined in Equation 6. Therefore, if the flux is nearly isotropic, it may be expressed as

$$F(z, E, \mu) \cong \frac{1}{4\pi} \left[\bar{\Phi}(z, E) + 3\mu J_z(z, E) \right] \quad (28)$$

Upon substituting Equation 28 into Equation 23 and carrying out the integrations:

$$\frac{\partial J_z(z, E)}{\partial z} + \sum_T(E) \bar{\Phi}(z, E) = \int \sum_S^o(E' \rightarrow E) \bar{\Phi}(E', z) dE' \quad (29)$$

Now substituting Equation 28 into Equation 20, multiplying by μ and integrating over $\hat{\Omega}$ yields:

$$2\pi \int_{-1}^1 \mu^2 \frac{1}{4\pi} \left[\frac{\partial \bar{\Phi}(z, E)}{\partial z} + 3\mu \frac{\partial J_z(z, E)}{\partial z} \right] + 2\pi \int_{-1}^1 \sum_T(E, \mu) \frac{\mu}{4\pi} \left[\bar{\Phi}(z, E) + 3\mu J_z(z, E) \right] d\mu = \frac{2\pi}{2} \sum_l \int dE' \int_{-1}^1 d\mu' \sum_S^l(E' \rightarrow E) P_l(\mu') F(z, E', \mu') \int_{-1}^1 P_l(\mu) \mu d\mu,$$

or

$$\frac{1}{2} \left[\frac{\mu^3}{3} \right]_{-1}^1 \frac{\partial \Phi(z, E)}{\partial z} + \frac{1}{2} \sum_T(E) 3 \left[\frac{\mu^3}{3} \right]_{-1}^1 J_z(z, E) =$$

$$\pi \int dE' \int_{-1}^1 d\mu' \sum_S'(E' \rightarrow E) P_1(\mu') \frac{1}{4\pi} \left[\Phi(E', z) + 3\mu' J_z(z, E') \right] \left[\frac{\mu^3}{3} \right]_{-1}^1,$$

or

$$\frac{1}{3} \frac{\partial \Phi(z, E)}{\partial z} + \sum_T(E) J_z(z, E) = \frac{1}{2 \cdot 3} \int dE' \sum_S'(E' \rightarrow E)$$

$$3 \left[\frac{\mu^3}{3} \right]_{-1}^1 J_z(z, E')$$

So finally,

$$\frac{\partial \Phi(z, E)}{\partial z} + 3 \sum_T(E) J_z(z, E) = \int \sum_S'(E' \rightarrow E) J_z(z, E') dE' \quad (30)$$

Equations 29 and 30 are the usual P(1) equations.

One possibility (as is done in GAM) for treating the spacial dependence in order to obtain a set of energy dependent equations is to integrate Equation 29 over some spacial region $\Delta \mathbf{z}$, and differentiate Equation 30 with respect to $\mathbf{z}$ before integrating over this same region. Equation 29 and 30 become:

$$\bar{J}(E) + \sum_{\tau} \bar{\Phi}(E) = \int \sum_s^{\circ} (E' \rightarrow E) \bar{\Phi}(E) dE', \quad (31)$$

and
$$\mathcal{L} \bar{\Phi}(E) + 3 \sum_{\tau} \bar{J}(E) = \int \sum_s^{\circ} (E' \rightarrow E) \bar{J}(E') dE', \quad (32)$$

where
$$\bar{J}(E) = \frac{1}{\Delta z} \int \frac{\partial J_z(z, E)}{\partial z} dz \quad (= \frac{1}{V} \int \vec{\nabla} \cdot \vec{J} dV = \frac{1}{V} \int \vec{J} \cdot d\vec{A}), \quad (33)$$

$$\bar{\Phi}(E) = \frac{1}{\Delta z} \int \Phi(z, E) dz \quad (= \frac{1}{V} \int \Phi dV), \quad (34)$$

and
$$\mathcal{L}(E) = \frac{\int \frac{\partial^2 \Phi(z, E)}{\partial z^2} dz}{\int \Phi(z, E) dE} \left(= \frac{\int \nabla^2 \Phi dV}{\int \Phi dV} \right). \quad (35)$$

The spatial dependence is now contained in the input quantity $\mathcal{L}(E)$.

The spatial dependence in the P(1) equations 29 and 30 can also be treated by means of a fourier transform, i.e. let

$$f(B, E, \mu) \equiv \int_{-\infty}^{\infty} F(z, E, \mu) e^{i B z} dz \approx \frac{1}{4\pi} \int_{-\infty}^{\infty} \left[\Phi(z, E) + 3\mu J_z(z, E) \right] e^{i B z} dz \quad (36)$$

also set

$$f(B, E, \mu) \approx \frac{1}{4\pi} \left[\phi(B, E) + 3\mu \psi(B, E) \right] \quad (37)$$

Multiplying Equation 29 by e^{iBz} and integrating over z yields

$$\int_{-\infty}^{\infty} \frac{\partial J_z(z, E)}{\partial z} e^{iBz} dz + \sum_T(E) \phi(B, E) = \int \sum_S^o(E' \rightarrow E) \phi(B, E') dE' \quad (38)$$

Now
$$\int_{-\infty}^{\infty} \frac{\partial}{\partial z} [J_z(z, E) e^{iBz}] dz = \int_{-\infty}^{\infty} \frac{\partial J_z(z, E)}{\partial z} e^{iBz} dz + iB \int_{-\infty}^{\infty} J_z(z, E) e^{iBz} dz$$

or

$$[J_z(z, E) e^{iBz}]_{z \rightarrow -\infty}^{z \rightarrow \infty} = \int_{-\infty}^{\infty} \frac{\partial J_z(z, E)}{\partial z} e^{iBz} dz - B_j(B, E). \quad (39)$$

Since $J(\infty, E) = J(-\infty, E) = 0$, substituting Equation 39 into Equation 38

yields
$$B_j(B, E) + \sum_T(E) \phi(B, E) = \int \sum_S^o(E' \rightarrow E) \phi(B, E') dE' \quad (40)$$

Similarly Equation 30 becomes

$$-iB \phi(B, E) + 3 \sum_T(E) i j(B, E) = i \int \sum_S^i(E' \rightarrow E) j(B, E') dE' \quad (41)$$

$$-B \phi(B, E) + 3 \sum_T(E) j(B, E) = \int \sum_S^i(E' \rightarrow E) j(B, E') dE' \quad (42)$$

Hence, in the P(1) approximation we obtain the following two equations from rewriting Equation 40 and multiplying Equation 42 by B:

$$[B_j(B, E)] + \sum_T(E) \varphi(B, E) = \int \sum_S^0(E' \rightarrow E) \varphi(B, E') dE' \quad (43)$$

$$-B^2 \varphi(B, E) + 3 \sum_T(E) [B_j(B, E)] = \int \sum_S^1(E' \rightarrow E) [B_j(B, E')] dE' \quad (44)$$

These equations are the same as equations (31) and (32) if we make the following identifications:

$$\begin{aligned} B_j(B, E) &\longrightarrow \bar{J}(E) \\ \varphi(B, E) &\longrightarrow \bar{\Phi}(E) \end{aligned} \quad (45)$$

$$B^2 \longrightarrow -\mathcal{L} \quad \text{i.e., the buckling.} \quad (46)$$

To see that B^2 represents the buckling recall that

$$\bar{\Phi}(z) = \iint F(z, E, \kappa) dE d\hat{\Omega},$$

so from Equations 36 and 37:

$$\varphi(B) = \int_{-\infty}^{\infty} \bar{\Phi}(z) e^{iBz} dz, \quad \text{also} \quad \bar{\Phi}(z) \sim \int_{-\infty}^{\infty} \varphi(B) e^{-iBz} dB \quad (47)$$

so

$$\frac{\partial^2 \bar{\Phi}}{\partial z^2} = -B^2 \bar{\Phi}(z).$$

Let us now derive from Equation 20 the B1 approximate set of equations. In equation 20 we assume that $\sum_T$ is independent of $\hat{\Omega}$, so $\sum_T = \sum_T(E)$. Multiplying Equation 20 by e^{iBz} , integrating over z , and making use of Equation 36, one obtains

$$\begin{aligned} \mu \int_{-\infty}^{\infty} \frac{\partial F(z, E, \mu)}{\partial z} e^{iBz} dz + \sum_T(E) f(B, E, \mu) = \frac{1}{2} \sum_{\ell} \int_0^{\infty} dE' \int_{-1}^1 d\mu' \\ \left\{ \sum_S^{\ell} (E' \rightarrow E) P_{\ell}(\mu) P_{\ell}(\mu') f(B, E', \mu') \right\} \end{aligned} \quad (48)$$

Since

$$\begin{aligned} \int_{-\infty}^{\infty} \mu \frac{\partial}{\partial z} (F(z, E, \mu) e^{iBz}) dz = \mu \int_{-\infty}^{\infty} \frac{\partial F(z, E, \mu)}{\partial z} e^{iBz} dz + \mu iB \\ \int_{-\infty}^{\infty} F(z, E, \mu) e^{iBz} dz \end{aligned}$$

$$\text{and } \mu \int_{-\infty}^{\infty} \frac{\partial}{\partial z} (F(z, E, \mu) e^{iBz}) dz = \mu [F(z, E, \mu) e^{iBz}]_{-\infty}^{\infty} = 0$$

$$\text{since } F(\infty, E, \mu) = F(-\infty, E, \mu) = 0$$

$$\text{we obtain } \mu \int_{-\infty}^{\infty} \frac{\partial F(z, E, \mu)}{\partial z} e^{iBz} dz = -iB\mu f(B, E, \mu)$$

and Equation 48 becomes

$$-i B \mu f(B, E, \mu) + \sum_T(E) f(B, E, \mu) = \frac{1}{2} \sum_L \int_0^\infty dE' \int_{-1}^1 d\mu' \left\{ \sum_S^L (E' \rightarrow E) P_L(\mu) P_L(\mu') f(B, E', \mu') \right\}$$

or

$$(1 - \mu \eta(B, E)) \sum_T(E) f(B, E, \mu) = \frac{1}{2} \sum_L \int_0^\infty dE' \int_{-1}^1 d\mu' \left\{ \sum_S^L (E' \rightarrow E) P_L(\mu) P_L(\mu') f(B, E', \mu') \right\} \quad (49)$$

where

$$\eta(B, E) = \frac{i B}{\sum_T(E)} \quad (50)$$

Now expand $f(B, E, \mu)$ in Legendre Polynomials,

$$f(B, E, \mu) = \sum_j f_j(B, E) P_j(\mu), \quad (51)$$

Equation 49 becomes

$$\begin{aligned} \sum_T(E) \sum_j f_j(B, E) P_j(\mu) &= \frac{1}{2} \sum_L \int_0^\infty dE' \int_{-1}^1 d\mu' \left\{ \sum_S^L (E' \rightarrow E) \frac{P_L(\mu)}{1 - \mu \eta(B, E)} \right. \\ &\quad \left. P_L(\mu') \sum_j f_j(B, E) P_j(\mu) \right\} = \frac{1}{2} \sum_L \int_0^\infty dE' \left\{ \sum_S^L (E' \rightarrow E) \frac{P_L(\mu)}{1 - \mu \eta(B, E)} \right. \\ &\quad \left. \frac{2}{(2L+1)} f_L(B, E) \right\} \end{aligned} \quad (52)$$

Multiply Equation 52 by $P_k(\mu)$ and integrate over μ :

$$\sum_T(E) f_k(B, E) \left(\frac{2}{2k+1} \right) = \sum_l \int_0^\infty dE' \left\{ \frac{1}{2l+1} \left[\int_{-1}^1 \frac{P_k(\mu) P_l(\mu) d\mu}{1 - \mu \eta(B, E)} \right] \right. \\ \left. \sum_S^l (E' \rightarrow E) f_l(B, E') \right\}$$

or

$$\frac{\sum_T(E) f_k(B, E)}{2k+1} = \sum_l \frac{A_{kl}}{2l+1} \int_0^\infty \sum_S^l (E' \rightarrow E) f_l(B, E') dE' \quad (53)$$

where $A_{kl} = \frac{1}{2} \int_{-1}^1 \frac{P_k(\mu) P_l(\mu)}{1 - \mu \eta(B, E)} d\mu \quad (54)$

or $A_{kl} = \frac{1}{\eta(B, E)} Q_k \left(\frac{1}{\eta(B, E)} \right) P_k \left(\frac{1}{\eta(B, E)} \right) \quad \text{for } l \leq k \quad (55)$

where P_l = Legendre polynomial of 1st kind,

Q_k = Legendre polynomial of 2nd kind.

$$A_{0,0} = \frac{\tan^{-1} \chi}{\chi}, \quad A_{0,1} = i \frac{(1 - A_{0,0})}{\chi}, \quad A_{1,0} = A_{0,1}, \quad A_{1,1} = -\frac{i}{\chi} A_{0,1} \quad (56)$$

where $\chi = \frac{\eta}{i} = \frac{B}{\sum_T} = \frac{-i A_{0,1}}{A_{1,1}}.$

Let $k = 0$ and take the first two terms of the expansion, i.e. $\ell = 0, 1$

$$\sum_T(E) f_0(B, E) = A_{0,0} \int_0^\infty \sum_S^0(E' \rightarrow E) f_0(B, E') dE' + \frac{A_{0,1}}{3} \int_0^\infty \sum_S^1(E' \rightarrow E) f_1(B, E') dE' \quad (57)$$

Let $k = 1$ and take the first two terms of the expansion, i.e. $\ell = 0, 1$

$$\frac{1}{3} \sum_T(E) f_1(B, E) = A_{1,0} \int_0^\infty \sum_S^0(E' \rightarrow E) f_0(B, E') dE' + \frac{A_{1,1}}{3} \int_0^\infty \sum_S^1(E' \rightarrow E) f_1(B, E') dE' \quad (58)$$

Substituting $\phi = 4\pi f_0$ and $j = \frac{4\pi}{3} f_1$ (from Equation 37) into

Equations 57 and 58:

$$\sum_T(E) \phi(B, E) = A_{0,0} \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE' + i A_{0,1} \int_0^\infty \sum_S^1(E' \rightarrow E) j(B, E') dE' \quad (59)$$

$$\sum_T(E) j(B, E) = (-i A_{1,0}) \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE' + A_{1,1} \int_0^\infty \sum_S^1(E' \rightarrow E) j(B, E') dE' \quad (60)$$

Multiply Equation 59 by $\frac{i A_{1,1}}{A_{0,1}}$ and add to Equation 60 to obtain:

$$\frac{i A_{1,1}}{A_{0,1}} \sum_T(E) \phi(B, E) + \sum_T(E) j(B, E) = \left(\frac{i A_{0,0} A_{1,1}}{A_{0,1}} - i A_{1,0} \right) \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE'$$

or

$$+ \frac{1}{\chi} \sum_T(E) \phi(B, E) + \sum_T(E) j(B, E) = \left(+ \frac{A_{00}}{\chi} - \frac{A_{00}^{-1}}{\chi} \right) \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE'$$

or

$$+ \sum_T(E) \phi(B, E) + \chi \sum_T(E) j(B, E) = + \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE'$$

or

$$\sum_T(E) \phi(B, E) + B j(B, E) = \int_0^\infty \sum_S^0(E' \rightarrow E) \phi(B, E') dE' \quad (61)$$

Multiply Equation 59 by $(i A_{10}/A_{00})$ and add to Equation 60

$$\frac{i A_{10}}{A_{00}} \sum_T(E) \phi(B, E) + \sum_T(E) j(B, E) = \left(- \frac{A_{10} A_{01}}{A_{00}} + A_{11} \right) \int_0^\infty \sum_S^1(E' \rightarrow E) j(B, E') dE'$$

or

$$- \frac{1 - A_{00}}{A_{00} \chi} \sum_T(E) \phi(B, E) + \sum_T(E) j(B, E) = \left(+ \frac{(1 - A_{00})^2}{A_{00} \chi^2} + \frac{1 - A_{00}}{\chi^2} \right) \int_0^\infty \sum_S^1(E' \rightarrow E) j(B, E') dE'$$

Multiply by $\frac{\chi^2 A_{00}}{1-A_{00}}$ to obtain

$$-B\phi(B,E) + \frac{\chi^2 A_{00}}{1-A_{00}} \sum_T (E) j(B,E) = (1-A_{00}+A_{00}) \int_0^\infty \sum_S' (E' \rightarrow E) j(B,E') dE'$$

or

$$-B\phi(B,E) + 3\gamma \sum_T (E) j(B,E) = \int_0^\infty \sum_S' (E' \rightarrow E) j(B,E') dE' \quad (62)$$

where $\gamma = \frac{\chi^2 A_{00}}{3(1-A_{00})}$. (63)

The B1 equations are given by Equations 61 and 62 where

$$\gamma(B,E) = \frac{\chi^2 A_{00}}{3(1-A_{00})} = \frac{1}{3} \frac{\chi \tan^{-1} \chi}{1 - \frac{1}{\chi} \tan^{-1} \chi}$$

or

$$\gamma(B,E) = \frac{1}{3} \frac{\chi^2 \tan^{-1} \chi}{\chi - \tan^{-1} \chi} = \frac{1}{3} \frac{\frac{B^2}{\sum_T^2} \tan^{-1} \left(\frac{B}{\sum_T} \right)}{\frac{B}{\sum_T} - \tan^{-1} \left(\frac{B}{\sum_T} \right)} . \quad (64)$$

Hence the P(1) equations (Equations 40 and 42) are a special case of the B(1) equations (Equations 61 and 62) obtained when $\gamma = 1$.

Let the thermal energy range extend from 0 - E_c ($E_c = 2.38$ for TNS).

Then Equation 61 becomes

$$B_j(B,E) + \left[\sum_a + \int_0^{E_c} \sum_S^o (E \rightarrow E') dE' + \int_{E_c}^\infty \sum_S^o (E \rightarrow E') dE' \right] \phi(B,E) = \int_0^{E_c} \sum_S^o (E' \rightarrow E) \phi(B,E') dE' + S^o(E), \quad (65)$$

where the source term
$$S^0(E) = \int_{E_c}^{\infty} \sum_S^0(E' \rightarrow E) \phi(B, E') dE'. \quad (66)$$

Assuming elastic isotropic scattering in the center of mass coordinate system, we have for each scattering isotope

$$\begin{aligned} \sum_S^0(E' \rightarrow E) &= \frac{\sum_S(E')}{E'(1-\alpha)} \quad \alpha E' \leq E \leq E' \\ &= 0 \quad \text{otherwise} \end{aligned} \quad (67)$$

where
$$\alpha = \left(\frac{A-1}{A+1} \right)^2.$$

If we assume that $\phi(B, E') = \frac{C}{E'}$, for $E' > E_c$, and if we let $c = 1$ in magnitude since the magnitude of the fluxes and currents that are calculated will not affect any of the flux and current averaged results then

$$S^0(E) = \sum_i \frac{er}{cm^2 \text{ sec.}} \int_{E_c}^{E/\alpha^i} \frac{\sum_S^i(E')}{E'(1-\alpha^i)} \frac{dE'}{E'}$$

where i signified the isotope. If $\sum_S^i(E)$ is treated as a constant

$$S^0(E) = \frac{er}{cm^2 \text{ sec.}} \sum_i \frac{\sum_S^i}{1-\alpha^i} \left[\frac{1}{E_c} - \frac{\alpha^i}{E} \right] \text{ for } \alpha E_c \leq E \leq E_c \quad (68)$$

otherwise $S^0(E) = 0$.

Also, from Equation 62

$$-B\phi(B,E) + 3\gamma(B,E) \left[\sum_0 + \int_0^{E_c} \sum_S^0(E \rightarrow E') dE' + \int_{E_c}^{\infty} \sum_S^0(E \rightarrow E') dE' \right] j(B,E) =$$

$$\int_0^{E_c} \sum_S'(E' \rightarrow E) j(B,E') dE' + S'(E) \quad (69)$$

where

$$S'(E) = \int_{E_c}^{\infty} \sum_S'(E' \rightarrow E) j(E') dE' \quad (70)$$

For each scattering isotope (isotropic elastic scattering in C.M.)

$$\sum_S' = \frac{3 \sum_S(E')}{E'(1-\alpha)} \mu_S \quad (71)$$

where μ_S is the scattering angle in the Lab System.

Therefore

$$\mu_S = \frac{A+1}{2} \sqrt{\frac{E}{E'}} - \frac{A-1}{2} \sqrt{\frac{E'}{E}}, \quad (72)$$

and

$$1 - \alpha = 1 - \left(\frac{A-1}{A+1} \right)^2 = \frac{4A}{(A+1)^2}, \quad (73)$$

So Equation 70 becomes

$$S'(E) = \int_{E_c}^{E/2} \frac{3 \sum_S(E') (1+A)^2}{E' 4A} \left(\frac{A+1}{2} \sqrt{\frac{E}{E'}} - \frac{A-1}{2} \sqrt{\frac{E'}{E}} \right) j(E') dE' \quad (74)$$

Now: Treat $\sum_S(E')$ as a constant, and factor $\frac{1}{2}\sqrt{\frac{E'}{E}}$ from the parenthesis term. Also (see equation 47) $J(z, E) = -D \nabla \Phi(z, E) + D i B \Phi(z, E)$; multiplying by $e^{i B z}$ and integrating over z yields $J(E') = D B \Phi(E')$ where the diffusion coefficient D is independent of E' .

In addition let $\varphi = \frac{c}{E'}$, then Equation 74 becomes

$$S'(E) = DB(3\sum_S) \frac{(1+A)^2}{8A} \left(\frac{ev}{cm^2 sec} \right) \int_{E_c}^{E/\alpha} \frac{1}{\sqrt{EE'}} \left[(A+1) \frac{E}{E'} - (A-1) \right] \frac{dE'}{E'} \quad (75)$$

or

$$S'(E) = DB(3\sum_S) \frac{(1+A)^2}{8A} \left\{ (A+1) \frac{\sqrt{E'}}{(E)^{3/2}} \left(-\frac{2}{3} \right) + 2 \frac{A-1}{\sqrt{E'}} \frac{1}{\sqrt{E'}} \right\}_{E_c}^{E/\alpha} \frac{ev}{cm^2 sec},$$

or

$$S'(E) = DB(3\sum_S) \frac{(1+A)^2}{4A} \left\{ (A+1) \frac{\sqrt{E'}}{\left(\frac{E}{2}\right)^{3/2}} \left(-\frac{1}{3} \right) + \frac{1}{3} (A+1) \frac{\sqrt{E'}}{(E_c)^{3/2}} + \frac{A-1}{\sqrt{E'}} \sqrt{\frac{\alpha}{E}} - \frac{A-1}{\sqrt{E'}} \frac{1}{\sqrt{E_c}} \right\} \frac{ev}{cm^2 sec},$$

or

$$S'(E) = DB(3\sum_S) \frac{(1+A)^2}{4A} \frac{ev}{cm^2 sec} \left\{ \frac{A+1}{3} \left[-\alpha^{3/2} \left(\frac{E_c}{E} \right) + \sqrt{\frac{E'}{E_c}} \right] + (A-1) \left[\alpha^{1/2} \left(\frac{E_c}{E} \right) - \sqrt{\frac{E'}{E}} \right] \right\},$$

now $\alpha^{3/2} = \frac{(A-1)^3}{(A+1)^3}$ and $\alpha^{1/2} = \frac{A-1}{A+1}$, so

$$S'(E) = \sum_i D_i B (3 \sum_s)_i \frac{(A_i-1)(A_i+1)^2}{4 A_i} \frac{1}{E_c} \left\{ \frac{1}{3 \alpha_i} \left[\sqrt{\frac{E}{E_c}} - \alpha_i^{3/2} \frac{E_c}{E} \right] + \sqrt{\alpha_i} \left(\frac{E_c}{E} \right) - \sqrt{\frac{E_c}{E}} \right\} \frac{ev}{cm^2 sec} \quad (76)$$

$\alpha E_c \leq E \leq E_c$

Otherwise $S'(E) = 0$.

APPENDIX II. EQUATIONS IN MATRIX FORM

From the B-1 equations (Equations 65 and 69, Appendix I) we may write for each energy of our fine energy mesh:

$$B_{jk} + \sum_{T_k} \phi_k - \sum_{l=1}^{99} \sum_{l,k}^{\circ} \phi_l \Delta_l = S_k^{\circ} \quad k=1, 2, \dots, 99 \quad (1)$$

Expression 1 represents 99 equations and 2 x 99 unknowns.

$$-B\phi_k + 3\gamma_k \sum_{T_k} j_k - \sum_{l=1}^{99} \sum_{l,k}' j_l \Delta_l = S_k' \quad (2)$$

Expression 2 represents 99 equations and 2 x 99 unknowns.

Expressions 1 and 2 represent 2 x 99 equations and 2 x 99 unknowns. Writing out a few equations from 1 and 2:

$$B_{j_1} + (\sum_{T_1} - \sum_{1,1}^{\circ} \Delta_1) \phi_1 - \sum_{2,1}^{\circ} \phi_2 \Delta_2 - \sum_{3,1}^{\circ} \phi_3 \Delta_3 - \dots - \sum_{99,1}^{\circ} \Delta_{99} \phi_{99} = S_1^{\circ}$$

$$B_{j_2} - \sum_{1,2}^{\circ} \phi_1 \Delta_1 + (\sum_{T_2} - \sum_{2,2}^{\circ} \Delta_2) \phi_2 - \sum_{3,2}^{\circ} \phi_3 \Delta_3 - \dots - \sum_{99,2}^{\circ} \Delta_{99} \phi_{99} = S_2^{\circ}$$

$$B_{j_3} - \sum_{1,3}^{\circ} \phi_1 \Delta_1 - \sum_{2,3}^{\circ} \phi_2 \Delta_2 + (\sum_{T_3} - \sum_{3,3}^{\circ} \Delta_3) \phi_3 - \dots - \sum_{99,3}^{\circ} \Delta_{99} \phi_{99} = S_3^{\circ}$$

⋮

$$B_{j_{99}} - \sum_{1,99}^{\circ} \phi_1 \Delta_1 - \sum_{2,99}^{\circ} \phi_2 \Delta_2 - \sum_{3,99}^{\circ} \phi_3 \Delta_3 - \dots + (\sum_{T_{99}} - \sum_{99,99}^{\circ} \Delta_{99}) \phi_{99} = S_{99}^{\circ}$$

$$-B\phi_1 + (3\gamma_1 \sum T_1 - \sum'_{1,1} \Delta_1) j_1 - \sum'_{2,1} j_2 \Delta_2 - \sum'_{3,1} j_3 \Delta_3 - \dots - \sum'_{qq,1} j_{qq} \Delta_{qq} = S'_1$$

$$-B\phi_2 - \sum'_{1,2} j_1 \Delta_1 + (3\gamma_2 \sum T_2 - \sum'_{2,2} \Delta_2) j_2 - \sum'_{3,2} j_3 \Delta_3 - \dots - \sum'_{qq,2} j_{qq} \Delta_{qq} = S'_2$$

$$-B\phi_3 - \sum'_{1,3} j_1 \Delta_1 - \sum'_{2,3} j_2 \Delta_2 + (3\gamma_3 \sum T_3 - \sum'_{3,3} \Delta_3) j_3 - \dots - \sum'_{qq,3} j_{qq} \Delta_{qq} = S'_3$$

⋮

$$-B\phi_{qq} - \sum'_{1,qq} j_1 \Delta_1 - \sum'_{2,qq} j_2 \Delta_2 - \sum'_{3,qq} j_3 \Delta_3 - \dots + (3\gamma_{qq} \sum T_{qq} - \sum'_{qq,qq} \Delta_{qq}) j_{qq} = S'_{qq}$$

In matrix form the above equations become:

$$\underline{B} \underline{j} + \underline{\alpha} \underline{\phi} = \underline{S}^o \quad (3)$$

$$\text{and } -\underline{B} \underline{\phi} + \underline{\beta} \underline{j} = \underline{S}' \quad (4)$$

where B = constant scalar

$\underline{j}$ = 99 component vector

$\underline{\phi}$ = 99 component vector

$\underline{S}^o$ = 99 component vector

$\underline{S}^1$ = 99 component vector

$\underline{\alpha}$ = 99 x 99 element matrix

$\underline{\beta}$ = 99 x 99 element matrix.

Multiplying (4) by B: $-B^2 \underline{\varphi} + B \underline{\beta} \underline{j} = B \underline{S}'$ (5)

Substituting (3) into (5): $-B^2 \underline{\varphi} + \underline{\beta} [\underline{S}^0 - \underline{\alpha} \underline{\varphi}] = B \underline{S}'$

or $-(B^2 + \underline{\beta} \underline{\alpha}) \underline{\varphi} = B \underline{S}' - \underline{\beta} \underline{S}^0$, or $(B^2 + \underline{\beta} \underline{\alpha}) \underline{\varphi} = \underline{\beta} \underline{S}^0 - B \underline{S}'$ (6)

and $\underline{j} = \frac{1}{B} \underline{S}^0 - \frac{1}{B} \underline{\alpha} \underline{\varphi}$ (7)

Since $B^2 \underline{\varphi} = B^2 \underline{1} \underline{\varphi}$ where $\underline{1}$ = unit matrix, we may write $B^2 \underline{\varphi} = \underline{B}^2 \underline{\varphi}$

where $\underline{B}^2$ is a diagonal matrix having elements of B^2 . Equation 6 becomes

$$\underline{\xi} \underline{\varphi} = \underline{\eta} \quad (8)$$

where

$$\xi_{kl} = \sum_j \beta_{kj} \alpha_{jl} \quad k \neq l,$$

and

$$\xi_{kk} = \sum_j \beta_{kj} \alpha_{kj} + B^2 ;$$

also

$$\eta_k = \sum_j \beta_{kj} S_j^0 - B S'_k .$$

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