ENU 6052 - RADIATION TRANSPORT BASICS & APPLICATIONS

INTRODUCTION

Statistical Nature of Matter

Typical macroscopic descriptions of physical phenomena are

$$N(t) = N_o e^{-\lambda t}$$

i.e., the population of radioactive nuclei remaining at time t, and

$$I(x) = I_o e^{-\Sigma x}$$

i.e., the intensity of a monovelocity particle beam reamining uncollided to a penetration x in an interactive medium. There are several conceptual difficulties inherent in these results. To resolve some of them, and provide an introduction to the material of these lectures, consider the radioactivity problem in more detail.

"As good as new" postulate:

The probability that a radionuclide decays in the time period t to $t + \Delta t$ is $\lambda\Delta t$ where λ is a constant which depends on the nuclear specie. Note that Δt must be "small," i.e., $\lambda\Delta t << 1$ and that the probability is t-independent. The quantity of interest, in studying the detailed meaning of the N(t) expression, is $Q_m^{\ell}(\Delta t, t)$ = probability that m nuclei decay in t to $t + \Delta t$ providing that there are ℓ nuclei present at t. Note that for small Δt, the "as good as new" postulate for each nucleus implies that $Q_m^{\ell}(\Delta t, t) = Q_m^{\ell}(\Delta t)$.

Binomial distribution:

$b_m^{\ell}(\xi)$ = probability that m entities (out of ℓ) experience an event if ξ is the probability that each experience the event.

$$b_m^{\ell}(\xi) = \frac{\ell!}{m!(\ell-m)!}\ \xi^m(1-\xi)^{\ell-m}$$

and has the properties

1. $b_m^{\ell}(0) = \delta_{mo}$

2. $b_m^{\ell}(1) = \delta_{m\ell}$

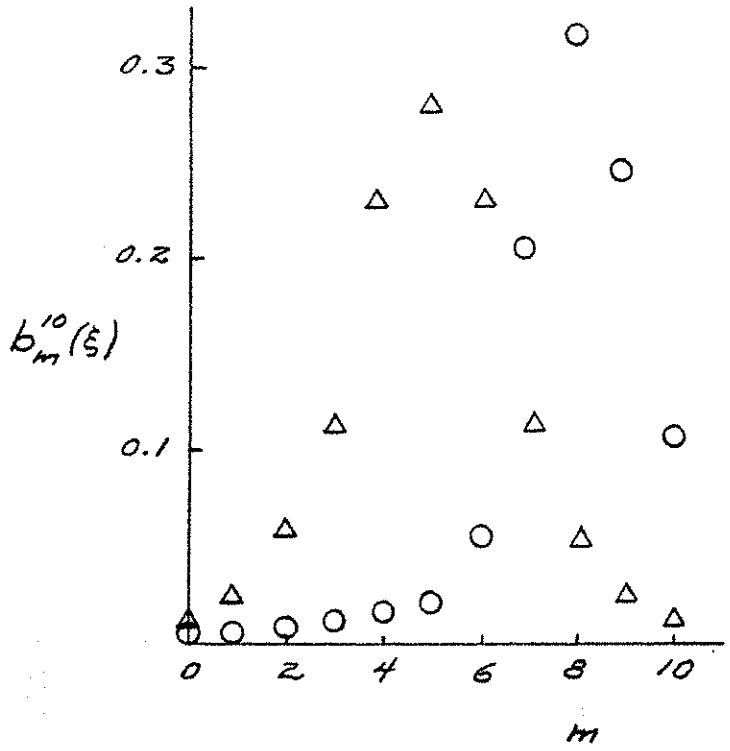
   where $\delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases}$

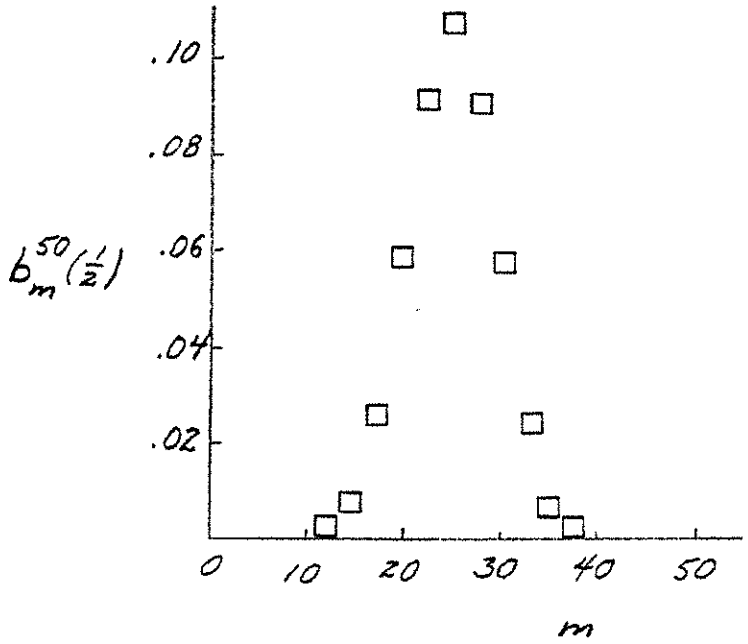
3. $\sum_{m=0}^{\ell} b_m^{\ell}(\xi) = 1$

4. $\sum_{m=0}^{\ell} m b_m^{\ell}(\xi) = \ell\xi$

5. $\sum_{m=0}^{\ell} m^2 b_m^{\ell}(\xi) = \ell\xi + \ell(\ell-1)\xi^2$

Examples are $\Delta(\xi = 0.5)$ $\circ(\xi = 0.8)$





Poisson distribution and normal distribution:

For $\xi \ll 1$ and $\ell \gg 1$,

$$b_m^{\ell}(\xi) \approx p_m^{\ell}(\xi) = \frac{(\ell\xi)^m e^{-\ell\xi}}{m!}$$

which is the Poisson probability distribution. An alternative approximation is the normal distribution which is defined for the continuous variable μ, i.e.,

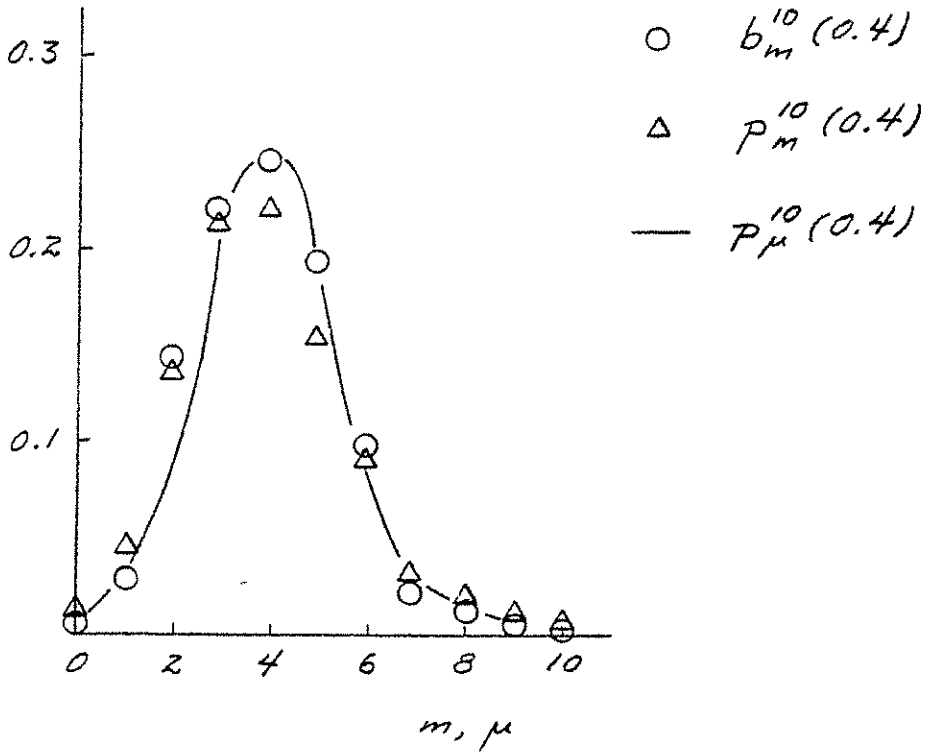
discrete $m \rightarrow$ continuous μ,

$$p_{\mu}^{\ell}(\xi) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp[-(\mu-\ell\xi)^2/2\sigma^2]$$

where $\sigma^2 = \ell\xi(1-\xi)$. $p_{\mu}^{\ell}(\xi)$ is a continuous probability distribution in the sense that

$p_{\mu}^{\ell}(\xi)d\mu$ = probability that μ in the range μ to $\mu + d\mu$ entities out of ℓ experience the event.

Example comparison of $b_m^{\ell}(\xi)$, $p_m^{\ell}(\xi)$ and $p_\mu^{\ell}(\xi)$. $\ell = 10 \quad \xi = 0.4$



Radioactivity relations:

$$Q_m^{\ell}(\Delta t) = b_m^{\ell}(\lambda \Delta t) \text{ for } \lambda \Delta t << 1.$$

Consider N_o radionuclei present at $t = 0$ and define

$P_j(t)$ = probability that j nuclei have not decayed by time t.

$N(t) = \sum_{j=0}^{N_o} jP_j(t)$ = "expected" (i.e., average) number of nuclei which have not decayed by t. Question - What temporal relation does N(t) satisfy?

Solution - For small Δt,

$$\sum_j jP_j(t + \Delta t) = \sum_{j,m} jP_{j+m}(t)Q_m^{j+m}(\Delta t)$$

$$= \sum_\ell \ell P_\ell(t) \sum_{m=0}^{\ell} Q_m^\ell(\Delta t) - \sum_\ell P_\ell(t) \sum_{m=0}^{\ell} mQ_m^\ell(\Delta t)$$

But, $\sum_{m=0}^{\ell} Q_m^\ell(\Delta t) = 1$ and

$$\sum_{m=0}^{\ell} mQ_m^\ell(\Delta t) = \sum_{m=0}^{\ell} mb_m^\ell(\lambda\Delta t) = \ell\lambda\Delta t$$

whence,

$$N(t + \Delta t) - N(t) = -\lambda N(t)\Delta t$$

$$\frac{N(t + \Delta t) - N(t)}{\Delta t} = -\lambda N(t)$$

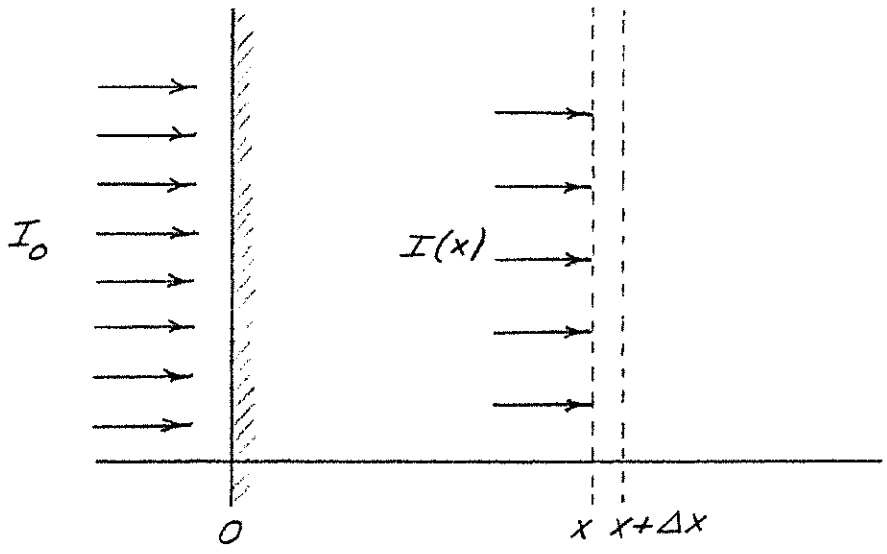
and from the limit as $\Delta t \to 0$,

$$\frac{dN(t)}{dt} = -\lambda N(t)$$

with solution $N(t) = N_o e^{-\lambda t}$

In the familiar radioactivity relation, N(t) actually means the statistical average result obtained with many measurements commencing with identical initial conditions.

Particle transport problem:



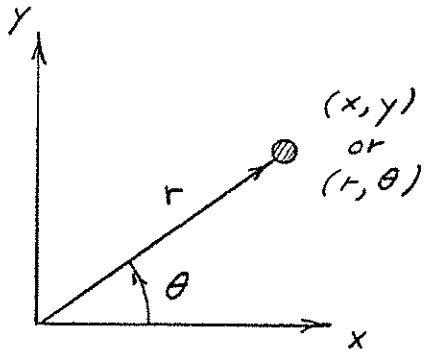
Consider a beam of monovelocity particles perpendicularly incident on a half-space of targets of uniform density. For each particle, the probability that the first interaction with a target occurs between x and $x + \Delta x$ is x-independent and, if Δx is small enough, is given by $\Sigma\Delta x$. If $Q_m^{\ell}(\Delta x)$ = probability that m particles have first interaction in x to $x + \Delta x$ with ℓ uninteracted particles at x, then $Q_m^{\ell}(\Delta x) = b_m^{\ell}(\Sigma\Delta x)$. And if $I(x) = \sum_j jP_j(x)$, then $\frac{dI(x)}{dx} = -\Sigma I(x)$ implies $I(x) = I_o e^{-\Sigma x}$.

Coordinate Transformations

Vector $\underline{x}$ means $(x_1, x_2, \ldots, x_n)$, e.g., location on a line $\underline{x}$ means x, Cartesian location on a plane $\underline{x}$ means (x,y), Cartesian location in configuration $\underline{x}$ means (x,y,z). A vector $\underline{x}$ can be expressed in alternate coordinates, i.e., $\underline{x}$ can be represented by

$$(x_1, x_2, \ldots, x_n) \text{ or } (u_1, u_2, \ldots, u_n),$$

e.g., location on a plane.



$r = r\ (x,y)$

$\theta = \theta\ (x,y)$

and if angle limits are set to yield one-to-one transformation

$x = x\ (r,\theta)$ $y = y\ (r,\theta)$

Differential element $d^n x$ means $dx_1 dx_2 dx_3 \ldots dx_n$, e.g., line $d^1 x$ means dx, Cartesian plane $d^2 x$ means dxdy, polar plane $d^2 x$ means $dr d\theta$, spherical polar configuration $d^3 x$ means $dr d\theta d\phi$. The function $f(\underline{x})$ means $f(x_1, x_2, \ldots x_n)$ and if the function is itself a vector, $\underline{f}(\underline{x})$ means $[f_1(x_1 \ldots x_n), \ldots f_m(x_1 \ldots x_n)]$.

Density Functions:

$f(\underline{x})$ will often represent the density of some physical property in the space of $\underline{x}$.

Examples are

1. Mass density along a line, i.e., $f(x)$ such that the mass between $x=a$ and $x=b$ $(a<b)$ is given by $\int_a^b f(x)dx$.

2. Particle density in configuration, i.e., $f(x,y,z)$ such that the number of particles in volume V is given by $\int_V f(x,y,z)dxdydz$.

3. Particle kinetic energy spectrum, i.e., $f(E)$ such that the number of particles with kinetic energy between E_1 and E_2 $(E_1 < E_2)$ is given by $\int_{E_1}^{E_2} f(E)dE$.

Transformation of coordinates:

One-dimensional case -

Let $u = u(x)$ be a one-to-one transformation $(x \to u)$ with inverse $x=x(u)$ describing transformation $(u \to x)$, and $f(x)$ be a density function such that $F = \int_a^b f(x)dx$ has some physical significance. Problem - To express F as an integral over u rather than x and thereby deduce the form of the density function in u-space.

Solution - $x = x(u)$ implies $dx = \frac{dx}{du}\,du$

and

$$F = \int_{u(a)}^{u(b)} f[x(u)]\,\frac{dx}{du}\,du$$

However, it is customary to choose integral limits such that

(lower limit) < (upper limit).

Moreover, if $u(x)$ is one-to-one, then it is monotonic. Whence,

$$F = \int_{\min u}^{\max u} f[x(u)]\,\left|\frac{dx}{du}\right|\,du$$

and conclude that

$$g(u) = f[x(u)] \left|\frac{dx}{du}\right|$$

is the density function in u-space such that $F = \int g(u)\, du$, e.g., $E = \frac{1}{2}mv^2$ ($v \geq 0$) and $f(v)$ represent particle speed spectrum.

$F = \int_{v_1}^{v_2} f(v)\, dv$ = number of particles with speed in range v_1 to v_2.

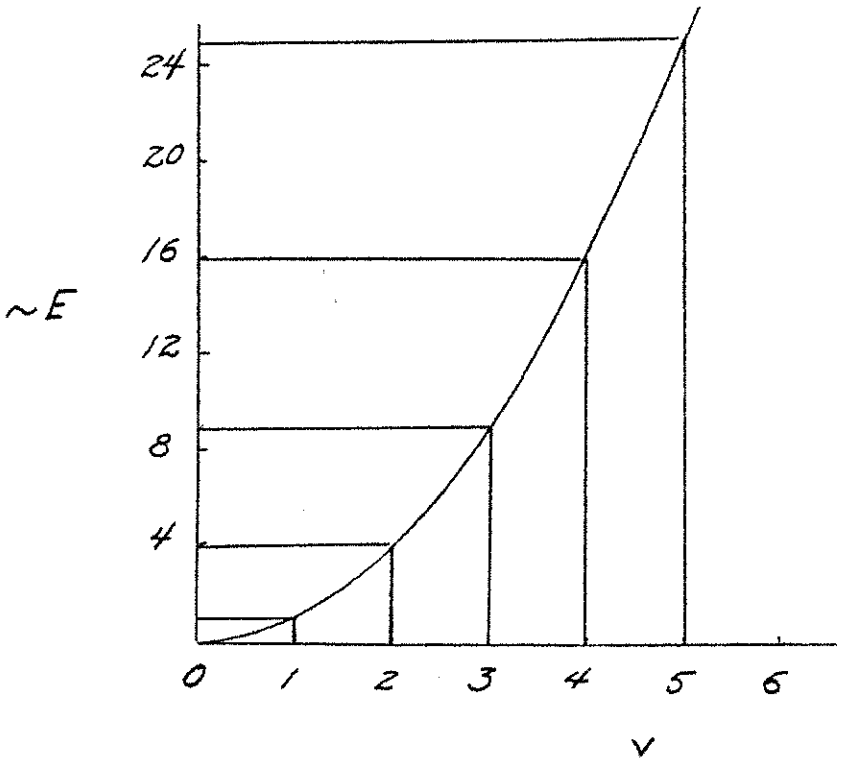
The corresponding particle kinetic energy spectrum is given by

$$g(E) = f\left(\sqrt{\frac{2E}{m}}\right) \sqrt{\frac{1}{2Em}}$$

and

$$F = \int_{E_1}^{E_2} g(E)dE, \quad E_i = \tfrac{1}{2}mv_i^2$$

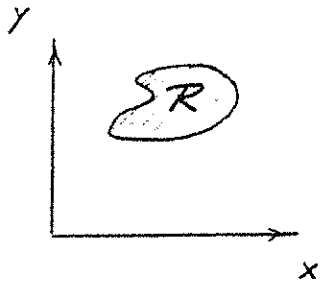
An explanation of the varying form of spectrum (density function) is aided by noting that equal intervals of v are transformed into unequal intervals of E as illustrated.



Thus, for example, it is expected that a constant density (spectrum) in speed space implies an energy spectrum which decreases with increasing E.

Two-dimensional case -

Let $u = u(x,y)$, $v = v(x,y)$ be a one-to-one transformation $(x,y) \to (u,v)$ with inverse $x = x(u,v)$, $y = y(u,v)$, i.e., $(u,v) \to (x,y)$.



$$F = \iint_R f(x,y)\, dxdy$$

$$F = \iint_R f[x(u,v),\ y(u,v)]\left|J\left(\frac{x,y}{u,v}\right)\right| dudv$$

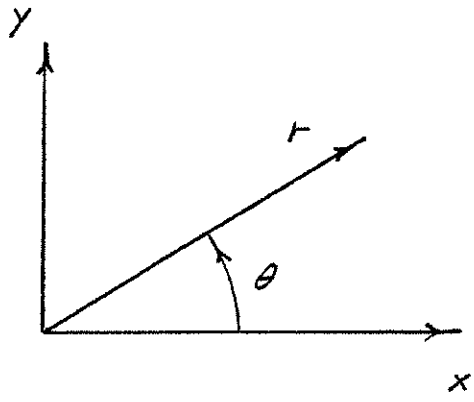
where the Jacobian of the transformation is defined by

$$J\left(\frac{x,y}{u,v}\right) = \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{vmatrix}$$

The density function in (u,v) - space is

$$g(u,v) = f[x(u,v),\ y(u,v)]\left|J\left(\frac{x,y}{u,v}\right)\right|$$

e.g.,



$$x = r\cos\theta$$

$$y = r\sin\theta$$

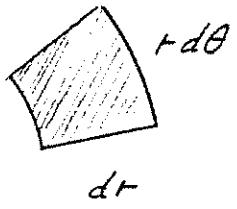
$$J\left(\frac{x,y}{r,\theta}\right) = r$$

Thus, $g(r,\theta) = f(r\cos\theta, r\sin\theta)\ r$

$$F = \iint_R g(r,\theta)\ dr d\theta, \text{ or equivalently,}$$

$$F = \iint_R \underbrace{f(r\cos\theta, r\sin\theta)}_{*} \underbrace{r\ dr d\theta}_{*}$$

*Note that the indicated grouping of factors is not in the spirit of expressing density functions and differential elements in (r,θ) - space. Rather, the grouping implies merely a change of coordinates for performing the integration $\iint_R f(x,y)\ dxdy$, and



r dr dθ is an area differential of the type dxdy, i.e., in (x,y) - space, not (r,θ) - space.

n-dimensional case -

Let $\underline{x} = \underline{x}(\underline{u})$ have inverse $\underline{u} = \underline{u}(\underline{X})$.

$$F = \int_R f(x)d^n x = \int_R g(u)d^n u$$

where

$$g(\underline{u}) = f[\underline{x}(\underline{u})]\ \left| J\left(\frac{\underline{x}}{\underline{\underline{u}}}\right)\right|$$

$$J\left(\frac{\underline{x}}{\underline{\underline{u}}}\right) = \begin{vmatrix} \frac{\partial x_1}{\partial u_1} & \frac{\partial x_1}{\partial u_2} & \cdots & \frac{\partial x_1}{\partial u_n} \\ \frac{\partial x_2}{\partial u_1} & & & \\ & & & \\ \frac{\partial x_n}{\partial u_1} & \cdots & & \frac{\partial x_n}{\partial u_n} \end{vmatrix}$$

Particle Density Distributions

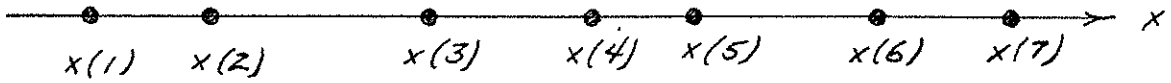
Configuration-space density:

Consider N particles labelled $\alpha = 1, 2, \ldots, N$. The configuration of these particles in 3-space is completely specified by the set of 3N numbers $\{\underline{r}(\alpha), \alpha = 1, 2, \ldots, N\}$.

There are at least two reasons why such a dynamic state description is unrealistic -

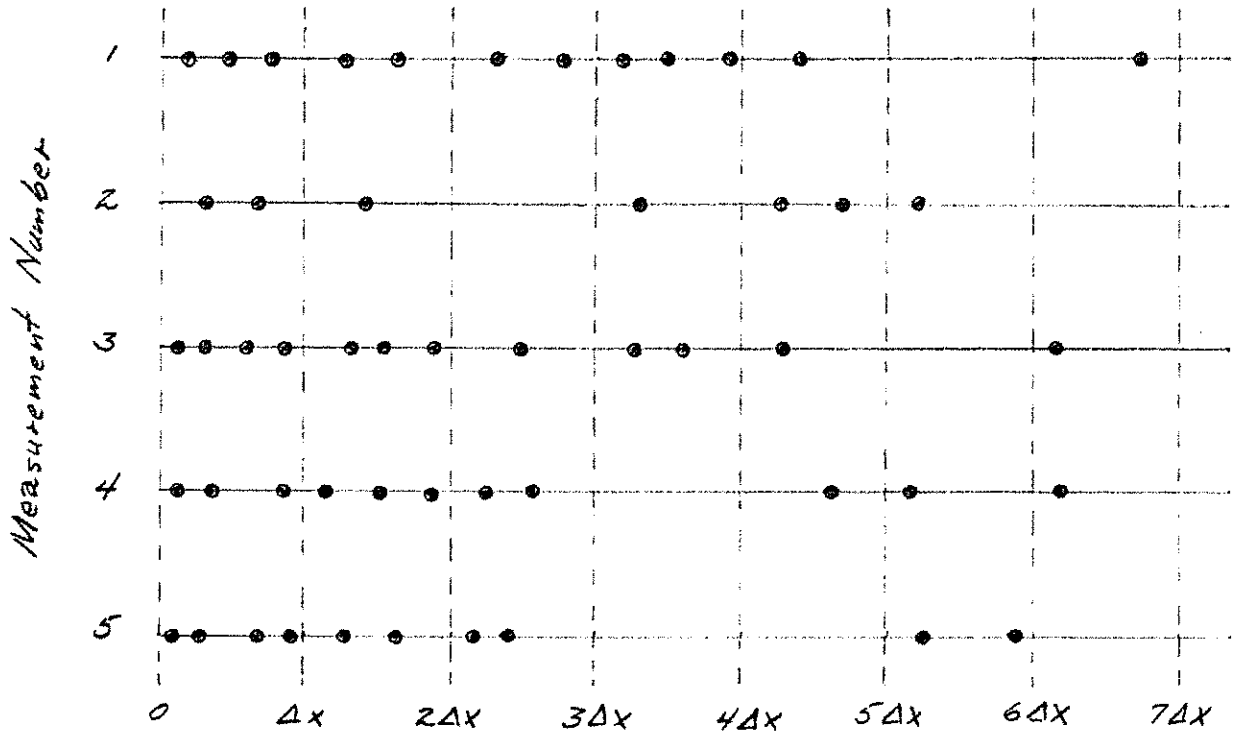
1. N of interest is often larger than 10^{20}.
2. Particle interactions are thought to be actually statistical in nature (quantum mechanics) and thus a precise specification is of questionable relevance.

Thus, there is motivation for developing the ideas of describing particles by statistical distributions and their moments (e.g., averages). For example, the one-dimensional particle configuration



is presumably unpredictable (i.e., with given initial conditions, identical experiments yield different results at time of measurement). Instead of specifying the set $\{x(\alpha)\}$ a particle density function is developed and defined in a probabilistic fashion.

For example, suppose the following is obtained in 5 measurements.



With respect to this set of measurements, define

$P_j(x,\Delta x)$ = probability of finding j particles in Δx at x.

If there are many more than 5 measurements performed, then often

$$\lim_{\Delta x \to 0} \quad P_j(x,\Delta x) = \delta_{j0}$$

and the limit is approached smoothly such that

$$N(x) = \lim_{\Delta x \to 0} \quad \frac{1}{\Delta x} \sum_j j P(x,\Delta x)$$

has a clear meaning,

$$\int_a^b N(x)dx = N(a<x<b) = \text{"expected" (or, average) number of particles}$$

found in the interval $a \leq x \leq b$ over many identical performances of the experiment. Generalizing to n-dimensional configuration space (n=1, a line; n=2, a surface; n=3, a volume). $N(\underline{r})$ is so defined such that

$$\int_R N(\underline{r}) d^n r = N(R)$$

i.e., the expected number of particles in region R.

Transformation of configuration density:

Let $\underline{r}' = \underline{r}'(\underline{r})$ be a one-to one transformation with inverse $\underline{r} = \underline{r}(\underline{r}')$. Then,

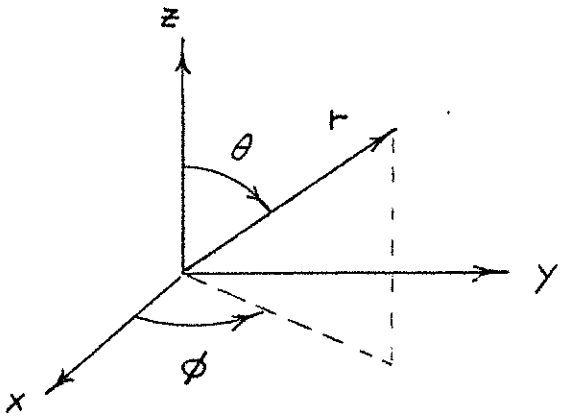
$$N(R) = \int_{\mathcal{R}} N(\underline{r}) d^n r = \int_R N'(\underline{r}') d^n r'$$

where

$$N'(\underline{r}') = N(\underline{r}(\underline{r}')) \left| J\left(\frac{\underline{r}}{\underline{r}'}\right) \right|$$

Note that N' represents the particle density function in $\underline{r}'$ - coordinates and is usually a different function of its variables than N is of its variables.

For example, consider the 3-space transformation from Cartesian coordinates (x,y,z) to spherical polar coordinates (r,θ,ϕ).



$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

$$0 \leq \theta \leq \pi$$

$$0 \leq \phi \leq 2\pi$$

$$J\left(\frac{x,y,z}{r,\theta,\phi}\right) = r^2\sin\theta$$

$N'(r,\theta,\phi) = N(r\sin\theta\cos\phi,\ r\sin\theta\sin\phi,\ r\cos\theta)r^2\sin\theta$ where $N'(r,\theta,\phi)$ is the particle density in spherical polar coordinates, and $N(x,y,z)$ is the particle density in Cartesian coordinates.

Moments of the configuration density:

Zeroth-order moments -

Restricting attention to the usual 3-space density $N(\underline{r})$ with $\underline{r} = (r_1,r_2,r_3)$, define the zeroth-order moments as

$$N = \iiint N(r_1,r_2,r_3)\ dr_1dr_2dr_3$$

$$N_1(r_1) = \iint N(r_1,r_2,r_2)dr_2dr_3$$

and similar definitions for

$N_1(r_2)$ and $N_1(r_3)$, and

$$N_2(r_1,r_2) = \int N(r_1,r_2,r_3)dr_3$$

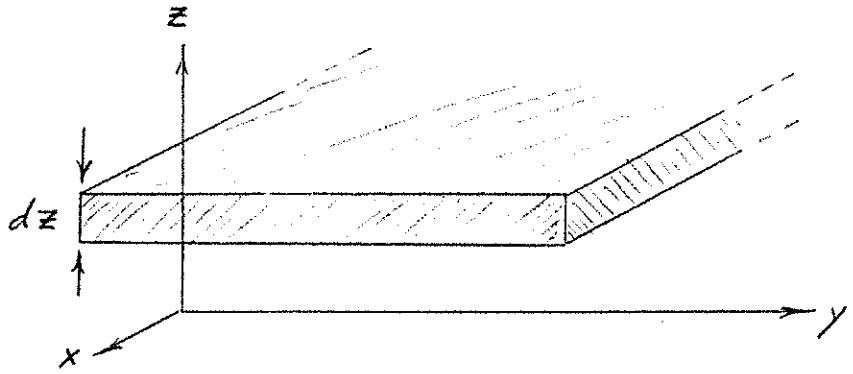
and similar definitions for $N_2(r_2,r_3)$ and $N_2(r_3r_1)$. Note that if a region (limits) are unspecified on an integral, then the usual meaning (in these notes) is to cover the entire relevant space of the variable. For example, the Cartesian 3-space zeroth-order particle densities are

$$N = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} N(x,y,z)dxdydz$$

and represents the total number of particles (everywhere).

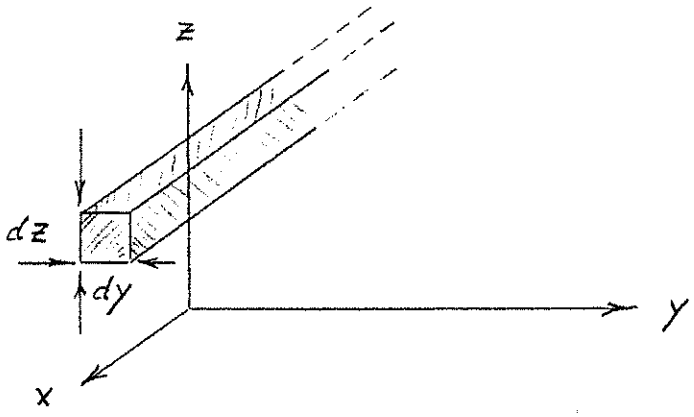
$$N_1(z) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} N(x,y,z)dxdy$$

and represents the particle density per illustrated relevant volume element



$$N_2(y,z) = \int_{-\infty}^{+\infty} N(x,y,z)dx$$

and represents the particle density per illustrated relevant volume element.



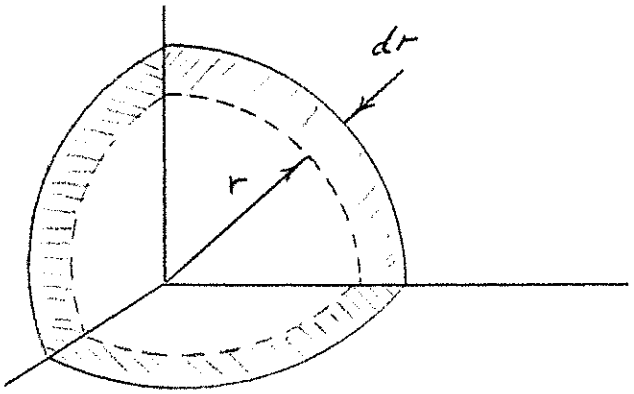
As another example, consider spherical polar 3-space and designate the particle density in spherical polar coordinates as $N'(r,\theta,\phi)$.

$$N = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} N'(r,\theta,\phi)\ dr d\theta d\phi$$

and, again represents the total number of particles.

$$N_1(r) = \int_0^{\pi} \int_0^{2\pi} N'(R,\theta,\phi)\ d\theta d\phi$$

and represents the particle density per illustrated spherical shell volume element.



Note that if the Cartesian 3-space density is a constant, i.e.,

$$N(x,y,z) = C, \text{ then}$$

$$N'(r,\theta,\phi) = Cr^2\sin\theta$$

and

$$N_1(r) = Cr^2 \int_0^{\pi} \int_0^{2\pi} \sin\theta d\theta d\phi$$

$$= 4\pi r^2 C$$

Higher-order moments -

Recall the one-dimensional example of particles distributed along the x-axis. A particular measurement yields $\{x(\alpha), \alpha=1, \ldots, N\}$ and the familiar definition of the average value of displacement x is

$$\langle x \rangle = \frac{1}{N} \sum_{\alpha=1}^{N} x(\alpha)$$

For the equivalent particle expected distribution, $N(x)dx$ = number of particles in dx about x and

$$\langle x \rangle = \frac{1}{N} \int_{-\infty}^{+\infty} xN(x)dx$$

Generalizing (in one-dimension),

$$\langle g(x)\rangle = \frac{1}{N}\int_{-\infty}^{+\infty} g(x)N(x)dx$$

where g(x) is any meaningful description of the particle location.

Generalizing to n-dimensions,

$$\langle g(\underline{r})\rangle = \frac{1}{N}\int g(\underline{r})N(\underline{r})d^n r$$

and, if g is a vector quantity itself,

$$\langle \underline{g}(\underline{r})\rangle = \frac{1}{N}\int \underline{g}(\underline{r})N(\underline{r})d^n r$$

Examples -

1. Let $g(\underline{r}) = r$ in 3-space and use spherical polar coordinates.

$$\langle r\rangle = \frac{1}{N}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} rN'(r,\theta,\phi)drd\theta d\phi$$

or, in terms of the Cartesian density N(x,y,z)

$$\langle r\rangle = \frac{1}{N}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} rN(x,y,z)r^2\sin\theta drd\theta d\phi$$

or, equivalently

$$\langle r\rangle = \frac{1}{N}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (x^2+y^2+z^2)^{\frac{1}{2}} N(x,y,z)dxdydz$$

2. Let $\underline{g}(\underline{r}) = \underline{r}$ and use spherical polar coordinates

$$\langle \underline{r}\rangle = \frac{1}{n}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} \underline{r}N'(r,\theta,\phi)drd\theta d\phi$$

An "isotropic" distribution is defined by N = N(r). For an isotropic distribution $\langle \underline{r}\rangle = 0$ but $\langle r\rangle = 0$ only if all particles are at the origin of coordinates.

Configuration-velocity space density:

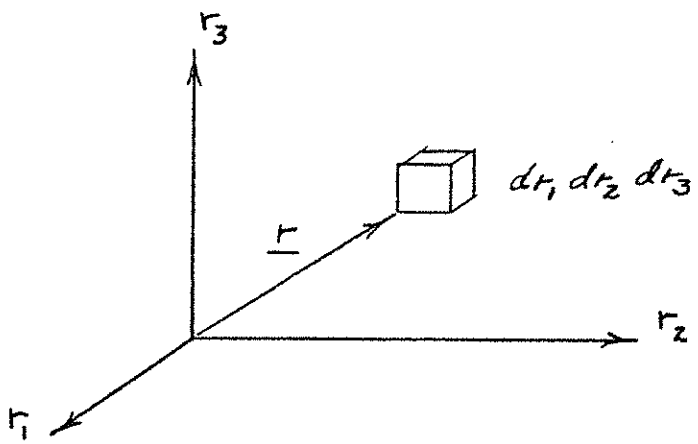
For each particle (labeled α) $\underline{r}(\alpha) = \underline{r}_\alpha(t)$ and $\underline{v}(\alpha) = \underline{v}_\alpha(t)$ are the particle trajectory relations and, thus, $\underline{r}(\alpha)$ is a function of $\underline{v}(\alpha)$. In order to describe the expected distribution of particles in both configuration (location) and velocity (energy and direction-of-travel), consider the 6-dimensional $(\underline{r}, \underline{v})$ - space where $\underline{r} = (r_1, r_2, r_3)$ describes location and $\underline{v} = (v_1, v_2, v_3)$ describes velocity. Note that in this abstract space $\underline{r}$ and $\underline{v}$ are considered as independent variables. The particle density $n(\underline{r},\underline{v},t)$ is defined such that $\int_{V_r}\int_{V_v} n(\underline{r},\underline{v},t)\, d^3r d^3v$ = the expected particle population in configuration volume V_r with velocities in the range of volume V_v in $\underline{v}$-space. An alternative particle distribution description is in terms of $\underline{r}$, E and $\hat{\Omega}$ where E is the particle kinetic energy and $\hat{\Omega}$ unit vector in the direction-of-travel, i.e., $E = \frac{1}{2}mv^2$ and $\hat{\Omega} = \frac{\underline{v}}{v}$, where m is the particle mass. The particle density $n(\underline{r},E,\hat{\Omega},t)$ is then defined such that

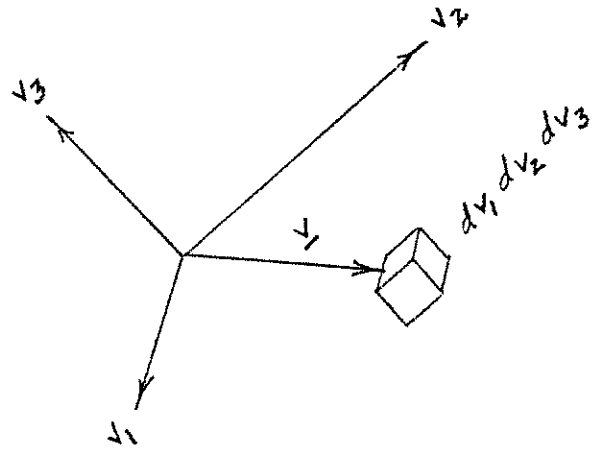
$$\int_V \int_{E_1}^{E_2} \int_W n(\underline{r},E,\hat{\Omega},t) d^3r dE d^2\Omega$$

is the expected particle population in configuration volume V with energy in the internal E_1 to E_2 and with direction-of-travel in the solid angle W, at time t.

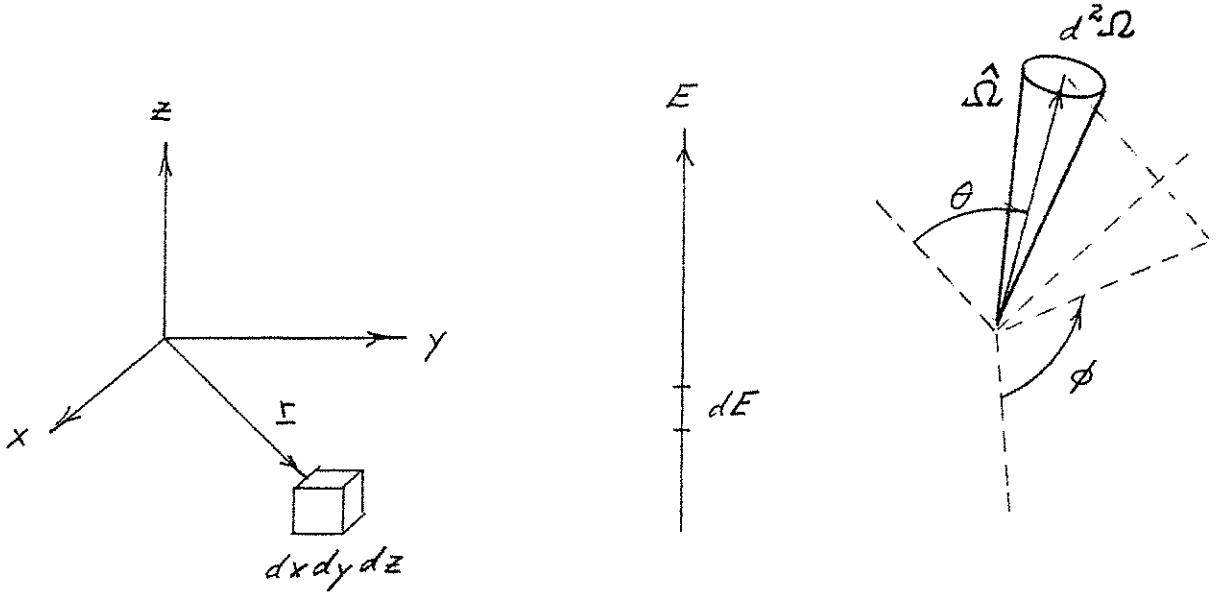
Examples of 6-dimensional coordinate systems -

1. $(\underline{r},\underline{v})$ - space, Cartesian in both $\underline{r}$ and $\underline{v}$.





2. $(\underline{r},E,\hat{\Omega})$ - space, Cartesian in $\underline{r}$ and spherical polar in $\hat{\Omega}$.



Transformation of $(\underline{r},\underline{v})$ coordinates:

Let $\underline{r}' = \underline{r}'(\underline{r},\underline{v})$, $\underline{v}' = \underline{v}'(\underline{r},\underline{v})$ be a one-to-one transformation with inverse $\underline{r} = \underline{r}(\underline{r}',\underline{v}')$, $\underline{v} = \underline{v}(\underline{r}',\underline{v}')$. Then $n'(\underline{r}',\underline{v}',t) = n[\underline{r}(\underline{r}',\underline{v}'), \underline{v}(\underline{r}',\underline{v}'),t]$ $\left|J\left(\frac{\underline{r},\underline{v}}{\underline{r}',\underline{v}'}\right)\right|$ A usual special case is the simpler transformation $\underline{r}' = \underline{r}'(\underline{r})$, $\underline{v}' = \underline{v}'(\underline{v})$. Then $n'(\underline{r}',\underline{v}',t) = n[\underline{r}(\underline{r}'), \underline{v}(\underline{v}'),t]$ $\left|J\left(\frac{\underline{r}}{\underline{r}'}\right)\right| \left|J\left(\frac{\underline{v}}{\underline{v}'}\right)\right|$

Moments of $n(\underline{r},\underline{v},t)$:

$N(\underline{r},t) = \int n(\underline{r},\underline{v},t)d^3v$ = number density in configuration space.

$N(\underline{v},t) = \int n(\underline{r},\underline{v},t)d^3r$ = averaged velocity spectrum.

$N(t) = \iint n(\underline{r},\underline{v},t)d^3rd^3v$ = total particle population.

$\bar{g}(\underline{r},t) = \frac{1}{N(\underline{r},t)} \int g(\underline{r},\underline{v},t)n(\underline{r},\underline{v},t)d^3v$ are $\underline{v}$-space moments (or averages) of relevant physical quantities g.

$\langle \bar{g} \rangle (t) = \frac{1}{N(t)} \iint g(\underline{r},\underline{v},t)\, n(\underline{r},\underline{v},t)\, d^3rd^3v$ are $(\underline{r},\underline{v})$-space moments (or averages) over total particle populations.

Delta Functions

Discrete index delta function:

δ_{mn} has previously been defined in these lectures as

$$\delta_{mn} = \begin{cases} 1 \text{ if } m=n \\ 0 \text{ if } m\neq n \end{cases}$$

where m and n are integers and are thus a discrete set. An important feature of δ_{mn} is the collapse of summations to a single term, i.e.,

$$\sum_n A_n \delta_{mn} = A_m$$

Note that if the set of terms $\{A_n\}$ is arbitrary, then this collapsing property leads directly to the definition and can therefore be itself considered a definition.

Dirac delta function:

The Dirac delta function plays the same role with continuous variables that δ_{mn} plays with a discrete index. In one-dimension, $\delta(x-a)$ is defined by the relation:

$$\int_{x_1}^{x_2} \delta(x-a)f(x)dx = \begin{cases} f(a) \text{ if } x_1 \leq a \leq x_2 \\ 0 \text{ if } a<x_1 \text{ or } a>x_2 \end{cases}$$

which implies that $\delta(x-a)$ can be considered as the limit of an "ordinary" function $F(x,a)$ with the properties

1. $\int_{-\infty}^{+\infty} F(x,a)dx = 1$
2. In the limit, $F(x,a) = 0$ everywhere in x except near $x = a$ where it must be highly peaked.

In n-dimensional space, $\delta(\underline{x}-\underline{a})$ is defined by

$$\int_R \delta(\underline{x}-\underline{a})f(\underline{x})d^n x = \begin{cases} f(\underline{a}) \text{ if } \underline{a} \text{ in } R \\ 0 \text{ if } \underline{a} \text{ is not in } R \end{cases}$$

For example, in Cartesian 3-space, the definition is satisfied if

$$\delta(\underline{r}-\underline{a}) = \delta(x-a_x)\delta(y-a_y)\delta(z-a_z)$$

Dirac delta functions are density distributions and thus transform as such, i.e., if $\underline{u} = \underline{u}(\underline{x})$ with inverse $\underline{x} = \underline{x}(\underline{u})$, then

$$\delta'(\underline{u}-\underline{b}) = \delta[\underline{x}(\underline{u})-\underline{a}]\left|J\left(\frac{\underline{x}}{\underline{u}}\right)\right|$$

where $\underline{b} = \underline{u}(\underline{a})$.

Interaction Rate Densities

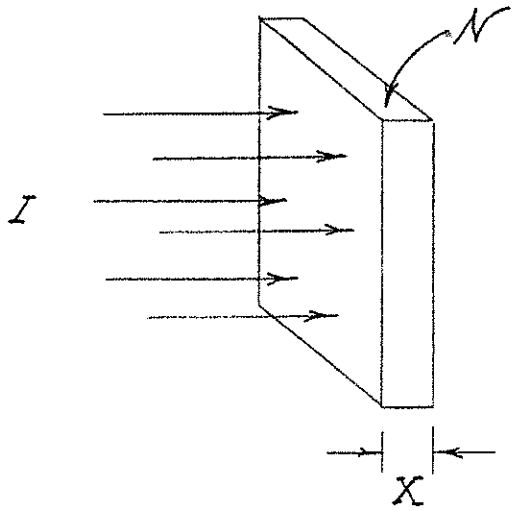
Binary interaction description:

Consider a beam of monovelocity particles perpendicularly incident on a "thin" slab of stationary targets. Let

I = particles beam intensity (in cm^{-2} sec^{-1})

N = target density (in cm^{-3})

X = target slab thickness (in cm)



Expect that the i-type particle-target interaction rate is proportional to

$$N \times I$$

and define the "microscopic cross section" for an i-type binary interaction by

$$\left\{\begin{matrix}\text{Interaction rate of} \\ \text{type i per cm}^2 \text{ of the} \\ \text{target slab}\end{matrix}\right\} = \sigma_i N \times I$$

Let F_i - i-type interaction rate density (in cm^{-3} sec^{-1}). For the slab experiment,

$$F_i = \frac{1}{X}(\sigma_i N \times I) = N\sigma_i I$$

Cross section and flux:

For the slab experiment, the "macroscopic cross section" is defined by $\Sigma_i = N\sigma_i$ (in cm^{-1}). Note that for a monovelocity particle beam, I = Nv. For the case of monoenergetic particles, define the particle flux by $\Phi = Nv$ (in cm^{-2} sec^{-1}) and the interaction rate density expression is generalized to

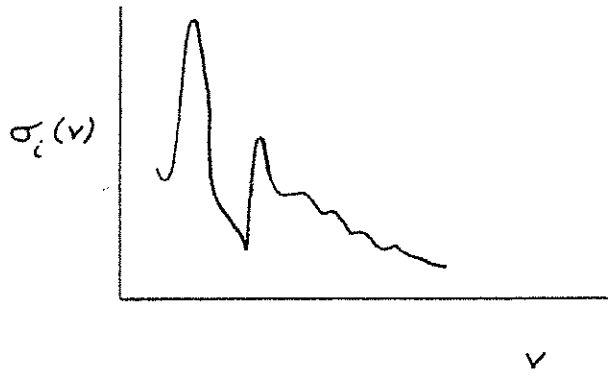
$$F_i = \Sigma_i \Phi \quad cm^{-3} sec^{-1}$$

for a monoenergetic (but, not necessarily monodirectional) particle distribution in a field of stationary targets.

Cross section energy-dependence:

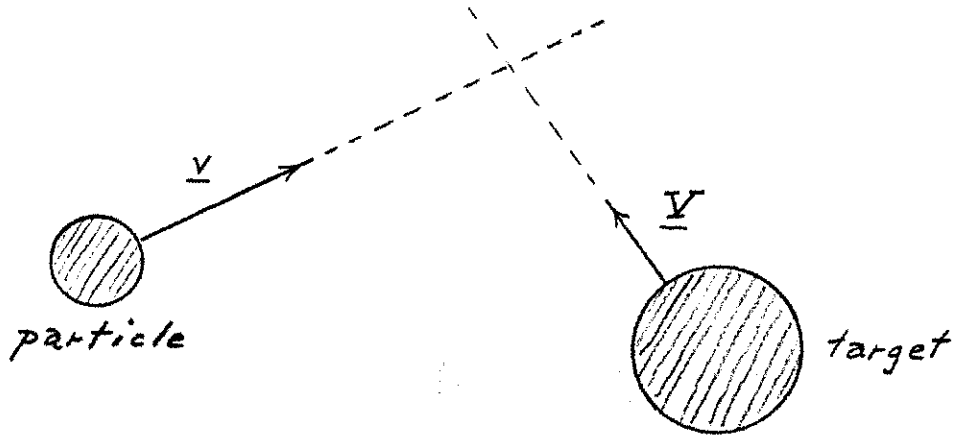
$F_i = N\sigma_i Nv$ for the slab experiment. Consider varying v and also varying $N \sim \frac{1}{v}$ such that Nv is v-independent. N is certainly v-independent. Usually find that $F_i = F_i(v)$ implies $\sigma_i = \sigma_i(v)$, i.e., the "interaction area" varies with the particle approach speed.

Example - neutron-nucleus resonance interaction



The case of moving targets:

Consider a particle with velocity v which interacts with a target with velocity V.



Precollision conditions.

In many cases, find that σ_i depends only on the "relative approach speed" $|\underline{v} - \underline{V}|$, i.e.,

$$\sigma_i = \sigma_i (|\underline{v} - \underline{V}|)$$

Consider the i-type interaction rate density of a particle distribution $n(\underline{v})$ with a target distribution $N(\underline{v})$. Define $f_i(\underline{v},\underline{V})$ by

$f_i(\underline{v},\underline{V})\ d^3v d^3V$ = i-type interaction rate density of particles in d^3v at $\underline{v}$ with targets in d^3V at $\underline{V}$.

$$f_i(\underline{v},\underline{V})\ d^3v d^3V = \sigma_i(|\underline{v} - \underline{V}|)|\underline{v} - \underline{V}| n(\underline{v}) d^3v N(\underline{V}) d^3V$$

In these terms

$$F_i = \iint f_i(\underline{v},\underline{V}) d^3v d^3V$$

$$F_i = \iint \sigma_i(|\underline{v}-\underline{V}|)|\underline{v}-\underline{V}| n(\underline{v}) N(\underline{V}) d^3v d^3V$$

Average macroscopic parameters:

Average cross section and integral flux -

It is often useful ~~useful~~ to define the integral particle flux by

$$\Phi = \int v n(\underline{v}) d^3v = N\overline{v}$$

and, to then express the i-type interaction rate density by

$$F_i = \overline{\Sigma}_i \Phi$$

The averaging process for the cross section has thereby been designated as

$$\overline{\Sigma}_i = \frac{\iint \sigma_i(|\underline{v}-\underline{V}|)|\underline{v} - \underline{V}| n(\underline{v}) N(\underline{V}) d^3v d^3V}{\int v n(\underline{v}) d^3v}$$

Examples -

1. Case of stationary targets, i.e., $N(\underline{V}) = N\delta(\underline{V})$ where N is the total target density (in cm^{-3}).

$$\bar{\Sigma}_i = \frac{N\int \sigma_i(v)vn(\underline{v})d^3v}{\int vn(\underline{v})d^3v}$$

$$= N\frac{\overline{v\sigma_i(v)}}{\bar{v}}$$

2. Case of stationary targets and monoenergetic particles, i.e., $n(\underline{v}) = n_2(\hat{\Omega})\,\delta(v-v_o)$ where $n_2(\hat{\Omega})$ is the particle direction-of-travel distribution.

$$\bar{\Sigma}_i = N\sigma_i(v_o)$$

3. Case of stationary targets and a classical equilibrium distribution of particles, i.e.,

$$n(\underline{v}) = N\left(\frac{m}{2\pi kT}\right)^{3/2} \exp[-mv^2/2kT]$$

$$\bar{v} = 2\left(\frac{2kT}{\pi m}\right)^{1/2} = KT^{1/2}$$

$$\bar{\Sigma}_i = N\frac{\overline{v\sigma_i(v)}}{KT^{1/2}}$$

4. Case of a $\frac{1}{v}$-cross section, i.e.,

$$\sigma_i(|\underline{v} - \underline{V}|) = \frac{C}{|\underline{v}-\underline{V}|} \quad .$$

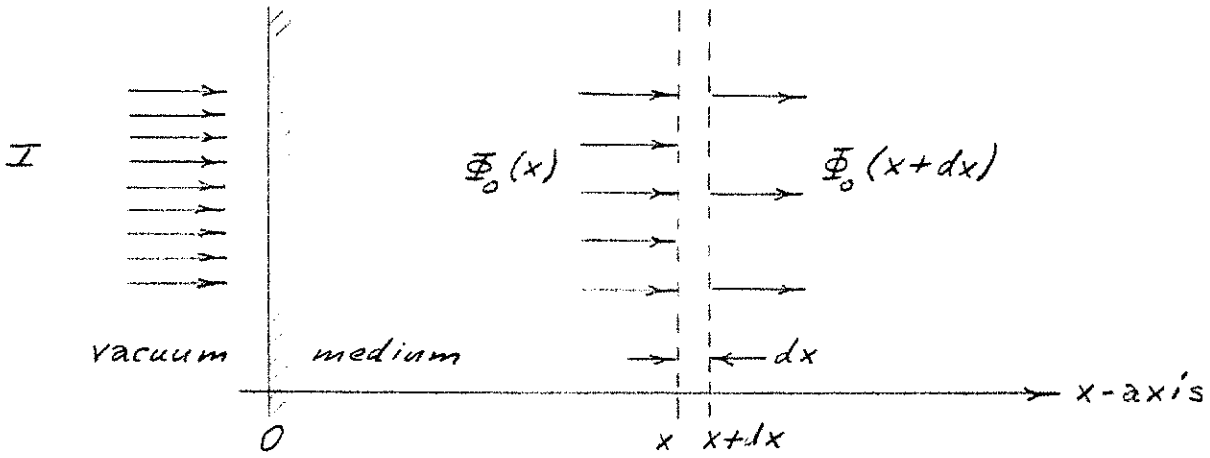
$$\bar{\Sigma}_i = N\frac{C}{\bar{v}} = N\sigma_i(\bar{\underline{v}})$$

5. Case of a $\frac{1}{v}$-cross section and a classical equilibrium particle distribution.

$$\bar{\Sigma}_i = N\frac{C}{KT^{1/2}}$$

Uncollided Particle Flux and Mean-Free-Path

The discussions employed to define the microscopic and macroscopic cross sections (σ_i and Σ_i) can also be used as the basis of a first particle transport discussion. Specifically, consider the determination of the uncollided particle flux in a medium that is "illuminated" by a monovelocity beam. For simplicity, consider a beam perpendicularly incident on the plane surface of a homogeneous "half-space." As illustrated, the incident beam



intensity is I, the medium surface is at x = 0, and the uncollided component of the particle flux is denoted $\Phi_o(x)$. The thin slab of medium between x and x+dx may be considered to be equivalent to the thin slab used in defining σ_i. Confining attention to only the uncollided particles, the beam incident on this thin slab (at x) is $\Phi_o(x)$, and, if there are first collisions (interactions) in the thin slab, then the change in the uncollided flux, $d\Phi_o(x)$, across dx is given by

$$d\Phi_o(x) = \Phi_o(x+dx) - \Phi_o(x)$$

and is a negative quantity. The first-collision rate density at x is given by

$$F_1(x) = \Sigma_t \Phi_o(x)$$

where the total cross section, Σ_t, is used because all types of first-interactions are counted. The first-collision rate per unit area of the thin slab at x is $F_1(x)dx$. First-collisions is the only mechanism for decreasing the uncollided flux, i.e., $F_1(x)dx$ has the same magnitude as $d\Phi_o(x)$. Whence,

$$d\Phi_o(x) = - F_1(x)dx = - \Sigma_t \Phi_o(x)dx$$

$$\frac{d\Phi_o(x)}{dx} = - \Sigma_t \Phi_o(x) \text{ and } \Phi_o(0) = I$$

The solution of the uncollided flux relation is

$$\Phi_o(x) = I\, e^{-\Sigma_t x}$$

Mean-free-path:

From the uncollided flux result a clear physical meaning of the total cross section can be deduced. The form of the result is immediately comparable to the radioactive nuclide decay relation, $N(t) = N_o \exp[-\lambda t]$. Recall the definition of the decay constant, λ. Specifically, $\lambda\Delta t$ is the probability that a radionucleus decay in the next time increment Δt (if $\lambda\Delta t << 1$). The statistical meaning of Σ_t is, in analogy, given by: $\Sigma_t \Delta x$ is the probability that a particle experience an interaction (any type) in the next Δx of particle travel (if $\Sigma_t \Delta x << 1$). Moreover, the equivalent "as good as new postulate" is: For a particle traveling in a medium, the probability that it interact with the targets of the medium in the next Δx of travel is independent of the distance traveled before that interaction. Moreover, $F_1(x) = \Sigma_t \Phi_o(x)$ only describes the statistical average of the first-interaction rate density at x. The statistical description is given by the binomial distribution $b^{\ell}_m(\Sigma_t \Delta x)$. Note also that the description in location of first-collision, x, can easily be changed to a description in terms of the time (the particle spends in the medium), t, using the relation $x = vt$ or $\Delta x = v\ \Delta t$.

Another route to deduce the physical meaning of Σ_t (which agrees with the above discussion) is to determine the average (or mean) distance (x) of particle travel in the medium to the first-collision. Using the derived $\Phi_o(x)$, the rate of first-collisions in dx at x (per unit area of this slab) is given by

$$F_1(x)dx = \Sigma_t \Phi_o(x)dx = \Sigma_t I\, e^{-\Sigma_t x}\, dx$$

and these first-collisions are clearly generated by particles which have traveled a distance x in the medium before the first-collision. The mean value of the distance traveled in the medium to the first-collision is thus

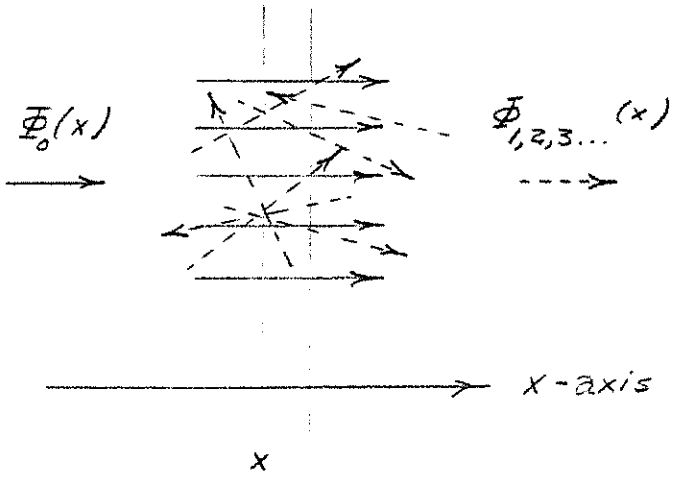
$$\langle x \rangle = \frac{\int_o^\infty x\, \Sigma_t I\, e^{-\Sigma_t x}\, dx}{\int_o^\infty \Sigma_t I\, e^{-\Sigma_t x}\, dx}$$

The denominator yields the total rate of first-interactions in a unit area of the entire half-space and must be equal to I, the incident beam intensity, to have a steady state (t-independent) problem. The numerator is equal to $1/\Sigma_t$. Whence,

$$\langle x \rangle = \frac{1}{\Sigma_t}$$

and the immediate interpretation: Σ_t is the inverse of the mean-free-path (of travel, x). The previously noted statistical meaning (viz., $\Sigma_t \Delta x$ is the probability of interaction for a particle travel distance Δx) is certainly consistent with this mean-free-path interpretation: $1/\Sigma_t \Delta x$ is the number of Δx distance increments required to "on the average" have one collision, which implies $\Delta x/\Sigma_t \Delta x$, or $1/\Sigma_t$, particle distance of travel to a collision.

It should be emphasized that in these discussions only the uncollided component of the particle flux has been considered. With reference to the illustration,



if particles are scattered (or, reemitted in any type of interaction), then the particle flux at x, $\Phi(x)$, has contributions from those particles which have had one ($\Phi_1(x)$) or more ($\Phi_2(x)$, $\Phi_3(x)$,...) collisions.

The more complex situation of $\Sigma_t = \Sigma_t(x)$ is easily approached with a change of variable defined by

$$\ell(x) = \int_a^x \Sigma_t(x')dx'$$

and termed the "optical variable," or "optical distance." So-defined, the origin of ℓ occurs at x = a. Often, the choice a = 0 is made and then $\ell = 0$ and x = 0 coincide. Since the mean-free-path at location x' is given by $1/\Sigma_t$, the integrand $\Sigma_t(x')dx'$ represents the fraction of a mean-free-path across the slab of thickness dx'. Whence, $\ell(x)$ represents the number of mean-free-paths between the plane at x and the plane at a (i.e., in the perpendicular, or x-direction).

The differential equation

$$\frac{d\Phi_o(x)}{dx} = -\Sigma_t(x)\ \Phi_o(x) \text{ and } \Phi_o(0) = I$$

is transformed to

$$\frac{d\Phi_o(\ell)}{d\ell} = -\Phi_o(\ell) \text{ and } \Phi_o(0) = I$$

if a = 0. Note that $\Phi_o(\ell) = \Phi_o(x(\ell))$. The solution takes the form

$$\Phi_o(\ell) = I\, e^{-\ell}$$

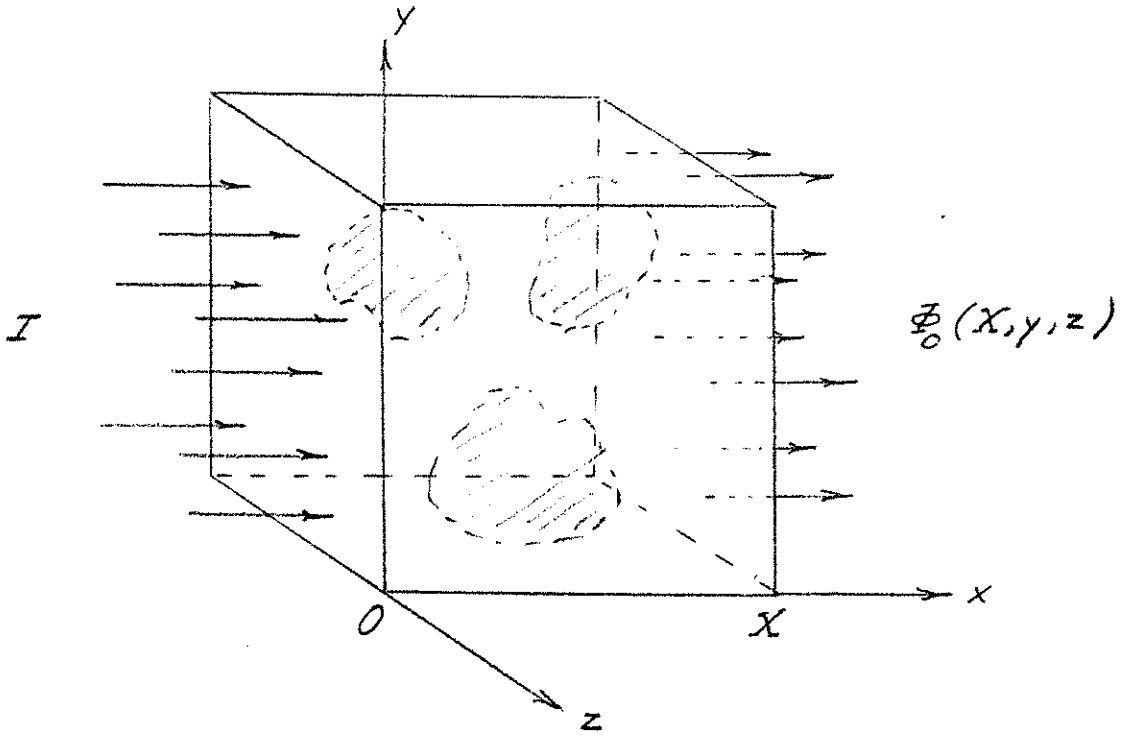
and, then transforming back to x yields

$$\Phi_o(x) = \Phi_o(\ell(x)) = I\, e^{-\ell(x)}$$

i.e.,

$$\Phi_o(x) = I \exp\left[-\int_o^x \Sigma_t(x')dx'\right]$$

As an example of immediate application of this initial transport problem solution, consider the uncollided particle flux which would emanate from a slab of thickness X which is uniformly and perpendicularly illuminated by a beam of intensity I.



The slab is neither thin nor uniform, i.e.,

$$\Sigma_t X = 0(1), \text{ or greater}$$

$$\Sigma_t = \Sigma_t(x,y,z)$$

The emerging, uncollided particle flux is given by

$$\Phi_o(X,y,z) = I\ e^{-\ell(X,y,z)}$$

i.e.,

$$\Phi_o(X,y,z) = I \exp\left[-\int_o^X \Sigma_t(x,y,z)dx\right]$$

If the uncollided flux is the only particle flux component of interest, then the above result immediately yields the "shielding" properties of the X-thick slab. As an example of another aspect of the solution, consider the case where the slab composition is uniform and only the target density, N, varies, i.e., $N = N(x,y,z)$ and

$$\Sigma_t(x,y,t) = \sigma_t\ N\ (x,y,z)$$

In this case, the result can be expressed as

$$\int_o^X N\ (x,y,z)dx = \frac{1}{\sigma_t}\ \ell n\left[\frac{I}{\Phi_o(X,y,z)}\right]$$

and a measurement of $\Phi_o(X,y,z)$ yields a determination of the x-direction, projected target densities in the X-thick slab.

It is rare that only the uncollided flux is relevant. The multiply-scattered flux components either represent unwanted noise in the determination of Φ_o, or they are of interest as being principally involved in the phenomena of interest. It is to the more complicated calculation of the entire flux, Φ, that we must eventually turn.

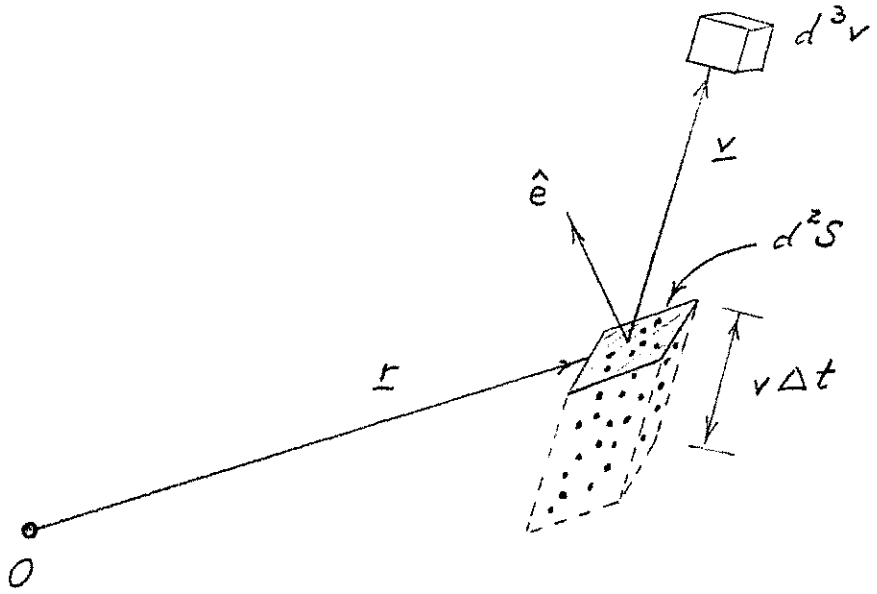
ELEMENTARY TRANSPORT RELATIONS

Particle Current

Consider a differential plane area element d^2S with unit normal vector $\hat{e}$ indicating the spatial orientation. The elemental area is located at $\underline{r}$ where the particle density is $n(\underline{r},\underline{v},t)$. In a small time interval Δt, the number of particles with velocities in d^3v which cross d^2S is given by

$$n(\underline{r},\underline{v},t)\ d^3v\ \Delta t \underline{v}\cdot\hat{e}\ d^2S$$

where $\underline{v}\cdot\hat{e} = \cos(\underline{v},\hat{e})$ with $(\underline{v},\hat{e})$ the angle between velocity $\underline{v}$ and unit normal $\hat{e}$. Note that a sign



convention has been thereby adopted relative to the arbitrarily chosen positive direction of $\hat{e}$, i.e.,

$$\underline{v}\cdot\hat{e} \gtrless 0 \text{ implies } \pm \text{ flow of particles.}$$

The flow rate of particles in d^3v across d^2S per unit area is given by

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t\, d^2S}\, n(\underline{r},\underline{v},t)\; d^3v\, \Delta t\; \underline{v}\cdot\hat{e}\; d^2S = n(\underline{r},\underline{v},t)\; d^3v\; \underline{v}\cdot\hat{e}$$

With respect to the direction $\hat{e}$, the positive (directed) component of the particle current, $J_+(\underline{r},t)$, is defined by

$$J_+(\underline{r},t) = \int_{\underline{v}\cdot\hat{e}>0} \underline{v}\cdot\hat{e}\; n(\underline{r},\underline{v},t)\; d^3v$$

and is equal to the rate of particle flow per unit area across a surface perpendicular to $\hat{e}$ at location $\underline{r}$ at time t; counting only particles with a positive component of $\underline{v}$ along the direction $\hat{e}$.

Similarly, with respect to the direction $\hat{e}$, the negative (directed) component of the particle current, $J_-(\underline{r},t)$, is defined by

$$J_-(\underline{r},t) = -\int_{\underline{v}\cdot\hat{e}<0} \underline{v}\cdot\hat{e}\; n(\underline{r},\underline{v},t)\, d^3v$$

and is equal to the rate of particle flow per unit area across a surface perpendicular to $\hat{e}$ at $\underline{r}$ and t; counting only particles with a negative component of $\underline{v}$ along the direction $\hat{e}$.

Clearly, the net rate of particle flow per unit area across a surface penpendicular to $\hat{e}$ at $\underline{r}$ and t is given by

$$J_+(\underline{r},t) - J_-(\underline{r},t) = \int \underline{v}\cdot\hat{e}\; n(\underline{r},\underline{v},t)\; d^3v$$

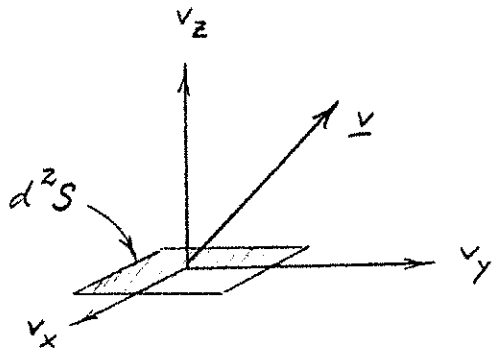
Defining the particle vector current by

$$\underline{J}(\underline{r},t) = \int \underline{v}\; n(\underline{r},\underline{v},t)\; d^3v$$

the net rate of particle flow per unit area across a surface perpendicular to an arbitrary direction $\hat{e}$ at location $\underline{r}$ and time t is $\hat{e}\cdot\underline{J}(\underline{r},t)$.

Case of an isotropic distribution:

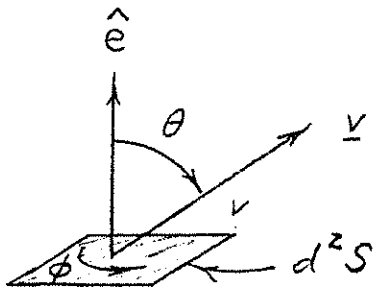
"Isotropic distribution" means that $n(\underline{r},\underline{v},t) = n(\underline{r},v,t)$ when expressed in velocity Cartesian 3-space. If Cartesian coordinates are



used for the $\underline{v}$-integration and v_z is chosen in the $\hat{e}$-direction, then

$$J_+(\underline{r},t) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{0}^{+\infty} v_z n(\underline{r},v,t)\, dv_x dv_y dv_z$$

The Cartesian $n(\underline{v})$ here actually depends on $|\underline{v}|$ only. Thus, it is more convenient to employ the illustrated spherical polar coordinates, with $\hat{e}$ the



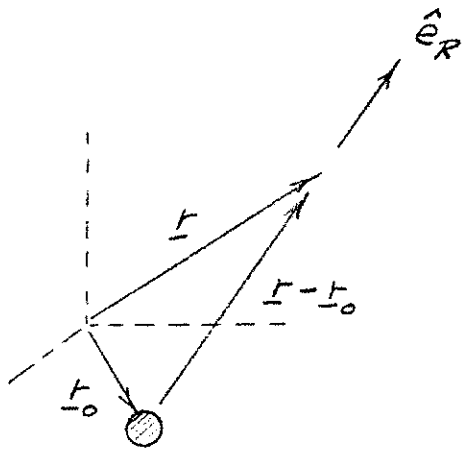
polar axis, for the integration, i.e.,

$$J_+(\underline{r},t) = \int_0^{\infty}\int_0^{\pi/2}\int_0^{2\pi} v\cos\theta n(\underline{r},v,t)v^2 \sin\theta dv d\theta d\phi$$

which reduces to $J_+(\underline{r},t) = \frac{1}{4} N(\underline{r},t)\ \bar{v}(\underline{r},t)$.

The Point Kernel

Consider a point (at $\underline{r}_o$), monoenergetic (speed v_o), steady source of particles emitting one particle per unit time isotropically into an infinite, homogeneous medium. Let



$R = |\underline{r} - \underline{r}_o|$ and

$$\hat{e}_R = \frac{\underline{r} - \underline{r}_o}{|\underline{r} - \underline{r}_o|}$$

$n_o(\underline{r},\underline{v})$ = the steady uncollided particle distribution resulting from the point source (i.e., the steady state point kernel),

$N_o(\underline{r})$ = the uncollided particle density $= \int n_o(\underline{r},\underline{v})\, d^3v$, and

$\underline{J}_o(\underline{r})$ = the uncollided particle current $= \int \underline{v} n_o(\underline{r},\underline{v})\, d^3v$.

Intuitively,

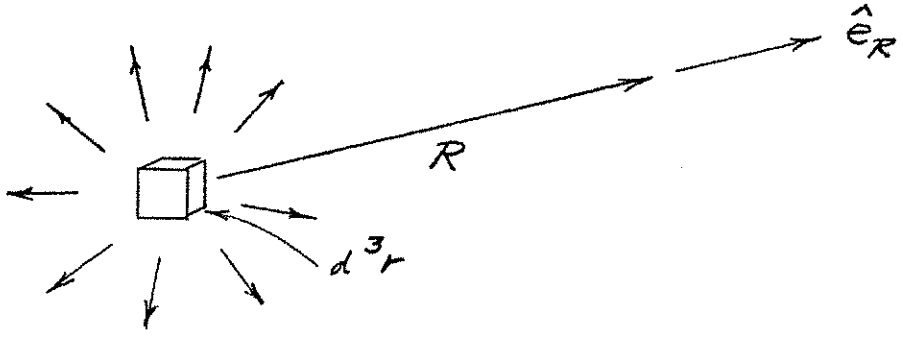
$$N_o(\underline{r}) = \frac{1/v_o}{4\pi R^2} \exp[-\Sigma_t R]$$

$$\underline{J}_o(\underline{r}) = \frac{1}{4\pi R^2} \exp[-\Sigma_t R]\, \hat{e}_R$$

and

$$n_o(\underline{r},\underline{v}) = \frac{1/v_o}{4\pi R^2} \exp[-\Sigma_t R]\, \delta\, (\underline{v} - v_o \hat{e}_R)$$

As an example of the use of these results consider a configuration volume element d^3r in which the rate of particle scattering collisions is $\Sigma_s \Phi(\underline{r}) d^3r$. Presuming that the scattering is isotropic, the volume element d^3r appears as an isotropic source of strength $\Sigma_s \Phi(\underline{r}) d^3r$.

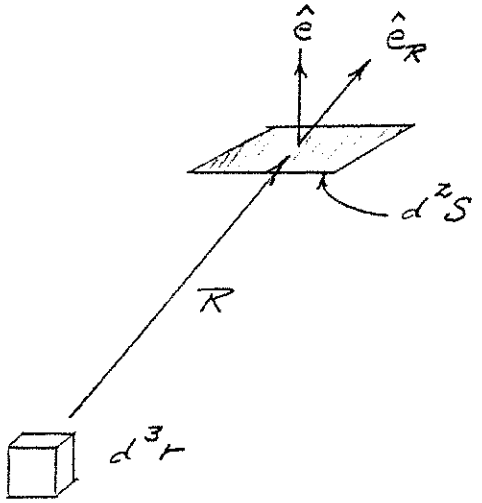


Denoting $d\underline{J}_o(R)$ as the uncollided particle current at R due to particles emanating from d^3r having had a scattering in d^3r,

$$d\underline{J}_o(\underline{R}) = \bar{\Sigma}_s \Phi(\underline{r}) d^3r \frac{1}{4\pi R^2} \exp[-\Sigma_t R] \hat{e}_R$$

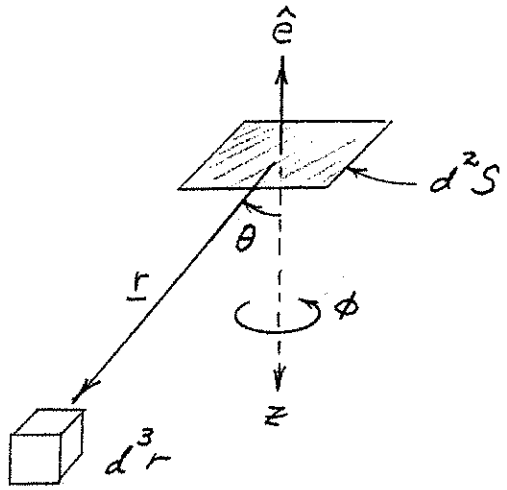
This result is now used to develop a heuristic derivation of Fick's diffusion law.

Fick's Law of Diffusion



Let dJ_+ represent the particle flow density rate thru d^2S due to particles which had last collision in d^3r, i.e.

$$dJ_+ = \Sigma_s \Phi(\underline{r}) d^3r \frac{1}{4\pi R^2} \exp[-\Sigma_t R] \hat{e}_R \cdot \hat{e}$$



In terms of the illustrated spherical polar configuration coordinates (i.e., with the origin at d^2S and polar axis, z, opposite to $\hat{e}$).

$$dJ_+ = \Sigma_s \Phi(\underline{r}) \frac{1}{4\pi r^2} \exp[-\Sigma_t r] \cos\theta r^2 \sin\theta dr d\theta d\phi$$

With the (unrealistic) presumption that the homogeneous medium is of infinite extent,

$$J_+ = \int_0^{\infty} \int_0^{\pi/2} \int_0^{2\pi} \frac{\Sigma_s}{4\pi} \Phi(\underline{r}) \exp[-\Sigma_t r] \cos\theta \sin\theta dr d\theta d\phi$$

For algebraic simplicity, suppose that $\Phi(\underline{r}) = \Phi(z)$ and employ the Taylor series expansion

$$\Phi(\underline{r}) = \Phi(0) + \left(\frac{\partial \Phi}{\partial z}\right)_0 (r\cos\theta) + \ldots$$

to obtain

$$J_+ = \frac{\Sigma_s}{2} \int_0^{\infty} \int_0^{\pi/2} [\Phi(0) + \left(\frac{\partial \Phi}{\partial z}\right)_0 (r\cos\theta) + \ldots] \exp[-\Sigma_t r] \cos\theta \sin\theta dr d\theta$$

With the (sometimes unrealistic) presumption that over the r-range (0, a few $1/\Sigma_t$) $\partial\Phi/\partial z$ is essentially constant and defining $\mu = \cos\theta$,

$$J_+ = \frac{\Sigma_s}{2} \int_0^{\infty} \int_0^{+1} [\Phi(0) + \left(\frac{\partial \Phi}{\partial z}\right)_0 r\mu] \exp[-\Sigma_t r] \mu dr d\mu$$

$$= \frac{\Sigma_s}{\Sigma_t} [\frac{1}{4} \Phi(0) + \frac{1}{6\Sigma_t} \left(\frac{\partial \Phi}{\partial z}\right)_0]$$

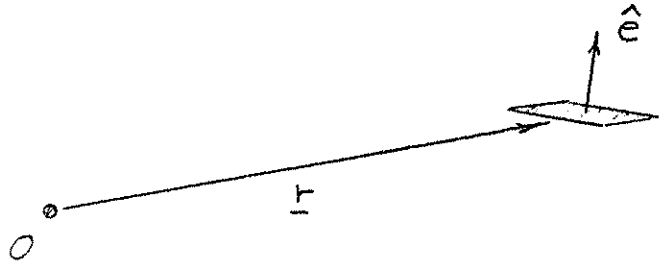
a more general (and accurate) result is

$$J_{\pm}(r) = \frac{1}{4} \Phi(\underline{r}) \mp \frac{1}{2} D \left(\frac{\partial \Phi}{\partial x_{\hat{e}}}\right)_{\underline{r}}$$

where, $x_{\hat{e}}$ is the distance measured along the + $\hat{e}$-direction, D is the diffusion coefficient

$$D = \frac{1}{3\Sigma_{tr}}$$

Σ_{tr} is the "transport cross section" (is equal to Σ_t for the case of isotropic scattering and weak absorption, $\Sigma_a << \Sigma_s$), and $\underline{r}$ is now the location of the surface thru which particles are passing with reference to an arbitrary origin, i.e.,



Note that

$$\hat{e} \cdot \underline{J}(\underline{r}) = J_+(\underline{r}) - J_-(\underline{r})$$

$$= - D \left(\frac{\partial \Phi}{\partial x_{\hat{e}}}\right)_{\underline{r}}$$

and that the gradient of $\Phi(\underline{r})$, denoted by $\nabla\Phi(\underline{r})$, is defined such that

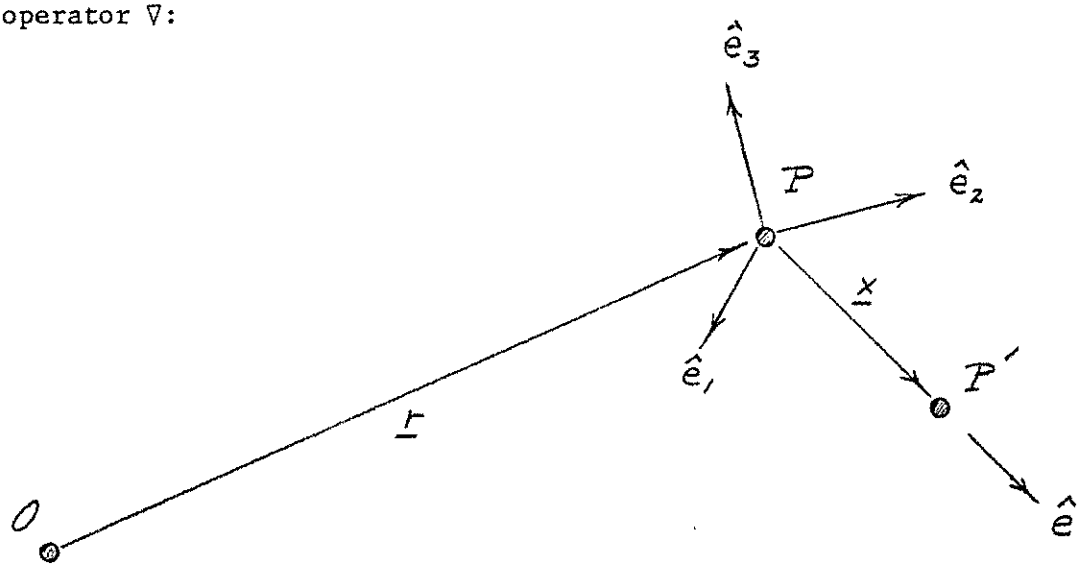
$$\hat{e} \cdot \nabla\Phi(\underline{r}) = \left(\frac{\partial \Phi}{\partial x_{\hat{e}}}\right)_{\underline{r}}$$

Whence, the relation

$$\underline{J}(\underline{r}) = - D \nabla\Phi(\underline{r})$$

which is Fick's law of diffusion.

The operator ∇:



Consider the orthogonal set of coordinates (x_1, x_2, x_3) at the point P with the respective unit vectors $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$. Presume that the x_i have distance dimension (e.g., cm). Let $F(\underline{r})$ be a scalar function and note

$$F(P') = F(P) + \left(\frac{\partial F}{\partial x_1}\right)_P x_1 + \left(\frac{\partial F}{\partial x_2}\right)_P x_2$$

$$+ \left(\frac{\partial F}{\partial x_3}\right)_P x_3 + O(x^2)$$

But, $(\hat{e}_1,\hat{e}_2,\hat{e}_3)$ is an orthonormal set and F(P') can be reexpressed

$$F(P') = F(P) + \left(\frac{\partial F}{\partial x_1}\,\hat{e}_1 + \frac{\partial F}{\partial x_2}\,\hat{e}_2 + \frac{\partial F}{\partial x_3}\,\hat{e}_3\right) \cdot \underline{x} + O(x^2)$$

where $\underline{x} = x_1\hat{e}_1 + x_2\hat{e}_2 + x_3\hat{e}_3$. Whence,

$$\frac{F(P') - F(P)}{x} = \left(\frac{\partial F}{\partial x_1}\,\hat{e}_1 + \frac{\partial F}{\partial x_2}\,\hat{e}_2 + \frac{\partial F}{\partial x_3}\,\hat{e}_3\right) \cdot \hat{e} + O(x)$$

and

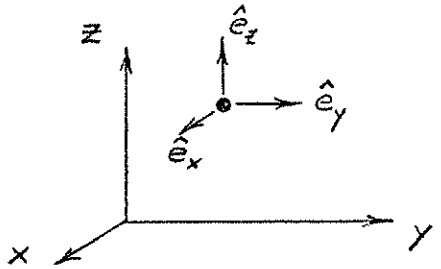
$$\lim_{x\to 0} \frac{F(P') - F(P)}{x} = \frac{\partial F}{\partial x_{\hat{e}}} = \hat{e} \cdot \nabla F(x_1,x_2,x_3)$$

where the operator ∇ is defined by

$$\nabla = \hat{e}_1 \frac{\partial}{\partial x_1} + \hat{e}_2 \frac{\partial}{\partial x_2} + \hat{e}_3 \frac{\partial}{\partial x_3}$$

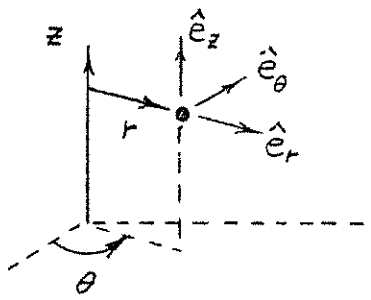
Examples --

1. Cartesian (x,y,z)



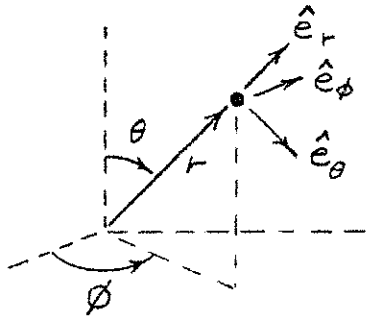
$$\nabla = \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z}$$

2. Cylindrical (r,θ,z)



$$\nabla = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_z \frac{\partial}{\partial z}$$

3. Spherical polar (r,θ,ϕ)

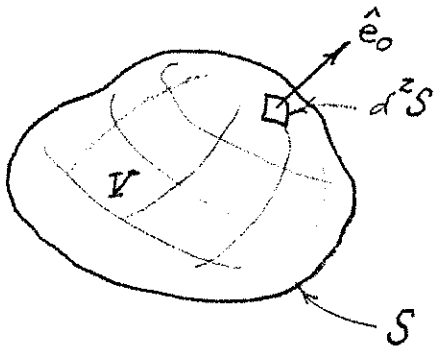


$$\nabla = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r\sin\theta} \frac{\partial}{\partial \phi}$$

Continuity Relations

Monoenergetic particles:

Consider the balance in population of monoenergetic particles in volume V enclosed by surface S.



$N(\underline{r},t)$ = particle density,

$\underline{J}(\underline{r},t)$ = particle current,

$s(\underline{r},t)$ = particle source rate density.

$\frac{\partial}{\partial t} \int_V N(\underline{r},t)\, d^3r$ = rate of change of the particle population in V, and has the following contributing terms:

1. $\int_V s(\underline{r},t)\, d^3r$ = rate of change due to particle sources.
2. $-\int_V \Sigma_a(\underline{r},t)\Phi(\underline{r},t)\, d^3r$ = rate of change due to particle absorption by targets.
3. $-\int_S \underline{J}(\underline{r},t) \cdot \hat{e}_o d^2S$ = rate of change due to net <u>outflow</u> of particles through S.

where $\hat{e}_o$ is the outward-directed unit normal vector to S.

Note that by Gauss' theorem,

$$\int_S \underline{J} \cdot \hat{e}_o d^2S = \int_V \nabla \cdot \underline{J}\, d^3r$$

Thus, if the particles are assumed to be stable,

$$\frac{\partial}{\partial t} \int_V N(\underline{r},t)\, d^3r = - \int_V \nabla \cdot \underline{J}(\underline{r},t)\, d^3r$$

$$- \int_V \Sigma_a(\underline{r},t)\phi(r,t)\, d^3r + \int_V s(\underline{r},t)\, d^3r$$

and, since V is entirely arbitrary

$$\frac{\partial N(r,t)}{\partial t} = - \nabla \cdot \underline{J}(\underline{r},t) - \Sigma_a(\underline{r},t)\Phi(\underline{r},t) + s(\underline{r},t)$$

which is the particle "continuity relation." For this assumed case of monoenergetic particles

$$\frac{\partial N(r,t)}{\partial t} = \frac{1}{v} \frac{\partial \Phi(r,t)}{\partial t}$$

which yields an expression for particle continuity in terms of the 2 dependent variables Φ and $\underline{J}$.

Polyenergetic particles:

In the more realistic case of particles with a range of kinetic energies, it is of interest to develop the particle population balance in E-space as well as in $\underline{r}$-space. Here, considering only the E-integrated population balance in $\underline{r}$-space,

$$\frac{\partial N(r,t)}{\partial t} = - \nabla \cdot \underline{J}(\underline{r},t) - \overline{\Sigma}_a(\underline{r},t)\phi(\underline{r},t) + s(\underline{r},t)$$

which is identical, in form, with the monoenergetic particle relation. Here,

$$N(\underline{r},t) = \int n(\underline{r},\underline{v},t)d^3v$$

$$\Phi(\underline{r},t) = \int vn(\underline{r},\underline{v},t)d^3v$$

$$\underline{J}(\underline{r},t) = \int \underline{v}n(\underline{r},\underline{v},t)d^3v$$

$$s(\underline{r},t) = \int s(\underline{r},\underline{v},t)d^3v$$

and $\overline{\Sigma}_a$ is the averaged particle absorption cross section as discussed in previous lectures. Moreover, in many cases,

$$\frac{\partial N(\underline{r},t)}{\partial t} = \frac{\partial}{\partial t}\left[\frac{\Phi(\underline{r},t)}{\overline{v}(\underline{r},t)}\right] \simeq \frac{1}{\overline{v}}\ \frac{\partial}{\partial t}\Phi(\underline{r},t)$$

where $\overline{v} = \dfrac{1}{n(\underline{r},t)} \int vn(\underline{r},\underline{v},t)\ d^3v$.

In these lectures, then, the general form of the particle population continuity relation is expressed as

$$\frac{1}{v}\ \frac{\partial}{\partial t}\ \Phi(\underline{r},t) = -\nabla \cdot \underline{J}(\underline{r},t) - \Sigma_a(\underline{r},t)\Phi(\underline{r},t) + s(\underline{r},t).$$

The diffusion approximation:

Fick's law of diffusion has been derived in the form

$$\underline{J}(\underline{r},t) = -D(\underline{r},t)\nabla\Phi(\underline{r},t)$$

This is an approximate relation between $\underline{J}$ and Φ which is valid if:

1. Distance to boundaries (or, to inhomogeneties) is much larger than $1/\Sigma_t$.
2. There is negligible variation in $\partial\Phi/\partial x_{\hat{e}}$ over distances of $1/\Sigma_t$, i.e., slowly varying $\Phi(\underline{r})$, or equivalently $\Sigma_a << \Sigma_s$.
3. There is negligible variation in $\Phi(t)$ over periods which are small relative to particle transit times.

The "diffusion approximation" to the particle population continuity relation is thus

$$\frac{1}{v}\ \frac{\partial}{\partial t}\ \Phi(\underline{r},t) = \nabla \cdot D(\underline{r},t)\nabla\Phi(\underline{r},t)$$

$$- \Sigma_a(\underline{r},t)\Phi(\underline{r},t) + s(\underline{r},t)$$

Note that, for the case of $D(\underline{r},t) = D(t)$ the operator ∇^2, defined by

$$\nabla^2 = \nabla \cdot \nabla$$

is relevant, i.e., the diffusion equation assumes the form

$$\frac{1}{v}\frac{\partial}{\partial t}\Phi(\underline{r},t) = D(t)\,\nabla^2\Phi(\underline{r},t)$$

$$- \Sigma_a(\underline{r},t)\Phi(\underline{r},t) + s(\underline{r},t)$$

Examples --

1. Cartesian coordinates (x,y,z)

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

2. Cylindrical coordinates (r,θ,z)

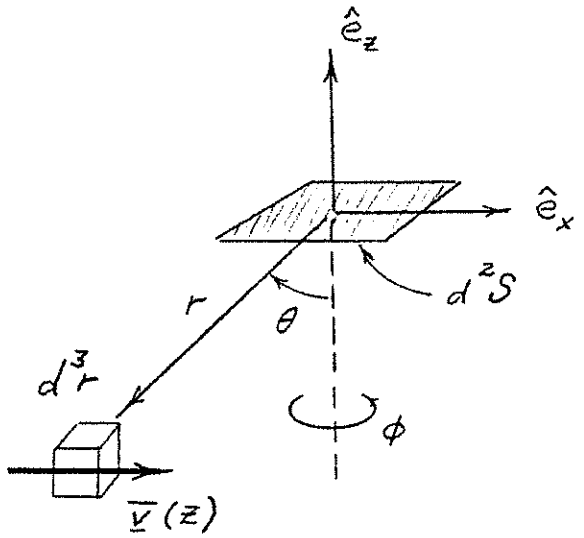
$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta} + \frac{\partial^2}{\partial \theta^2}$$

3. Spherical polar coordinates (r,θ,φ)

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2}{\partial \phi^2}$$

Viscosity and Thermal Conductivity

Viscosity:



Consider a fluid characterized by $n(\underline{r}) = n = \text{constant}$, and $\overline{\underline{v}}(\underline{r}) = \overline{\underline{v}}(z) = \overline{v}_x(z)\hat{e}_x$.

From the Fick's law derivation

$$dJ_+ = \frac{\Sigma_s \Phi}{4\pi} \exp[-\Sigma_t r] \cos\theta\sin\theta dr d\theta d\phi$$

Let $p_{xz}\hat{e}_x$ denote the net flow of particle momentum transfer through d^2S per unit area. Then

$$p_{xz} \simeq \frac{\Sigma_s \Phi m}{z} \int_0^\infty \int_0^\pi \exp[-\Sigma_t r]\ \overline{v}_x(r\cos\theta)\cos\theta\sin\theta dr d\theta$$

Note that it is assumed that Φ is approximately constant even though $\overline{v}_x$ is varying and that the ϕ-integration averages v_x at each value of θ.

$$p_{xz} \simeq \frac{\Sigma_s \Phi m}{2} \int_0^\infty \int_0^\pi \exp[-\Sigma_t r]\left[\overline{v}_x(0) - (r\cos\theta)\ \left(\frac{d\overline{v}_x}{dz}\right)_0\right]\cos\theta\sin\theta dr d\theta$$

i.e.,

$$p_{xz} = -\mu\left(\frac{d\overline{v}_x}{dz}\right)_0$$

where $\mu = \frac{1}{3}\frac{\Sigma_s}{\Sigma_t^2} m\Phi = Dm\Phi$ is the fluid "coefficient of viscosity." In three-dimensions, the result is

$$p_{ij} = -\mu \frac{\partial \overline{v}_i}{\partial x_j}$$

Thermal Conductivity:

Consider a fluid characterized by $n(\underline{r}) = n = \text{constant}$ and $\overline{v^2}(\underline{r}) = \overline{v^2}(z)$. Let Q_z denote the net rate of particle kinetic energy transfer through d^2S per unit area, i.e.,

$$Q_z = \frac{\Sigma_s \Phi m}{4} \int_0^\infty \int_0^\pi \exp[-\Sigma_t r]\ \overline{v^2}(r\cos\theta)\cos\theta\sin\theta dr d\theta$$

Moreover, if the particle distribution is locally in classical equilibrium,

then

$$\frac{1}{2}\,m\overline{v^2}(z) = \frac{3}{2}\,kT(z)$$

and

$$Q_z \simeq \frac{3}{4}\,k\Sigma_s \int_0^{\infty}\int_0^{\pi} \exp[-\Sigma_t r]\; T(r\cos\theta)\cos\theta\sin\theta\, dr\, d\theta$$

$$Q = -\kappa\left(\frac{dT}{dz}\right)_0$$

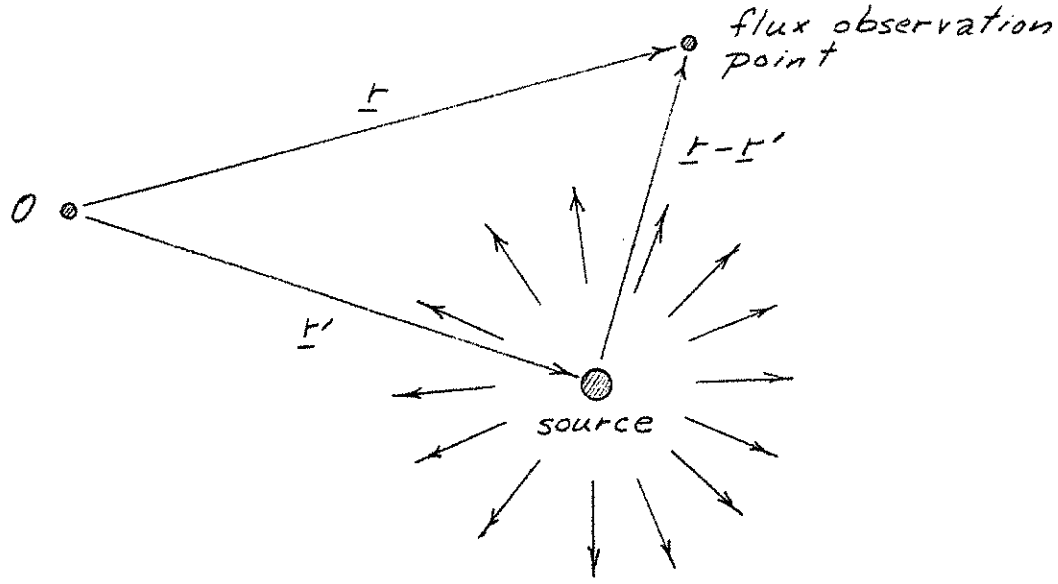
where $\kappa = \frac{1}{2}\,k\Phi\frac{\Sigma_s}{\Sigma_t^2} = \frac{3}{2}\,k\Phi D$ is the fluid "coefficient of thermal conductivity." Q_z is identified as the "heat flow density." In three-dimensions

$$\underline{Q} = -\kappa\nabla T$$

MONOENERGETIC PARTICLE TRANSPORT RELATIONS

Point Source Kernels

To motivate a careful understanding and analysis of the particle transport process, consider the details of a particular problem--Determine the particle flux, $\Phi(\underline{r})$, resulting from a unit strength, monoenergetic, steady point source of particles located at $\underline{r}'$ and emitting isotropically into an infinite, homogeneous medium. Two solution approaches have already been discussed in these notes. It is the relation between the two solution results that is addressed here.



The uncollided particle flux, $\Phi_o(\underline{r})$, has been previously discussed and is given by

$$\Phi_o(\underline{r}) = \frac{1}{4\pi|\underline{r} - \underline{r}'|^2} \exp[-\Sigma_t|\underline{r} - \underline{r}'|]$$

For reasons which will become apparent, denote this particle flux result by $G_o(\underline{r},\underline{r}')$, i.e.,

$G_o(\underline{r},\underline{r}')$ = the uncollided particle flux at $\underline{r}$ due to a unit strength, monoenergetic, steady, isotropic point source at $\underline{r}'$ in an infinite, homogeneous medium.

As a first detailed problem employing the derived particle diffusion equation, consider the unit strength, point source problem. Specifically--Find the particle flux, $\Phi(\underline{r})$, due to a source at $\underline{r}'$ using the steady state diffusion relation. In order to gain obvious symmetry, move the origin of spherical polar coordinates to the point source. Then $\Phi(\underline{r}) \rightarrow \Phi(r)$ and the diffusion equation can be stated

$$L^2 \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) \Phi(r) - \Phi(r) = 0$$

except at $r = 0$ where there is a suitable source condition. The "diffusion length," L, has been defined by the relation

$$L^2 = \frac{D}{\Sigma_a}$$

The general solution is

$$\Phi(r) = A \frac{1}{r} e^{-r/L} + C \frac{1}{r} e^{+r/L}$$

and the boundary (and source) conditions are

$$\text{(I)} \quad \lim_{r \to \infty} \Phi(r) = 0$$

$$\text{(II)} \quad \lim_{r \to 0} 4\pi r^2 \left(-D \frac{d\Phi}{dr}\right) = 1$$

Whence, the solution

$$\Phi(r) = \frac{1}{4\pi \Sigma_a L^2} \frac{e^{-r/L}}{r}$$

Spacial moments:

As expected, $\int_0^\infty \Sigma_a \Phi(r)\, 4\pi r^2 dr = 1$ which leads to the general spatial (r) moment relation

$$\langle r^n \rangle = \int_0^\infty r^n \Sigma_a \Phi(r)\, 4\pi r^2 dr = (n+1)! L^n$$

e.g., $\langle r \rangle = 2L$ and $\langle r^2 \rangle = 6L^2$. Note that $\langle r^2 \rangle \neq \langle r \rangle^2$.

Green's function:

As for the uncollided flux problem, there are useful reasons for denoting the particle flux result by $G_D(\underline{r},\underline{r}')$, i.e.,

$G_D(\underline{r},\underline{r}')$ = the particle flux at $\underline{r}$ due to a unit strength, monoenergetic, steady, isotropic point source at $\underline{r}'$ in an infinite, homogeneous medium, where the diffusion approximation (equation) has been employed to determine the result.

From the $\Phi(r)$ result obtained placing $\underline{r}'$ at the origin of $\underline{r}$-coordinates, it readily follows that

$$G_D(\underline{r},\underline{r}') = \frac{1}{4\pi\Sigma_a L^2 |\underline{r} - \underline{r}'|} \exp[-|\underline{r} - \underline{r}'|/L]$$

which should be compared with the uncollided particle flux Green's function

$$G_o(\underline{r},\underline{r}') = \frac{1}{4\pi|\underline{r} - \underline{r}'|^2} \exp\ [-|\underline{r} - \underline{r}'|/\Lambda]$$

where Λ denotes the mean-free-path, i.e., $\Lambda = 1/\Sigma_t$.

Use of Green's functions:

The two Green's functions, $G(\underline{r},\underline{r}')$, just described are certainly different in their functional form, i.e.,

$$G_D \sim \frac{1}{R} e^{-R/L}$$

and

$$G_o \sim \frac{1}{R^2} e^{-R/\Lambda}$$

where R is the distance between source location, $\underline{r}'$, and flux observation location, $\underline{r}$. However, both results are trying to describe the particle flux at $\underline{r}$ due to a unit strength, monoenergetic, steady, isotropic point source at $\underline{r}'$ in an infinite, homogeneous medium. The relation between these two results is considered later. Here, consider the general use of Green's

function results to determine particle flux due to complex source distributions.

Green's functions are generated by solution of linear analytical problems where the inhomogeneity (or, source) is singular - e.g., in the present problem, point sources are considered, i.e, $s(\underline{r}) \sim \delta(\underline{r} - \underline{r}')$. Since the problems are linear, the solution for a more complex source is given by the "sum" of the relevant Green's functions weighted with the distributed source density, i.e., the particle flux, $\Phi(\underline{r})$, due to a distributed source density, $s(\underline{r}')$, is given by

$$\Phi(\underline{r}) = \int G(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

if $G(\underline{r},\underline{r}')$ is the Green's function which describes the physical process correctly. If diffusion is the accurate transport description, then

$$\Phi(\underline{r}) = \int G_D(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

Or, if free-flight transport is the process, then

$$\Phi(\underline{r}) = \int G_o(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

Relation between free-flight and diffusion:

Using a method based on calculation of successive "orders-of-scattering" a relation between free-flight transport and the diffusion approximation will be developed. The purpose of this development at this point in these lectures is two-fold: 1. To qualitatively indicate the general idea of a transport calculation. 2. To show the inadequacy of knowing only the free-flight and diffusion description in studying general transport problems (and thus motivate a more careful consideration of the transport of particles in matter).

Calculation of the uncollided particle flux -

If $s(\underline{r}')$ represents a particle source distribution, then

$$\Phi_o(\underline{r}) = \int G_o(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

is the uncollided particle flux generated by the source distribution. Moreover,

$$F_1(\underline{r}) = \Sigma_t\Phi_o(\underline{r})$$

is the first-collision density rate.

Calculation of the once-collided particle flux -

If scattering is isotropic, then $\Sigma_s F_1(\underline{r}')/\Sigma_t$ represents an isotropic source distribution of once-collided particles. Whence,

$$\Phi_1(\underline{r}) = \int G_o(\underline{r},\underline{r}') \frac{\Sigma_s}{\Sigma_t} F_1(\underline{r}')d^3r' = \int G_o(\underline{r},\underline{r}')\ \Sigma_s\Phi_o(\underline{r}')d^3r'$$

is the once-collided particle flux. Moreover,

$$F_2(\underline{r}) = \Sigma_t\Phi_1(\underline{r})$$

is the second-collision density rate.

Calculation of higher-order-collided particle flux -

In general,

$$\Phi_m(\underline{r}) = \int G_o(\underline{r},\underline{r}')\Sigma_s\Phi_{m-1}(\underline{r}')d^3r'$$

is the m-collided particle flux (i.e., if scattering is isotropic and G_o is particle-energy-independent). In such cases then,

$$\Phi_m(\underline{r}) = \Sigma_s^m \int\int \cdots \int G_o(\underline{r},\underline{r}')G_o(\underline{r}',\underline{r}'')\ldots G_o(\underline{r}^{(m)},\underline{r}^{(m+1)})s(\underline{r}^{(m+1)})$$
$$d^3r'\ d^3r''\ldots d^3r^{(m+1)}$$

Calculation of particle flux -

If $\Phi(\underline{r})$ represents the particle flux (i.e., including all orders-of-collisions) due to the source distribution $s(\underline{r}')$, then

$$\Phi(\underline{r}) = \sum_{m=0}^{\infty} \Phi_m(\underline{r})$$

There usually is some integer, M, such that

$$\Phi(\underline{r}) \approx \sum_{m=0}^{M} \Phi_m(\underline{r})$$

and it is reasonable to presume that $M = 0(\Sigma_s/\Sigma_a)$. Two limiting examples have already been considered, i.e.,

1. Case of high absorption, i.e.,

   $\Sigma_a >> \Sigma_s$ implies $M \approx 0$ and

   $$\sum_{m=0}^{M} \Phi_m(\underline{r}) \to \Phi_o(\underline{r}) \approx \int G_o(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

2. Case of weak absorption, i.e,

   $\Sigma_a << \Sigma_s$ implies $M >> 1$ and

   $$\sum_{m=0}^{M} \Phi_m(\underline{r}) \to \Phi(\underline{r}) \approx \int G_D(\underline{r},\underline{r}')s(\underline{r}')d^3r'$$

   i.e., the diffusion approximation.

If M is between these two limiting cases (or, if scattering is anisotropic, or, transport is particle-energy-dependent) then the orders-of-scattering technique is either tedious or impossible to apply and a direct consideration of the complicated particle transport process is required. The remainder of this section of these notes is devoted to development and solution of a specific form of the Boltzmann transport equation with application to relevant physical and engineering problems.

Monoenergetic Particle Transport Equation

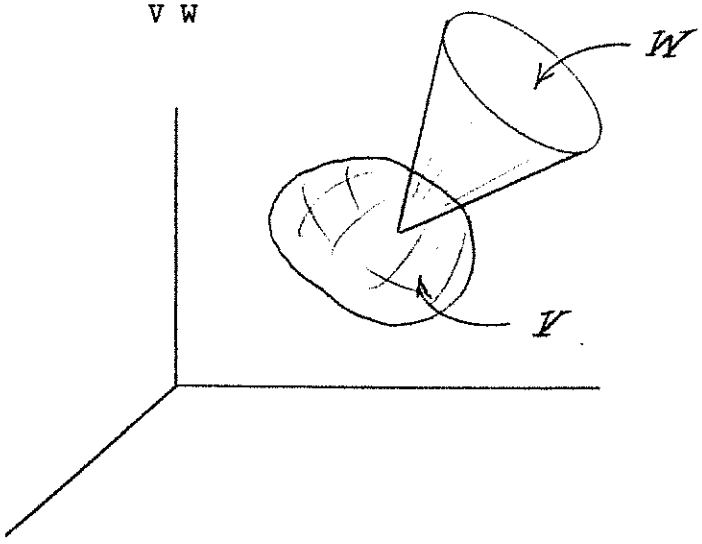
Presuming that the particles of interest are essentially moving points (i.e., with no relevant external or internal structure), the distribution independent coordinates are location, $\underline{r}$, velocity, $\underline{v}$, and time, t. Alternatively, and more useful for the present discussion, the independent coordinates can be chosen as $\underline{r}$, energy, E, direction-of-travel, $\hat{\Omega}$, and t. In order to somewhat simplify the development, understanding, and application of transport relations, an often-used approach is to separately consider the independent variables (or groups of variables). In this section of these notes, the variable dependencies $(\underline{r},\hat{\Omega},t)$ are considered and thus monoenergetic particle transport is addressed. The next section treats the E-dependence and is devoted to particle E-spectrum determination as well as energy deposition (in matter) considerations.

In the most complicated monoenergetic particle transport problem, $n(\underline{r},\hat{\Omega},t)$ is the relevant particle density distribution, i.e.,

$n(\underline{r},\hat{\Omega},t)$ = expected particle population per unit volume (e.g., per cubic centimeter) at $\underline{r}$, per unit solid angle (e.g., per steradian) at $\hat{\Omega}$, at time t.

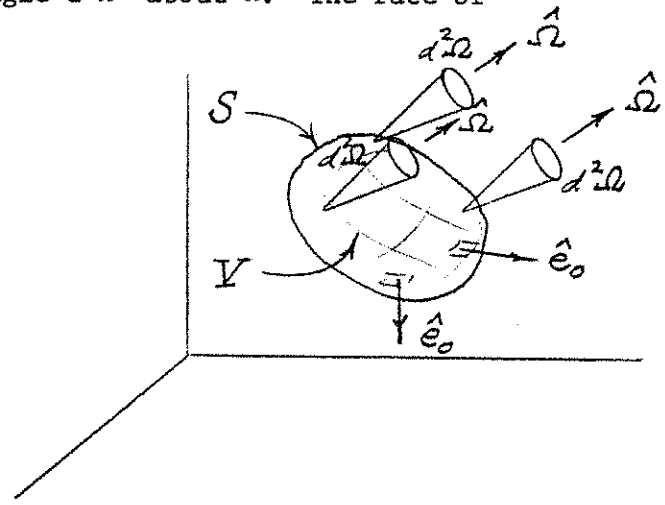
The number of particles in volume V with direction of travel in the solid angle W at time t is given by

$$\int_V \int_W n(\underline{r},\hat{\Omega},t)\,d^2\Omega\; d^3r$$



where all the particles have the same energy (i.e., truly monoenergetic) or, for some reason particle energy is an irrelevant variable and thus particles are counted independent of their energy.

Consider the particle population change in an arbitrary volume V surrounded by a closed surface S with local, outward-directed, unit normal $\hat{e}_o$. Consider only those particles with velocity directions in the incremental solid angle $d^2\Omega$ about $\hat{\Omega}$. The rate of



change of the expected population of relevant particles (i.e., those in V and $d^2\Omega$) is

$$d^2\Omega \frac{\partial}{\partial t} \int_V n(\underline{r},\hat{\Omega},t)d^3r$$

and has the contributing terms:

1. $d^2\Omega \int_S \hat{e}_o \cdot v\hat{\Omega} n(\underline{r},\hat{\Omega},t)d^2S$ = net rate of loss of particles from V with velocity directions in $d^2\Omega$ at time t due to flow through S.

2. $d^2\Omega \int_V \Sigma_t(\underline{r},t)vn(\underline{r},\hat{\Omega},t)d^3r$ = rate of loss of particles in V with precollision velocity direction in $d^2\Omega$ at time t due to binary collisions.

3. $d^2\Omega \int_V d^3r \int_{4\pi} c(\underline{r},t)f(\underline{r},t;\hat{\Omega}'\rightarrow\hat{\Omega})\Sigma_t(\underline{r},t)vn(\underline{r},\hat{\Omega}',t)d^2\Omega'$ = rate of gain of particles in V with velocity directions in $d^2\Omega$ at time t due to the production of secondary particles caused by collisions of particles in V with all possible precollision velocity directions.

4. $d^2\Omega \int_V s(\underline{r},\hat{\Omega},t)d^3r$ = rate of gain of particles in V with velocity directions in $d^2\Omega$ at time t due to independent particle emission sources.

In term (3) two new functions describing the particle interaction process are introduced. They are:

$c(\underline{r},t)$ = the expected number of secondary particles released per collision of the particles of interest (e.g., $c = \Sigma_s/\Sigma_t$ if scattering is the only collision type from which particles emanate)

$f(\underline{r},t;\hat{\Omega}'\rightarrow\hat{\Omega})$ = the normalized secondary particle direction of emission ($\hat{\Omega}$) distribution due to a precollision particle with velocity direction $\hat{\Omega}'$ (i.e., $fd^2\Omega$ is the fraction of particles emitted into $d^2\Omega$ about $\hat{\Omega}$)

It should be noted that term (3) includes the contribution of particle scattering from all direction increments into $d^2\Omega$ about $\hat{\Omega}$ and all these scatterings are described by binary (point) collisions. With intent, the continuous deviation of a particle direction-of-travel which would result from long-range force fields has not been included in this initial, simplified discussion. It should also be realized that there are numerous situations where long-range forces are of negligible importance and the relations being developed have meaningful application to such cases.

Gauss's vector field theorem applied to term (1) yields

$$\int_S \hat{e}_o \cdot v\hat{\Omega}n(\underline{r},\hat{\Omega},t)d^2S = \int_V \nabla \cdot v\hat{\Omega}n(\underline{r},\hat{\Omega},t)d^3r$$

Moreover, including the fact that v and $\hat{\Omega}$ are $\underline{r}$-independent,

$$\int_S \hat{e}_o \cdot v\hat{\Omega}n(\underline{r},\hat{\Omega},t)d^2S = \int_V v\hat{\Omega} \cdot \nabla n(\underline{r},\hat{\Omega},t)d^3r$$

Combining the contributing terms (with proper sign according to gain or loss rate) and realizing that both $d^2\Omega$ and V are arbitrary gives the Boltzmann transport equation,

$$\frac{\partial}{\partial t} n(\underline{r},\hat{\Omega},t) = - v\hat{\Omega}\cdot\nabla n(\underline{r},\hat{\Omega},t) - v\Sigma_t(\underline{r},t)n(\underline{r},\hat{\Omega},t)$$

$$+ c(\underline{r},t)v\Sigma_t(\underline{r},t) \int_{4\pi} f(\underline{r},t;\hat{\Omega}'\rightarrow\hat{\Omega})n(\underline{r},\hat{\Omega}',t)d^2\Omega' + s(\underline{r},\hat{\Omega},t)$$

In terms of the particle flux, $\Phi(\underline{r},\hat{\Omega},t) = vn(\underline{r},\hat{\Omega},t)$, the transport equation is

$$\frac{1}{v}\frac{\partial}{\partial t}\Phi(\underline{r},\hat{\Omega},t) = - \hat{\Omega}\cdot\nabla\Phi(\underline{r},\hat{\Omega},t) - \Sigma_t(\underline{r},t)\Phi(\underline{r},\hat{\Omega},t)$$

$$+ c(\underline{r},t)\Sigma_t(\underline{r},t) \int f(\underline{r},t;\hat{\Omega}'\rightarrow\hat{\Omega})\Phi(\underline{r},\hat{\Omega}',t)d^2\Omega' + s(\underline{r},\hat{\Omega},t)$$

In this monoenergetic particle formulation of the relation describing the transport process, it makes little computational or conceptual difference in using n or Φ as the dependent variable. Both formulations will be employed - the choice depending on the nature of the problem.

Conservation relations:

Consider the operation $\int d^2\Omega$ applied to the particle transport equation. Term-by-term the results are

$$\int \frac{\partial}{\partial t} n(\underline{r},\hat{\Omega},t)\, d^2\Omega = \frac{\partial}{\partial t}\int n(\underline{r},\hat{\Omega},t)d^2\Omega = \frac{\partial}{\partial t} N(\underline{r},t)$$

$$\int v\hat{\Omega}\cdot\nabla n(\underline{r},\hat{\Omega},t)d^2\Omega = \nabla\cdot\int v\hat{\Omega}n(\underline{r},\hat{\Omega},t)d^2\Omega = \nabla\cdot\underline{J}(\underline{r},t)$$

$$\int v\Sigma_t(\underline{r},t)n(\underline{r},\hat{\Omega},t)d^2\Omega = v\Sigma_t(\underline{r},t)N(\underline{r},t)$$

$$\int cv\Sigma_t \int f(\hat{\Omega}'\rightarrow\hat{\Omega})n(\hat{\Omega}')d^2\Omega' d^2\Omega$$

$$= \int cv\Sigma_t n(\hat{\Omega}') \int f(\hat{\Omega}'\rightarrow\hat{\Omega})d^2\Omega d^2\Omega' = cv\Sigma_t N(\underline{r},t)$$

$$\int s(\underline{r},\hat{\Omega},t)d^2\Omega = s(\underline{r},t)$$

Whence,

$$\frac{\partial}{\partial t} N(\underline{r},t) = -\nabla\cdot\underline{J}(\underline{r},t) + [c(\underline{r},t) - 1]v\Sigma_t(\underline{r},t)N(\underline{r},t) + s(\underline{r},t)$$

an equation which describes conservation of particle $\underline{r}$-space population density. Note that multiplication of this conservation relation by the particle mass, m, yields an equation expressing conservation of mass (i.e., the simplest of the equations of fluid dynamics).

More relations of fluid dynamics can be generated from performing various $\hat{\Omega}$-space moments of the transport equation. Such relations are far more meaningful when applied to the energy-dependent transport relation. However, the general idea can be briefly illustrated here. For example, consider the operation $\int d^2\Omega\, m\underline{v}$ applied to the particle transport equation. The left-hand side of the relation is

$$\int m\underline{v}\,\frac{\partial}{\partial t}\,n(\underline{r},\hat{\Omega},t)\,d^2\Omega = mv\,\frac{\partial}{\partial t}\int \hat{\Omega}n(\underline{r},\hat{\Omega},t)\,d^2\Omega$$

$$= mv\,\frac{\partial}{\partial t}\,[\bar{\hat{\Omega}}(\underline{r},t)N(\underline{r},t)] = \frac{\partial}{\partial t}\,[m\underline{\bar{v}}\,(\underline{r},t)N(\underline{r},t)]$$

and represents the rate of change of the net particle momentum per unit volume of $\underline{r}$-space. The right-hand side terms include discussions of complexity unwarranted at this point in these lectures. The resulting relation expresses conservation of particle momentum and is thus an "equation of motion" for the "fluid" of particles (i.e., a form of the Navier-Stokes equation of fluid dynamics).

Analytical Resolution of the Boltzmann Equation

To illustrate techniques for attempting analytical resolution of the Boltzmann transport relation just derived, three approaches are outlined here. For algebraic "simplicity" attention is restricted to a special class of problems. The Boltzmann equation we are considering has already included the simplifications of:

1. No long-range forces and short-range forces described by binary interaction cross sections.
2. Monoenergetic particles.

3. Cross sections independent of direction of particle travel ($\hat{\Omega}$).

4. Stable particles (i.e., no particle population change due to disintegration).

To these add the following restrictions:

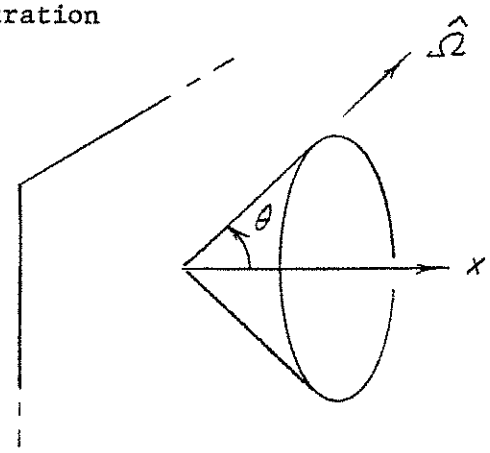
5. Homogeneous, steady state target medium (i.e., c and Σ_t are constants and $f(\hat{\Omega}'\rightarrow\hat{\Omega})$ is $\underline{r}$ and t-independent).

6. Isotropic emission of particles following a particle collision (i.e., $f(\hat{\Omega}'\rightarrow\hat{\Omega}) = 1/4\pi$).

7. Particles in steady state (i.e., $n = n(\underline{r},\hat{\Omega})$, or $\Phi = \Phi(\underline{r},\hat{\Omega})$).

8. Plane symmetry.

In detail, the restriction problems with plane symmetry means that $(\underline{r},\hat{\Omega}) \rightarrow (x,\theta)$, where the position coordinate, x, and the direction-of-travel coordinate, θ, are defined by the illustration



Clearly, in order to actually achieve plane symmetry all medium boundaries or discontinuities would need to be in the form of infinite planes perpendicular to the x-axis, and particle sources would be required which are in the form of x-planes with emission-direction symmetrically distributed about the x-axis.

The restriction of plane symmetry as well as the other seven simplifications listed above are never completely descriptive of a real problem. However, techniques for analytical resolution of more general transport problems are usually based on the ideas outlined here for this greatly simplified case.

For this case, the dependent variable appears always as $vn(x,\theta)$ and therefore the flux (Φ) equation requires less symbols to express. In addition

$$\hat{\Omega}\cdot\nabla\Phi(x,\theta) \rightarrow \cos\theta \frac{\partial}{\partial x}\Phi(x,\theta)$$

$$\int_{4\pi} f(\hat{\Omega}'\rightarrow\hat{\Omega})\phi(x,\theta')d^2\Omega' \rightarrow \frac{1}{2}\int_0^{\pi}\Phi(x,\theta')\sin\theta'd\theta'$$

is more naturally expressed in terms of the direction-cosine, $\mu = \cos\theta$, i.e., $\Phi \rightarrow \Phi(x,\mu)$ and

$$\hat{\Omega}\cdot\nabla\Phi \rightarrow \mu\frac{\partial}{\partial x}\Phi(x,\mu)$$

$$\int_{4\pi} f\,\Phi\, d^2\Omega' \rightarrow \frac{1}{2}\int_{-1}^{+1}\Phi(x,\mu')d\mu'$$

In these terms, the relevant Boltzmann equation is

$$\mu\frac{\partial}{\partial x}\Phi(x,\mu) + \Sigma_t\Phi(x,\mu) = \frac{c\Sigma_t}{2}\int_{-1}^{+1}\Phi(x,\mu')d\mu' + s(x,\mu)$$

It is to this relation that the three solution approaches discussed in these notes are applied.

Approach 1. Eigenvalues and functions of the Boltzmann operator:

Consider the homogeneous form of the Boltzmann equation ($s = 0$) and include effects of s by boundary conditions. Thus,

$$\left(\mu\frac{\partial}{\partial x} + \Sigma_t\right)\Phi(x,\mu) = \frac{c\Sigma_t}{2}\int_{-1}^{+1}\Phi(x,\mu')d\mu'$$

Translational invariance of this equation suggests solutions of the form

$$\Phi(x,\mu) = \Psi(\ell,\mu)e^{-x/\ell}$$

where $\Psi(\ell,\mu)$ must then satisfy

$$\left(-\frac{\mu}{\ell} + \Sigma_t\right)\Psi(\ell,\mu) = \frac{c\Sigma_t}{2}\int_{-1}^{+1}\Psi(\ell,\mu')d\mu'$$

It is found that acceptable values of ℓ fall into a discrete and a continuous spectrum. The continuum in ℓ is for real ℓ in the range

$$-1/\Sigma_t \leq \ell \leq 1/\Sigma_t$$

The discrete values of ℓ, are $\ell = \pm L$ with $c < 1$ implying that L is real and $c > 1$ implying that L is imaginary.

The eigenfunction set $\{\Psi(\ell,\mu)\}$ is orthogonal in the sense

$$\int_{-1}^{+1} \mu\Psi(\ell,\mu)\Psi(\ell',\mu)d\mu = 0 \text{ for } \ell \neq \ell'$$

which can be expressed as

$$\int_{-1}^{+1} \mu\Psi(\ell,\mu)\ \Psi(\ell',\mu)d\mu = \begin{cases} C_\ell \delta_{\ell\ell'}, & \ell \text{ and } \ell' \text{ discrete} \\ C_\ell \delta(\ell-\ell'), & \ell \text{ and } \ell' \text{ continuous.} \end{cases}$$

The general solution of the homogeneous equation is in the form

$$\Phi(x,\mu) = A(+L)\Psi(+L,\mu)e^{-x/L} + A(-L)\Psi(-L,\mu)e^{x/L} + \int_{-1/\Sigma_t}^{+1/\Sigma_t} A(\ell)\Psi(\ell,\mu)e^{-x/\ell}d\ell$$

where the set of expansion coefficients $\{A(\ell)\}$ is evaluated by boundary conditions with the aid of the orthogonality relations.

Approach 2. Expansion in direction-dependent functions:

Assume that the set of functions $\{\Omega_\ell(\mu)\}$ is complete for $-1 \leq \mu \leq +1$ and use the expansion

$$\Phi(x,\mu) = \sum_\ell F_\ell(x)\Omega_\ell(\mu)$$

in the homogeneous form of the transport equation, i.e.,

$$\sum_\ell [\mu\Omega_\ell(\mu)\ \frac{d}{dx} F_\ell(x) + \Sigma_t\Omega_\ell(\mu)F_\ell(x)] = \frac{c\Sigma_t}{2}\sum_\ell F_\ell(x)\int_{-1}^{+1} \Omega_\ell(\mu')d\mu'$$

A particular example of a useful function set is the Legendre polynomials $\{P_\ell(\mu)\}$ which, in addition to being complete, are orthogonal on $-1 \leq \mu \leq +1$ in the sense

$$\int_{-1}^{+1} P_\ell(\mu)P_{\ell'}(\mu)d\mu = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

and obey the recurrence relation

$$(\ell+1)P_{\ell+1}(\mu) - (2\ell+1)\mu P_\ell(\mu) + \ell P_{\ell-1}(\mu) = 0.$$

For simplicity of physical interpretation, redefine the expansion coefficients, $F_\ell(x)$, such that

$$\Phi(x,\mu) = \sum_\ell \frac{2\ell+1}{4\pi}\Phi_\ell(x)P_\ell(\mu)$$

and note that, with this redefinition,

$$\Phi_\ell(x) = 2\pi\int_{-1}^{+1}\Phi(x,\mu)P_\ell(\mu)d\mu = \int\Phi(x,\mu)P_\ell(\mu)d^2\Omega$$

For example,

$\Phi_o(x) = \int\Phi(x,\mu)d^2\Omega = \Phi(x)$, the particle flux

$\Phi_1(x) = \int\Phi(x,\mu)\mu d^2\Omega = J_x(x)$, the particle net current

The transport equation becomes

$$\sum_\ell \frac{2\ell+1}{4\pi}\left[\mu P_\ell(\mu)\frac{d}{dx}\Phi_\ell(x) + \Sigma_t P_\ell(\mu)\Phi_\ell(x) - \frac{c\Sigma_t}{2}\Phi_\ell(x)\int_{-1}^{+1}P_\ell(\mu')d\mu'\right] = 0$$

which, using orthogonality and the recurrence relation, takes the form

$$\sum_\ell \left[(\ell+1)P_{\ell+1}(\mu)\frac{d}{dx}\Phi_\ell(x) + \ell P_{\ell-1}(\mu)\frac{d}{dx}\Phi_\ell(x) + (2\ell+1)P_\ell(\mu)\Sigma_t\Phi_\ell(x) - c\Sigma_t\Phi_\ell(x)\delta_{\ell o}\right] = 0$$

or equivalently,

$$\sum_\ell \left[\ell\frac{d}{dx}\Phi_{\ell-1}(x) + (\ell+1)\frac{d}{dx}\Phi_{\ell+1}(x) + (2\ell+1)\Sigma_t\Phi_\ell(x) - c\Sigma_t\Phi_\ell(x)\delta_{\ell o}\right]P_\ell(\mu) = 0$$

Recognizing that the set $\{P_\ell(\mu)\}$ is linearly independent,

$$\ell \frac{d}{dx} \Phi_{\ell-1}(x) + (\ell+1) \frac{d}{dx} \Phi_{\ell+1}(x) + (2\ell+1)\Sigma_t\Phi_\ell(x) - c\Sigma_t\Phi_\ell(x)\delta_{\ell o} = 0$$

i.e., an infinite set of coupled differential equations in terms of the expansion coefficient functions, $\Phi_\ell(x)$.

The P_N-approximation:

A method for truncating the above set of differential equations is to presume that $\Phi_\ell(x) = 0$ for $\ell > N$ and only retain the first $N + 1$ equations. As an example, consider the P_1-approximation equations

$$\frac{d\Phi_1(x)}{dx} + (1-c)\Sigma_t\Phi_o(x) = 0$$

$$\frac{d\Phi_o(x)}{dx} + 3\Sigma_t\Phi_1(x) = 0$$

which imply

$$\frac{1}{3\Sigma_t} \frac{d^2\Phi_o(x)}{dx^2} - (1-c)\Sigma_t\Phi_o(x) = 0$$

Defining the diffusion coefficient $D = 1/3\Sigma_t$, and identifying $\Phi_o(x)$ and $\Phi_1(x)$ as particle flux and current respectively, the above relations are

$$D \frac{d^2\Phi(x)}{dx^2} - (1-c)\Sigma_t\Phi(x) = 0, \text{ the diffusion equation}$$

$$J_x(x) = - D \frac{d\Phi(x)}{dx}, \text{ Fick's law of diffusion}$$

Note that the solution of the homogeneous diffusion equation is of the form

$$\Phi(x) = B_+e^{-x/L_1} + B_-e^{x/L_1}$$

where the diffusion length, L_1, is defined by

$$L_1 = \left(\frac{D}{(1-c)\Sigma_t}\right)^{1/2}$$

Approach 3. Moments method:

Including an extraneous source, $s(x,\mu)$, the transport equation is

$$(\mu \frac{\partial}{\partial x} + \Sigma_t)\Phi(x,\mu) = \frac{c\Sigma_t}{2} \int_{-1}^{+1} \phi(x,\mu')d\mu' + s(x,\mu)$$

Using the Legnedre polynomial expansions

$$\Phi(x,\mu) = \sum_{\ell} \frac{2\ell+1}{4\pi} \Phi_\ell(x)P_\ell(\mu)$$

$$s(x,\mu) = \sum_{\ell} \frac{2\ell+1}{4\pi} s_\ell(x)P_\ell(\mu)$$

reduces the transport description to the set of differential equations

$$\frac{\ell}{2\ell+1} \frac{d}{dx} \Phi_{\ell-1}(x) + \frac{\ell+1}{2\ell+1} \frac{d}{dx}\Phi_{\ell+1}(x) + (1-c\delta_{\ell o})\Sigma_t\Phi_\ell(x) = s_\ell(x)$$

Define the particle flux distribution moments and particle source moments by

$$\Phi_{\ell m} = \int_{-\infty}^{+\infty} x^m\Phi_\ell(x)dx = \int_{-\infty}^{+\infty} dx x^m \int P_\ell(\mu)\phi(x,\mu)d^2\Omega$$

$$s_{\ell m} = \int_{-\infty}^{+\infty} x^m s_\ell(x)dx = \int_{-\infty}^{+\infty} dx x^m \int P_\ell(\mu)s(x,\mu)d^2\Omega$$

For example,

$$\ell = 0: \quad \Phi_{om} = \int_{-\infty}^{+\infty} dx x^m \int\Phi(x,\mu)d^2\Omega = \int_{-\infty}^{+\infty} x^m\Phi(x)dx$$

Therefore $\frac{\Phi_{om}}{\Phi_{oo}} = \langle x^m \rangle$, i.e., the configuration moments of the particle distribution.

$$m = 0: \quad \Phi_{\ell o} = \int_{-\infty}^{+\infty} dx \int P_\ell(\mu)\Phi(x,\mu)d^2\Omega = \int_{-\infty}^{+\infty} \overline{P_\ell(\mu)}\ (x)\Phi(x)dx$$

Therefore $\frac{\Phi_{\ell o}}{\Phi_{oo}} = \langle P_\ell(\mu) \rangle$, i.e., the direction-of-travel moments of the particle distribution.

In order to obtain an equation relating the $\{\Phi_{\ell m}\}$ with the set $\{s_{\ell m}\}$ perform the operation

$$\int_{-\infty}^{+\infty} x^m(\text{equation above in } \Phi_\ell,\ \Phi_{\ell-1},\ \Phi_{\ell+1},\ s_\ell)dx$$

and note that

$$\int_{-\infty}^{+\infty} \frac{d\Phi_\ell}{dx}\, x^m dx = (x^m \Phi_\ell)_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} m x^{m-1} \Phi_\ell(x)\, dx = \not{\Phi}_{\ell,\ m-1}$$

Whence, the relation

$$(1-c\delta_{\ell o})\Sigma_t \Phi_{\ell m} = s_{\ell m} + \frac{m}{2\ell+1}\left[\ell \Phi_{\ell-1,\ m-1} + (\ell+1)\Phi_{\ell+1,\ m-1}\right]$$

In many problems, the source moment set $\{s_{\ell m}\}$ is given, or can be obtained from a given source distribution $s(x,\mu)$, and the particle flux solution is sought. The results, here, indicate a systematic, algebraic technique of obtaining as many members of the particle flux moment set $\{\Phi_{\ell m}\}$ as is practical, or desired. From the particle flux moments either certain physical descriptions are immediately evident (such as problem scales), or an attempt can be made to artificially construct the particle distribution, $\Phi(x,\mu)$. It should be carefully noted that although there is an infinite sequence of algebraic moment relations, they are coupled such that $\Phi_{\ell m}$ depends only on $\Phi_{\ell-1,\ m-1}$ and $\Phi_{\ell+1,\ m-1}$. Thus, a systematic progression of obtaining moments given $\{\Phi_{\ell o}\}$ is generated. The set $\{\Phi_{\ell o}\}$ depends only on $\{s_{\ell o}\}$ and is thus presumed given. The following matrix indicates the systematic progression in the calculation of moments.

$\ell\rightarrow$		0	1	2	...	$\ell-1$	ℓ	$\ell+1$	...
m $\downarrow$	0	Φ_{00}	Φ_{10}	Φ_{20}			$\Phi_{\ell 0}$	direction moments (presumed given)	
	1	Φ_{01}							
	2	Φ_{02}							
	$\vdots$								
	$m-1$					$\Phi_{\ell-1,\ m-1}$		$\Phi_{\ell+1,\ m-1}$	
	m	Φ_{0m}					$\Phi_{\ell m}$		
	$m+1$								
	$\vdots$	configuration moments							

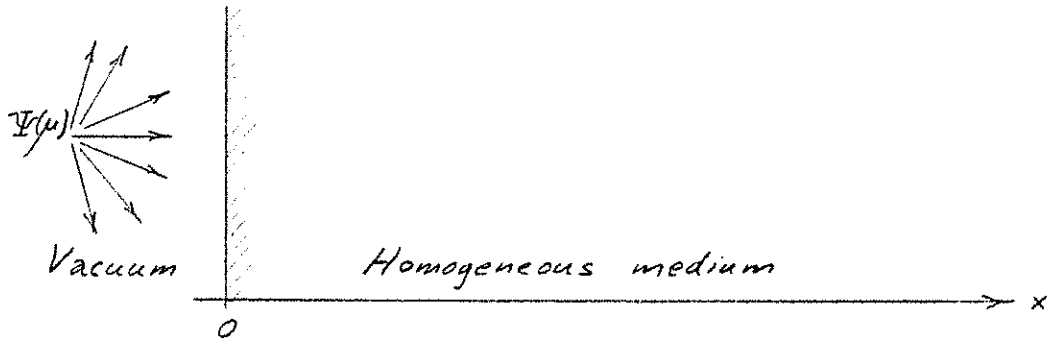
Application and Validity of Analytical Methods

In terms of the analytical approaches just described, attention can now be focused on application to physical problems. Such considerations help to clarify the details of the methods as well as illustrate their limitations.

Use and validity of P_N-approximations will be illustrated by application to the problem of determining the reflection properties of a homogeneous half-space. Use of the moments method will be illustrated by application to the problem of determining the effects of source emission distributions.

Reflection properties of a half-space:

Consider the problem of a radiation flux illuminating the plane surface of a homogeneous half-space. With reference to the illustration, a



homogeneous medium in the positive x half-space is illuminated by a particle flux with a prescribed angular description, i.e.,

$$\Phi(0,\mu) = \Psi(\mu) \text{ for } 0 \leq \mu \leq +1$$

The emerging radiation flux, $\Phi(0,\mu)$ for $-1 \leq \mu \leq 0$, completely describes the reflection properties of the half-space as dictated by the parameters of the medium and the incident illumination. Note that we have already discussed a more restricted descriptive quantity, R, the reflection coefficient, defined by

$$R = \frac{J_-(0)}{J_+(0)}$$

Certainly R can be evaluated via radiation flux illumination and emerging descriptions, viz.

$$J_+(0) = 2\pi \int_0^{-1} \mu\Psi(\mu)d\mu \quad \text{and} \quad J_-(0) = -2\pi \int_{-1}^{0} \mu\Phi(0,\mu)d\mu$$

Thus, the problem is fully directed toward determining the emerging radiation flux, $\Phi(0,\mu)$ for $-1 \leq \mu \leq 0$.

The P_N-approximation is summarized by the truncation

$$\Phi(x,\mu) = \sum_{n=0}^{N} \frac{2n+1}{4\pi} \Phi_n(x) P_n(\mu)$$

and the equation set (for isotropic emission)

$$n \frac{d}{dx} \Phi_{n-1}(x) + (n+1) \frac{d}{dx} \Phi_{n+1}(x) + (2n+1)\Sigma_t(1-c\delta_{no})\Phi_n(x) = 0$$

with $n = 0, 1, 2, \ldots, N$ and $\Phi_{N+1}(x) = 0$.

P_1-approximation--

The particle flux is given by

$$\Phi(x,\mu) = \frac{1}{4\pi} \Phi_0(x) + \frac{3}{4\pi} \Phi_1(x)\mu$$

and the relevant equations are

$$\frac{d}{dx} \Phi_1(x) + \Sigma_t(1-c) \Phi_0(x) = 0$$

$$\frac{d}{dx} \Phi_0(x) + 3\Sigma_t \Phi_1(x) = 0$$

We have previously discussed the manipulation of these relations to generate Fick's law and the diffusion equation. Let us now approach the solution of the problem in a manner analogous to finding eigenvalues and eigenfunctions of the Boltzmann equation (Approach 1, page 3-13). Specifically: Translational

invariance suggests the form

$$\Phi_n(x) = \Psi_n(\ell)\ e^{-x/\ell} \text{ for } n = 0,1$$

Whence,

$$\ell\Sigma_t(1-c)\Psi_0(\ell) - \Psi_1(\ell) = 0$$

$$-\Psi_0(\ell) + 3\ell\Sigma_t\ \Psi_1(\ell) = 0$$

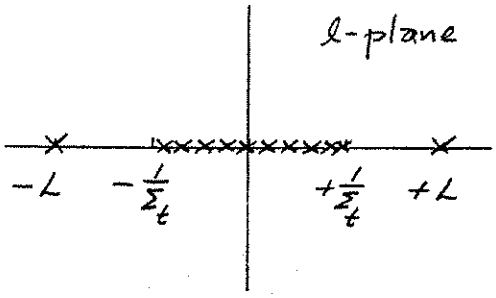
i.e., two linear, algebraic, homogeneous equations in the two unknown $\Psi_0(\ell)$ and $\Psi_1(\ell)$. The condition for non-trivial solution (where the trivial solution is $\Psi_0(\ell) = \Psi_1(\ell) = 0$) is

$$\begin{vmatrix} \ell\Sigma_t(1-c) & -1 \\ -1 & 3\ell\Sigma_t \end{vmatrix} = 0$$

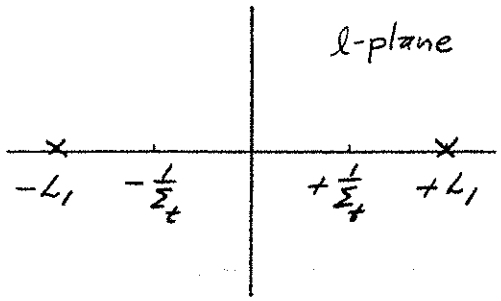
which reduces to $\ell = \pm L_1$ where

$$L_1 = [3(1-c)]^{-1/2}\ \Sigma_t^{-1}$$

The eigenvalues $\pm L_1$ are the P_1-approximation to the discrete pair of eigenvalues $\pm L$ discussed on page 3-14. For a $c<1$ problem, the eigenvalue spectrum for the exact solutions (Approach 1) can be compared to the eigenvalue spectrum of the P_1-approximation (Approach 2) via the illustration



Approach 1
Exact solution



Approach 2
P_1-approximation

The P_1-approximation eigenfunctions are easily extracted from the above relations. Specifically,

$$\frac{\Psi_1(\ell)}{\Psi_0(\ell)} = \frac{1}{3\ell\Sigma_t}$$

yields $\Psi_1(\pm L_1)/\Psi_0(\pm L_1) = \pm 1/3L_1\Sigma_t$. Whence, acceptable solutions of the exponential form are

$$\Phi(x,\mu) = \frac{\Psi_0(+L_1)}{4\pi}\left[1 + \frac{1}{L_1\Sigma_t}\mu\right]e^{-x/L_1}$$

and

$$\Phi(x,\mu) = \frac{\Psi_0(-L_1)}{4\pi}\left[1 - \frac{1}{L_1\Sigma_t}\mu\right]e^{+x/L_1}$$

i.e., a general solution of the form

$$\Phi(x,\mu) = A\left[1 + \frac{1}{L_1\Sigma_t}\mu\right]e^{-x/L_1} + C\left[1 - \frac{1}{L_1\Sigma_t}\mu\right]e^{+x/L_1}$$

In the half-space reflection problem, the boundary conditions are

(I) $\lim_{x \to \infty} \Phi(x,\mu) = 0$

(II) A condition descriptive of the entrance particle flux $\Psi(\mu)$.

Boundary condition (I) implies $C = 0$ and thus

$$\Phi(x,\mu) = A\left[1 + \frac{1}{L_1\Sigma_t}\mu\right]e^{-x/L_1}$$

In particular

$$\Phi(0,\mu) = A\left[1 + \frac{1}{L_1\Sigma_t}\mu\right]$$

Clearly, the application of boundary condition (II) cannot accurately describe an arbitrary illumination $\Psi(\mu)$, $0 \leqq \mu \leqq +1$. To satisfy the P_1-approximation, the linear μ-form is required and only the very restricted case of

$$\Psi(\mu) = A[1 + \frac{1}{L_1 \Sigma_t} \mu] \text{ for } 0 \leqq \mu \leqq +1$$

would give direction-of-travel pointwise agreement. It is therefore usually required to develop less rigorous boundary conditions which are, at least, intuitively satisfactory. An example is to establish entrance particle current agreement, i.e., apply boundary condition (II) as

$$2\pi \int_0^{+1} \mu\Phi(0,\mu)d\mu = 2\pi \int_0^{+1} \mu\Psi(\mu)d\mu = I$$

which is merely a statement that $J_+(0) = I$. Using this arbitrarily chosen condition yields

$$A = \frac{I}{\pi[1 + 2/3L_1 \Sigma_t]}$$

and the problem of characterizing the emerging radiation is solved, i.e.,

$$\Phi(0,\mu) = \frac{I}{\pi[1 + 2/3L_1 \Sigma_t]} [1 + \mu/L_1 \Sigma_t]$$

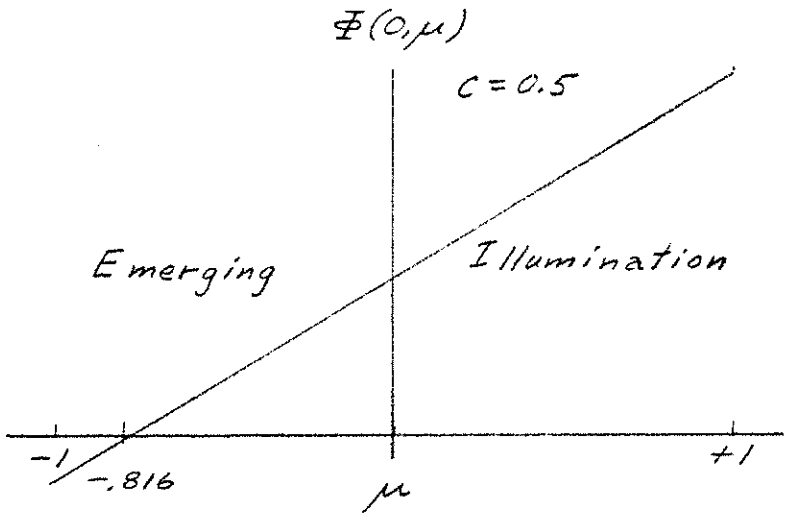
for $-1 \leqq \mu \leqq +1$ which includes the emerging direction contribution. In passing, note that

$$\frac{1}{L_1 \Sigma_t} = [3(1-c)]^{1/2}$$

and thus the expected result that half-space reflection properties are only a function of c and, for example, are independent of Σ_t. Rewriting the emission distribution as

$$\Phi(0,\mu) = A[1 + \sqrt{3(1-c)}\mu] \text{ for } -1 \leqq \mu \leqq 0$$

illustrates another limitation of the P_1-approximation. If $1/3(1-c) < 1$, i.e., if $0 < c < 2/3$, then $\Phi(0,\mu) < 0$ in the range of emerging directions which is a physical impossibility. The case of $c = 0.5$ is illustrated to indicate the clear limitations of the P_1-approximation applied to this problem.



Finally, with perseptive disbelief for cases where $c < 2/3$, the calculation of the reflection coefficient proceeds via

$$J_-(0) = -2\pi \int_{-1}^{0} \frac{I}{\pi[1 + 2/3L_1\Sigma_t]} \mu[1 + \mu/L_1\Sigma_t]d\mu$$

to the familiar "diffusion approximation" result

$$R = \frac{J_-(0)}{I} = \frac{1 - 2/3L_1\Sigma_t}{1 + 2/3L_1\Sigma_t} = \frac{1 - 2D/L_1}{1 + 2D/L_1}$$

P_2-approximation--

The particle flux is given by

$$\Phi(x,\mu) = \frac{1}{4\pi} \Phi_0(x) + \frac{3}{4\pi} \Phi_1(x)\mu + \frac{5}{4\pi} \Phi_2(x) [\frac{3}{2}\mu^2 - \frac{1}{2}]$$

and the relevant equations are

$$\frac{d}{dx}\ \Phi_1(x) + \Sigma_t(1-c)\ \Phi_0(x) = 0$$

$$\frac{d}{dx}\ \Phi_0(x) + 2\ \frac{d}{dx}\ \Phi_2(x) + 3\Sigma_t\ \Phi_1(x) = 0$$

$$2\ \frac{d}{dx}\ \Phi_1(x) + 5\Sigma_t\ \Phi_2(x) = 0$$

Same methods as used in the P_1-approximation give now

$$\ell\Sigma_t(1-c)\ \Psi_0(\ell) - \Psi_1(\ell) + 0 = 0$$

$$-\ \Psi_0(\ell) + 3\ell\Sigma_t\Psi_1(\ell) - 2\ \Psi_2(\ell) = 0$$

$$0 \quad - 2\ \Psi_1(\ell) + 5\ell\Sigma_t\Psi_2(\ell) = 0$$

where

$$\Phi_n(x) = \Psi_n(\ell)e^{-x/\ell} \text{ for } n = 0, 1, 2$$

For non-trivial solution,

$$\begin{vmatrix} \ell\Sigma_t(1-c) & -1 & 0 \\ -1 & 3\ell\Sigma_t & -2 \\ 0 & -2 & 5\ell\Sigma_t \end{vmatrix} = 0$$

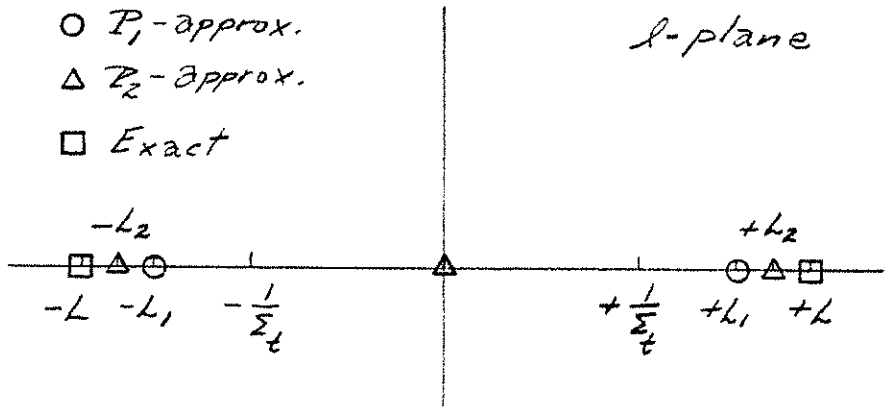
i.e.,

$$15(1-c)\ell^3\Sigma_t^3 - [5 + 4(1-c)]\ell\Sigma_t = 0$$

which reduces to $\ell = 0$ and $\pm L_2$ where

$$L_2 = \left[\frac{1}{3(1-c)} + \frac{4}{15}\right]^{1/2} \Sigma_t^{-1}$$

The eigenvalues $\pm L_2$ are the P_2-approximation to the discrete pair of eigenvalues $\pm L$. Comparing the discrete eigenvalues of the various approaches for a $c < 1$ problem yields the illustration



The P_2-approximation eigenfunctions are extracted from the above relations and yield the two ratios

$$\frac{\Psi_1(\ell)}{\Psi_0(\ell)} = \ell\Sigma_t(1-c)$$

$$\frac{\Psi_2(\ell)}{\Psi_0(\ell)} = \frac{3}{2}\ell^2\Sigma_t^2(1-c) - \frac{1}{2}$$

Whence $\Psi_1(\pm L_2)/\Psi_0(\pm L_2) = \pm L_2\Sigma_t(1-c)$ and $\Psi_2(\pm L_2)/\Psi_0(\pm L_2) = 3L_2^2\Sigma_t^2(1-c)/2-1/2$; acceptable solutions for the particle flux take the form

$$\Phi(x,\mu) = \frac{\Psi_0(+L_2)}{4\pi}\left[1 + 3L_2\Sigma_t(1-c)\mu + 5\left(\frac{3}{2}L_2^2\Sigma_t^2(1-c) - \frac{1}{2}\right)\left(\frac{3}{2}\mu^2 - \frac{1}{2}\right)\right]e^{-x/L_2}$$

In summary, the P_2-approximation solution to this problem yields a better asymptotic eigenvalue than does the P_1-approximation (i.e., L_2 is closer to L than is L_1). Moreover, a more complete angular distribution is generated. However, because the additional eigenvalue, $\ell = 0$, is of no use in satisfying boundary values, there is no more flexibility found for

more completely specifying the illuminating particle flux $\Psi(\mu)$. For this reason, the next approximation used in problems such as the one considered is the P_3-approximation.

P_3-approximation--

The particle flux is given by

$$\Phi(x,\mu) = \frac{1}{4\pi}\Phi_0(x) + \frac{3}{4\pi}\Phi_1(x)\mu + \frac{5}{4\pi}\Phi_2(x)\left[\frac{3}{2}\mu^2 - \frac{1}{2}\right] + \frac{7}{4\pi}\Phi_3(x)\left[\frac{5}{2}\mu^3 - \frac{3}{2}\mu\right]$$

and the relevant equations are

$$\frac{d}{dx}\Phi_1(x) + \Sigma_t(1 - c)\Phi_0(x) = 0$$

$$\frac{d}{dx}\Phi_0(x) + 2\frac{d}{dx}\Phi_2(x) + 3\Sigma_t\Phi_1(x) = 0$$

$$2\frac{d}{dx}\Phi_1(x) + 3\frac{d}{dx}\Phi_3(x) + 5\Sigma_t\Phi_2(x) = 0$$

$$3\frac{d}{dx}\Phi_2(x) + 7\Sigma_t\Phi_3(x) = 0$$

Using $\Phi_n(x) = \Psi_n(\ell)e^{-x/\ell}$ for n = 0, 1, 2, 3 yields the set of relations

$$\ell\Sigma_t(1 - c)\Psi_0(\ell) - \Psi_1(\ell) + 0 + 0 = 0$$

$$-\Psi_0(\ell) + 3\ell\Sigma_t\Psi_1(\ell) - 2\Psi_2(\ell) + 0 = 0$$

$$0 - 2\Psi_1(\ell) + 5\ell\Sigma_t\Psi_2(\ell) - 3\Psi_3(\ell) = 0$$

$$0 + 0 - 3\Psi_2(\ell) + 7\ell\Sigma_t\Psi_3(\ell) = 0$$

and the resulting condition for non-trivial solution,

$$\begin{vmatrix} \ell\Sigma_t(1 - c) & -1 & 0 & 0 \\ -1 & 3\ell\Sigma_t & -2 & 0 \\ 0 & -2 & 5\ell\Sigma_t & -3 \\ 0 & 0 & -3 & 7\ell\Sigma_t \end{vmatrix} = 0$$

i.e.,

$$105(1-c)\ell^4\Sigma_t^4 - [55(1-c)+35]\ell^2\Sigma_t^2 + 9 = 0$$

Whence,

$$\ell^2\Sigma_t^2 = \frac{35+55(1-c)}{210(1-c)} \left\{ 1 \pm \left[1 - \frac{3780(1-c)}{[35+55(1-c)]^2} \right]^{1/2} \right\}$$

Note that

$$[35+55(1-c)]^2 = 1225 + 3850(1-c) + 3025(1-c)^2$$

and defining $\varepsilon(c)$ by

$$\varepsilon(c) = \frac{3780(1-c)}{[35+55(1-c)]^2}$$

it is easily concluded that, for $0 < c < 1$, $0 < \varepsilon(c) < 1$. Moreover, as $c \to 1$, $\varepsilon(c) \to 0$. To indicate further relevant numerical details, consider a case with c sufficiently close to unity such that the approximation

$$[1 - \varepsilon(c)]^{1/2} \simeq 1 - \frac{1}{2}\varepsilon(c)$$

can be employed. Thus,

$$\ell^2\Sigma_t^2 \simeq \frac{35+55(1-c)}{210(1-c)} \quad [1 \pm (1-\varepsilon(c)/2)]$$

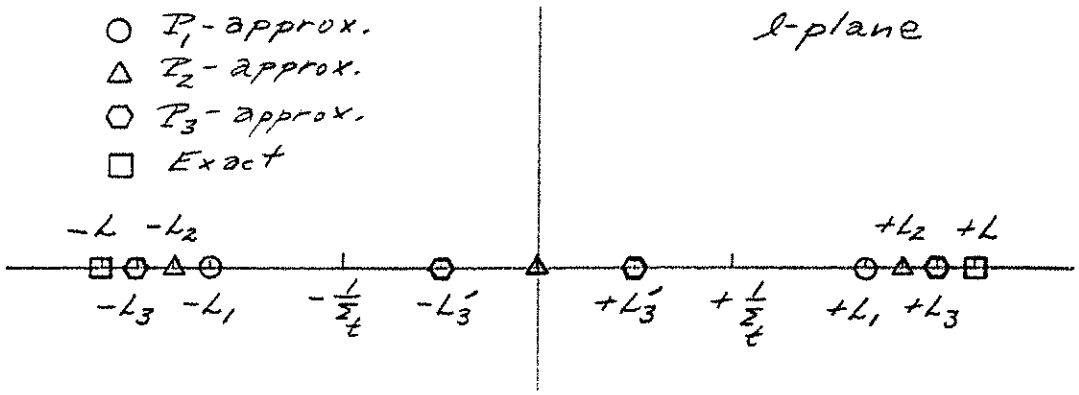
Whence, the solutions

$$\ell = \pm L_3 \text{ where } L_3 = \left[\frac{1}{3(1-c)} + \frac{11}{21} \right]^{1/2} \Sigma_t^{-1}$$

$$\ell = \pm L_3' \text{ where } L_3' = \left[\frac{9}{35+55(1-c)} \right]^{1/2} \Sigma_t^{-1}$$

The eigenvalues $\pm L_3$ and $\pm L_3'$ are the P_3-approximation to the discrete pair of eigenvalues $\pm L$ and the continuum of eigenvalues between $-1/\Sigma_t$ and $+1/\Sigma_t$, respectively. Comparing the eigenvalues of the various approaches for a

c < 1 problem now yields the illustration



The P_3-approximation eigenfunctions are extracted from the above relations and yield the three ratios

$$\frac{\Psi_1(\ell)}{\Psi_0(\ell)} = \ell\Sigma_t(1 - c)$$

$$\frac{\Psi_2(\ell)}{\Psi_0(\ell)} = \frac{3}{2}\ell^2\Sigma_t^2(1-c) - \frac{1}{2}$$

$$\frac{\Psi_3(\ell)}{\Psi_0(\ell)} = \frac{5}{2}\ell^3\Sigma_t^3(1-c) - \frac{5+4(1-c)}{6}\ell\Sigma_t$$

Acceptable solutions for the particle flux take the form

$$\Phi(x,\mu) = A\left[1 + 3\frac{\Psi_1(+L_3)}{\Psi_0(+L_3)}\mu + 5\frac{\Psi_2(+L_3)}{\Psi_0(+L_3)}\left(\frac{3}{2}\mu^2 - \frac{1}{2}\right) + 7\frac{\Psi_3(+L_3)}{\Psi_0(+L_3)}\left(\frac{5}{2}\mu^3 - \frac{3}{2}\mu\right)\right]e^{-x/L_3}$$

$$+ A'\left[1 + 3\frac{\Psi_1(+L_3')}{\Psi_0(+L_3')}\mu + 5\frac{\Psi_2(+L_3')}{\Psi_0(+L_3')}\left(\frac{3}{2}\mu^2 - \frac{1}{2}\right) + 7\frac{\Psi_3(+L_3')}{\Psi_0(+L_3')}\left(\frac{5}{2}\mu^3 - \frac{3}{2}\mu\right)\right]e^{-x/L_3'}$$

Exclusion of the otherwise acceptable solution forms which vary as $\exp(+x/L_3)$ and $\exp(+x/L_3')$ has already invoked the boundary condition that $\Phi(x,\mu) \to 0$ as $x \to \infty$. The two coefficients, A and A', are determined solely by conditions descriptive of the entrance particle flux $\Psi(\mu)$. Thus, like the P_2-approximation, the present solution yields a progressively better asymptotic eigenvalue (i.e., L_3 is closer to L than is either L_1 or L_2), and a more complete angular distribution is generated. In contrast to the P_2-approximation, the additional eigenvalue pair $\ell = \pm L_3'$ and their associated eigenfunctions provide additional flexibility in more completely characterizing the illuminating flux.

In the P_3-approximation $\Phi(0,\mu)$ has the form

$$\Phi(0,\mu) = A\ (C_0 + C_1\mu + C_2\ \mu^2 + C_3\ \mu^3)$$

$$+ A'\ (C_0' + C_1'\mu + C_2'\ \mu^2 + C_3'\ \mu^3)$$

where the C_n and C_n' are known functions of the half-space medium parameters. The cubic μ-form is required and only the very restricted case of

$$\Psi(\mu) = A_0 + A_1\mu + A_2\mu^2 + A_3\mu^3 \text{ for } 0 \leq \mu \leq +1$$

and the fortuity to find that there exist an A and A' which satisfy the simultaneous over-specified set of relations

$$A_0 = AC_0 + A'C_0'$$

$$A_1 = AC_1 + A'C_1'$$

$$A_2 = AC_2 + A'C_2'$$

$$A_3 = AC_3 + A'C_3'$$

yields direction-of-travel pointwise agreement between the solution $\Phi(0,\mu)$ and the illumination boundary condition $\Psi(\mu)$. It is, therefore, again required to develop less rigorous, but intuitively satisfactory, boundary conditions. Using the same approach as was applied to this problem under the P_1-approximation, an example is to require

$$2\pi \int_0^{+1} \mu\Phi(0,\mu)\,d\mu = 2\pi \int_0^{+1} \mu\Psi(\mu)\,d\mu = I$$

and

$$2\pi \int_0^{+1} \mu^3\Phi(0,\mu)\,d\mu = 2\pi \int_0^{+1} \mu^3\Psi(\mu)\,d\mu = H$$

which is a statement that not only $J_+(0) = I$, but that the average value of μ-cubed is also in agreement with the illumination conditions (i.e., a one-step better description of the actual illumination).

Using these two arbitrarily chosen boundary conditions yields

$$A = \frac{1}{\pi} \frac{\beta' I - \alpha' H}{\alpha\beta' - \alpha'\beta}$$

$$A' = \frac{1}{\pi} \frac{\alpha H - \beta I}{\alpha\beta' - \alpha'\beta}$$

where

$$\alpha = C_0 + \frac{2}{c} C_1 + \frac{1}{2} C_2 + \frac{2}{5} C_3$$

$$\alpha' = C_0' + \frac{2}{3} C_1' + \frac{1}{2} C_2' + \frac{2}{5} C_3'$$

$$\beta = \frac{1}{2} C_0 + \frac{2}{5} C_1 + \frac{1}{3} C_2 + \frac{2}{7} C_3$$

$$\beta' = \frac{1}{2} C_0' + \frac{2}{5} C_1' + \frac{1}{3} C_2' + \frac{2}{7} C_3'$$

Thus, the problem of characterizing the emerging radiation is solved. In addition, the calculation of the reflection coefficient proceeds via

$$J_-(0) = -2\pi \int_{-1}^{0} \mu\Phi(0,\mu)\,d\mu$$

which yields

$$J_-(0) = \overline{\alpha}\,\frac{\beta' I - \alpha' H}{\alpha\beta' - \alpha'\beta} + \overline{\alpha}'\,\frac{\alpha H - \beta I}{\alpha\beta' - \alpha'\beta}$$

where

$$\overline{\alpha} = C_0 - \frac{2}{3}C_1 + \frac{1}{2}C_2 - \frac{2}{5}C_3$$

$$\overline{\alpha}' = C_0' - \frac{2}{3}C_1' + \frac{1}{2}C_2' - \frac{2}{5}C_3'$$

The reflection coefficient is now easily expressed in terms of half-space material parameters (the $\alpha,\alpha',\beta,\beta'$, $\overline{\alpha}$ and $\overline{\alpha}'$) and illumination description (the I and H) as

$$R = \frac{J_-(0)}{I} = \frac{\overline{\alpha}}{I}\,\frac{\beta' I - \alpha' H}{\alpha\beta' - \alpha'\beta} + \frac{\overline{\alpha}'}{I}\,\frac{\alpha H - \beta I}{\alpha\beta' - \alpha'\beta}$$

An alternative algebraic reduction--

Beginning with the P_N-approximation set of couple differential equations for the functions $\{\Phi_n(x),\ n = 0,1,2,\ldots,N\}$, i.e.,

$$n\,\frac{d}{dx}\,\Phi_{n-1}(x) + (n+1)\,\frac{d}{dx}\,\Phi_{n+1}(x) + (2n+1)\Sigma_t(1-c\delta_{no})\Phi_n(x) = 0$$

with $n = 0,1,2,\ldots,N$ and $\Phi_{N+1}(x) = 0$, another, more direct, algebraic reduction is possible for problems such as the one just detailed. The approach follows the general path of that covered in Approach 1 (page 3-13). Specifically, translational invariance of the equation set suggests solutions of the form

$$\Phi_n(x) = \Psi_n(\ell)e^{-x/\ell}$$

In fact, using this form of solution actually generates a recurrence relation for the "eigenfunction" set $\{\Psi_n(\ell)\}$, viz.

$$n\,\Psi_{n-1}(\ell) - (2n+1)\,(1 - c\delta_{no})\,\ell\Sigma_t\Psi_n(\ell) + (n+1)\Psi_{n+1}(\ell) = 0$$

As written, the relation among the $\Psi_n(\ell)$ is reminiscent of the equivalent recurrence relation for the Legendre polynomials. Moreover, since these solutions will eventually be linearly combined (summed) with coefficients chosen to match arbitrary boundary conditions, an arbitrary normalization, say $\Psi_0(\ell) = 1$, may be employed. The desired function set is then generated by the recurrence relation, viz.

$$\Psi_0(\ell) = 1$$

$$\Psi_1(\ell) = (1-c)\ell\Sigma_t$$

$$\Psi_2(\ell) = \frac{3}{2}(1-c)\ell^2\Sigma_t^2 - \frac{1}{2}$$

$$\Psi_3(\ell) = \frac{5}{2}(1-c)\ell^3\Sigma_t^3 - \frac{5+4(1-c)}{6}\ell\Sigma_t$$

$$\Psi_4(\ell) = \frac{35}{8}(1-c)\ell^4\Sigma_t^4 - \frac{35+55(1-c)}{24}\ell^2\Sigma_t^2 + \frac{3}{8}$$

etc.

and, as expected, bears a resemblence to the Legendre polynomial set. The P_N-approximation is accomplished by using only $n = 0,1,2\ldots,N$ and setting $\Psi_{N+1}(\ell) = 0$.

It is no surprise that the set $\{\Psi_n(\ell)\}$ so-generated is identical to the functions found in the earlier discussion. What, perhaps, is a surprise is that the previously determined P_N-approximation secular equations (condition for non-trivial solution) is precisely the same as the relation $\Psi_{N+1}(\ell) = 0$. In fact, comparing the secular conditions and the present requirement yields:

P_1-approx. secular cond. = $[2\ \Psi_2(\ell) = 0]$

P_2-approx. secular cond. = $[6\ \Psi_3(\ell) = 0]$

P_3-approx. secular cond. = $[24\ \Psi_4(\ell) = 0]$

It can be shown, with some algebraic effort, that these results generalize to

$$P_N\text{-approx. secular cond.} = [(N+1)!\ \Psi_{N+1}(\ell) = 0]$$

Since it is relatively easy to generate the set $\{\Psi_n(\ell)\}$, this is a useful relation. The existence of the relation lends a sense of consistency to this method of truncating the expansion of $\Phi(x,\mu)$.

Source emission distribution effects:

Consider the problem of a single, plane radiation source in an infinite, homogeneous medium. We shall employ the moments method (Approach 3) to estimate, in a relatively simple manner, the influence of the source angular emission distribution on the resulting radiation flux.

The flux and source moments have been previously defined as

$$\Phi_{nm} = \int_{-\infty}^{+\infty} \int_{4\pi} x^m P_n(\mu)\, \Phi(x,\mu)\, dx d^2\Omega$$

$$s_{nm} = \int_{-\infty}^{+\infty} \int_{4\pi} x^m P_n(\mu)\, s(x,\mu)\, dx d^2\Omega$$

If the plane source is positioned at the origin of x, then $s(x,\mu) = s(\mu)\delta(x)$ and the set of source moments is generated by

$$s_{nm} = 2\pi\delta_{mo} \int_{-1}^{+1} P_n(\mu)\, s(\mu)\, d\mu = s_n \delta_{mn}$$

For the purpose of detailing a specific problem, consider the case where $s(\mu)$ is a symmetric, quadratic function of the direction variable μ, i.e.,

$$s(\mu) = A + C\mu^2 \text{ for } -1 \leq \mu \leq +1$$

In terms of the Legendre polynomial expansion of the source emission distribution,

$$s(\mu) = \frac{1}{4\pi}\ s_o + \frac{5}{4\pi}\ s_2\ \left(\frac{3}{2}\mu^2 - \frac{1}{2}\right)$$

Clearly,

$$A = \frac{1}{4\pi}\left(s_o - \frac{5}{2}\, s_2\right)$$

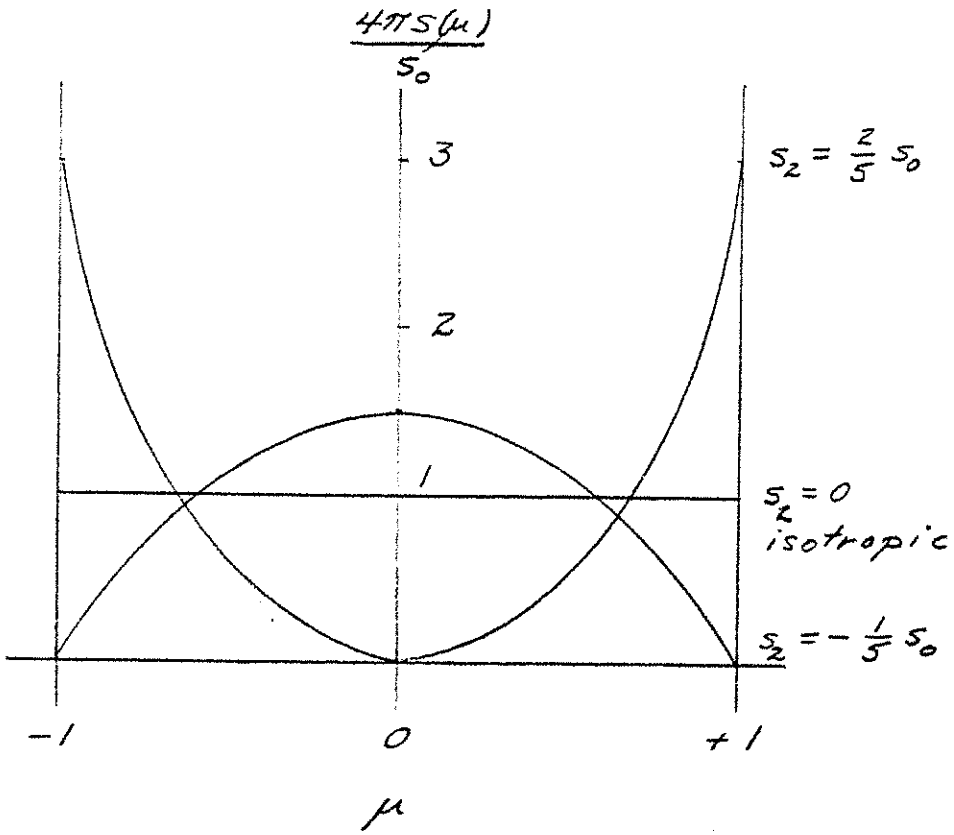
$$C = \frac{15}{8\pi}\, s_2$$

With the (angular integrated) strength of the source, s_0, fixed, the limits on s_2 which generate a positive-definite ($s(\mu) \geq 0$ for $-1 \leq \mu \leq +1$) source distribution are found by requiring $A \geq 0$ and $s(\pm 1) \geq 0$, viz.

$$A \geq 0 \;\rightarrow\; s_2 \leq \frac{2}{5}\, s_0$$

$$s(\pm 1) \geq 0 \;\rightarrow\; s_2 \geq -\frac{1}{5}\, s_0$$

Whence, $-s_0/5 \leq s_2 \leq 2s_0/5$. The limiting cases, depicting the range of symmetric, quadratic source emission distributions of physical relevance are illustrated.



With s_0 and s_2 (within the required limits) chosen, the source moment matrix is established, i.e.,

m ↓ \ n →	0	1	2	3	...
0	s_0	0	s_2	0	
1	0	0	0	0	
2	0	0	0	0	
3	0	0	0	0	
⋮					

The radiation flux moment set $\{\Phi_{n,m}\}$ is generated by the previously derived set of relations

$$-\frac{m}{2n+1}\left[n\Phi_{n-1,m-1} + (n+1)\Phi_{n+1,m-1}\right] + \Sigma_t(1-c\delta_{no})\Phi_{n,m} = s_{n,m}$$

The resulting low index corner of the flux moment matrix is

m ↓ \ n →	0	1	2	...
0	$\frac{s_0}{\Sigma_t(1-c)}$	0	$\frac{s_2}{\Sigma_t}$	
1	0	$\frac{1}{3\Sigma_t^2}\left(\frac{s_0}{1-c} + 2\,s_2\right)$	0	
2	$\frac{2}{3\Sigma_t^3(1-c)}\left(\frac{s_0}{1-c} + 2\,s_2\right)$	0		
⋮				

One technique of using the determined flux moments for practical calculation purposes is to formulate a guess of the functional form of the radiation flux and then apply the exact moments in the "optimization" of that guess. For example, in the present problem spatial symmetries imply that $\Phi(x,\mu) = \Phi(-x,-\mu)$. Moreover, previous lectures suggest an exponential form for the x-variable and a polynomial form for the μ-variable. Whence, the guess

$$\Phi(x,\mu) = A[1 \pm BP_1(\mu) + CP_2(\mu)]e^{\pm x/\ell}$$

where the upper and lower signs are applied to $x > 0$ and $x < 0$, respectively. The choice of using four descriptive parameters (A,B,C,ℓ) is based on the intention of employing the four flux moments found previously (i.e., Φ_{00}, Φ_{02}, Φ_{20} and Φ_{11}) for parameter optimization. In detail,

$$\Phi_{00} = 2\pi \int_{-\infty}^{+\infty} \int_{-1}^{+1} \Phi(x,\mu)\,dx\,d\mu = 8\pi A\ell$$

$$\Phi_{02} = 2\pi \int_{-\infty}^{+\infty} \int_{-1}^{+1} x^2\Phi(x,\mu)\,dx\,d\mu = 16\pi A\ell^3$$

$$\Phi_{20} = 2\pi \int_{-\infty}^{+\infty} \int_{-1}^{+1} P_2(\mu)\Phi(x,\mu)\,dx\,d\mu = \frac{8\pi}{5} A\ell C$$

$$\Phi_{11} = 2\pi \int_{-\infty}^{+\infty} \int_{-1}^{+1} xP_1(\mu)\Phi(x,\mu)\,dx\,d\mu = \frac{8\pi}{3} A\ell^2 B$$

which yield the relations

$$\ell = \left[\frac{\Phi_{02}}{2\Phi_{00}}\right]^{1/2} \qquad A = \frac{1}{4\pi}\left[\frac{\Phi_{00}^3}{2\Phi_{02}}\right]^{1/2}$$

$$B = 3\left[\frac{2}{\Phi_{00}\Phi_{02}}\right]^{1/2}\Phi_{11} \qquad C = \frac{5\Phi_{20}}{\Phi_{00}}$$

Using the flux moments derived previously for this problem in terms of the source emission parameters s_0 and s_2,

$$\ell = \left[\frac{1}{3\Sigma_t^2} \left(\frac{1}{1-c} + \frac{2\ s_2}{s_0} \right) \right]^{1/2}$$

$$A = \frac{\sqrt{3}}{8\pi} \frac{s_0}{1-c} \left[\frac{1}{1-c} + \frac{2\ s_2}{s_0} \right]^{-1/2}$$

$$B = \sqrt{3}(1-c) \left[\frac{1}{1-c} + \frac{2\ s_2}{s_0} \right]^{1/2}$$

$$C = 5(1-c) \frac{s_2}{s_0}$$

These results used in the guessed form for the radiation flux, $\Phi(x,\mu)$, give a solution which is optimized in the sense that the moments Φ_{00}, Φ_{02}, Φ_{20} and Φ_{11} are exactly correct.

A comment about diffusion theory--

If, in the above discussion of application of the moments method, $s_2 = 0$, then the results are descriptive of the radiation flux generated by a single, isotropic plane source located at $x = 0$. For this case

$$\Phi_{00} = \frac{s_0}{\Sigma_t(1-c)} \qquad \Phi_{02} = \frac{2\ s_0}{3\Sigma_t^3(1-c)^2}$$

from which

$$\langle x^2 \rangle = \frac{\Phi_{02}}{\Phi_{00}} = 2 \frac{1}{3\Sigma_t^2(1-c)} = 2\ L_1^2$$

where L_1 represents (as previously) the asymptotic (actually, only) eigenvalue obtained in the P_1-approximation.

It is interesting to note that if a P_1-approximation to the present problem is used, the result

$$\Phi(x) = \Phi_0(x) = A \exp[-|x|/L_1]$$

is obtained. Whence, if $\langle x^2 \rangle_1$ represents the second x-moment under P_1-theory,

$$\langle x^2 \rangle_1 = \frac{\int_0^\infty x^2 e^{-x/L_1} dx}{\int_0^\infty e^{-x/L_1} dx} = 2L_1^2$$

Thus, $\langle x^2 \rangle = \langle x^2 \rangle_1$. That is, the rather surprising result that however well, or badly, the P_1-approximation yields valid representations of flux solutions, or parameters based on flux solutions, it always gives the exact second x-moment. There are certain physically interesting problems which can be demonstrated to depend primarily on $\langle x^2 \rangle$ (e.g., the probability that radiation will emerge from a finite slab having been generated in the interior) and, these problems are well-described by diffusion theory even when material parameters dictate that the P_1-approximation is invalid.

Numerical Resolution of the Boltzmann Equation

The previous two sections of these lecture notes are devoted to the description and use of techniques which are primarily analytic. By "analytic" is meant that results may be formulated in general functional forms which indicate the influence of relevant parameters on the trend of solutions. Numerical evaluation of the analytic results is only required to visualize the details of these results. In this section, solution techniques are analytically generated which require extensive numerical computation to yield any meaningful information. These approaches are termed "numerical resolutions" and two of them are outlined here. Again, for algebraic and notational simplicity, attention is restricted to the special class of radiation transport problems which are described by the list of simplifications used in considering

analytical approaches (viz., items numbered 1 through 8 on pages 3-11 and 3-12 of these lecture notes). The relevant form of the Boltzmann equation is (from page 3-13)

$$\mu \frac{\partial}{\partial x} \Phi(x,\mu) + \Sigma_t \Phi(x,\mu) = \frac{c\Sigma_t}{2} \int_{-1}^{+1} \Phi(x,\mu')d\mu' + s(x,\mu)$$

It is to this relation that the two numerical solution approaches discussed in these notes are applied.

Approach 1. The discrete ordinates method:

The primary objective of the discrete ordinates approach is to reduce the integral term of the Boltzmann equation to algebraic terms. The emission of particles in collision (e.g., scattering) is described only in the discrete set of directions-of-travel $\{\mu_n,\ n = 1,2,\ldots,N\}$. With this procedure employed to reduce the integral term, it makes sense to use the same idea on the other terms in the equation. Thus, the transport equation takes the form

$$\mu_n \frac{d}{dx} \Phi(x,\mu_n) + \Sigma_t \Phi(x,\mu_n) = \frac{c\Sigma_t}{2} \sum_{n'=1}^{N} w_{n'} \Phi(x,\mu_{n'}) + s(x,\mu_n)$$

$$\text{for } n = 1,2,3,\ldots,N$$

where the w_n are "weight" functions suitably chosen with reference to the discrete directions μ_n so as to optimize the summation approximation to the actual integral term. The set $\{\mu_n, w_n; n=1,2,\ldots,N\}$ is termed the quadrature set and the choice thereof is important in developing a valid approximation to the solution of the transport equation.

An example of the generation of weight functions is illustrated by the use of trapezoidal quadrature. In this case, it is presumed that $\Phi(x,\mu)$ varies linearly with μ between any two successive quadrature directions, say μ_{n-1} and μ_n, i.e.,

$$\Phi(x,\mu) = \frac{\mu-\mu_{n-1}}{\mu_n-\mu_{n-1}} \Phi(x,\mu_n) + \frac{\mu_n-\mu}{\mu_n-\mu_{n-1}} \Phi(x,\mu_{n-1})$$

$$\text{for } \mu_{n-1} \leq \mu \leq \mu_n$$

With this presumption, the contribution to the integral term, $\int\Phi(x,\mu')d\mu'$, from the interval μ_{n-1} to μ_n is

$$\int_{\mu_{n-1}}^{\mu_n} \Phi(x,\mu')d\mu' = \frac{1}{2}(\mu_n-\mu_{n-1})\Phi(x,\mu_n) + \frac{1}{2}(\mu_n-\mu_{n-1})\Phi(x,\mu_{n-1})$$

Similarily,

$$\int_{\mu_n}^{\mu_{n+1}} \Phi(x,\mu')d\mu' = \frac{1}{2}(\mu_{n+1}-\mu_n)\Phi(x,\mu_{n+1}) + \frac{1}{2}(\mu_{n+1}-\mu_n)\Phi(x,\mu_n)$$

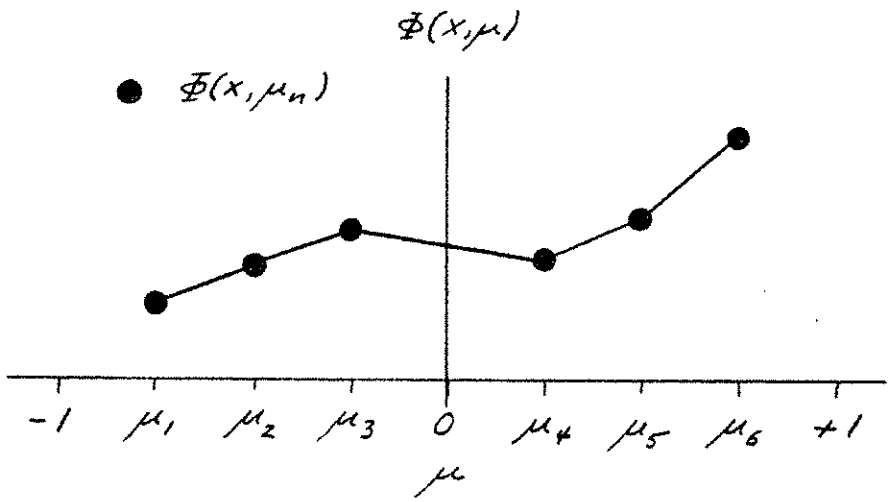
and, these two μ-interval contributions contain the only terms in which $\Phi(x,\mu_n)$ appear. Thus, the contribution to $\int\Phi(x,\mu')d\mu'$ from the quadrature direction μ_n is

$$\frac{1}{2}(\mu_{n+1}-\mu_{n-1})\Phi(x,\mu_n)$$

and the weight function is identified as

$$w_n = \frac{1}{2}(\mu_{n+1}-\mu_{n-1})$$

This result only applies to the case of trapezoidal quadrature and is based on the presumption that $\Phi(x,\mu)$ is as illustrated. Other assumptions



on the functional form, or moments, of $\Phi(x,\mu)$ lead to different quadrature sets.

It is instructive to examine solution of the homogeneous (s = 0) form of the discrete ordinates transport equation along the same lines as applied to the P_N-approximation. The equation is invariant with respect to translation of x which suggests the solution form

$$\phi(x,\mu_n) = \Psi(\ell,\mu_n)e^{-x/\ell}$$

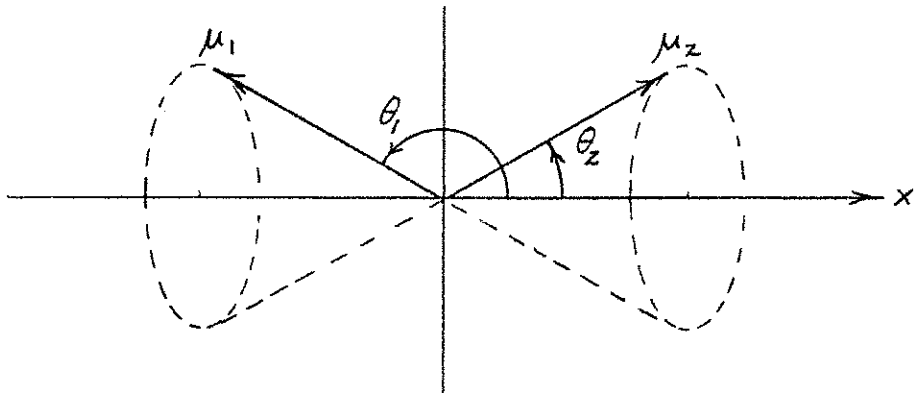
Whence,

$$(\mu_n - \ell\Sigma_t)\Psi(\ell,\mu_n) + \frac{c\ell\Sigma_t}{2}\sum_{n'=1}^{N} w_{n'}\Psi(\ell,\mu_{n'}) = 0$$

$$\text{for } n = 1,2,3,\ldots,N$$

which is a set of N linear algebraic, homogeneous equations in the N unknowns $\{\Psi(\ell,\mu_n),\ n = 1,2,\ldots,N\}$.

For the purpose of clarifying use of this result, consider details of the problem characterized by N = 2, $\mu_1 = -\mu_2$, and $w_1 = w_2 = 1$. The discrete direction symmetry chosen is as illustrated



where $\theta_1 = \pi - \theta_2$, $\mu_1 = \cos\theta_1$, $\mu_2 = \cos\theta_2$. The equation set now has only the

two members

$$[\mu_1 - \ell\Sigma_t(1-c/2)]\Psi(\ell,\mu_1) + \frac{c\ell\Sigma_t}{2}\ \Psi(\ell,\mu_2) = 0$$

$$[\mu_2 - \ell\Sigma_t(1-c/2)]\Psi(\ell,\mu_2) + \frac{c\ell\Sigma_t}{2}\ \Psi(\ell,\mu_1) = 0$$

Using $\mu_1 = -\mu_2$ and requiring non-trivial solutions for $\Psi(\ell,\mu_1)$ and $\Psi(\ell,\mu_2)$ generates a secular equation with solutions

$$\ell = \pm L \qquad \text{where} \qquad L = +\frac{\mu_2}{\Sigma_t\sqrt{1-c}}$$

The eigenvalues ($\pm L$) can be set at a desired value by suitable choice of the quadrature direction μ_2. For example, if μ_2 is chosen to be $1/\sqrt{3}$ (which corresponds to $\theta_2 = 54.7°$), then $L = L_1$, i.e., the P_1-approximation result.

In a later section of these notes the solution just obtained (i.e., for $N = 2$, $\mu_1 = \mu_2$, $w_1 = w_2 = 1$) will be applied to a specific physical problem. Here, it is of further general clarification of the discrete ordinates idea to consider the discrete μ-dependence of the radiation flux for positive x, i.e.,

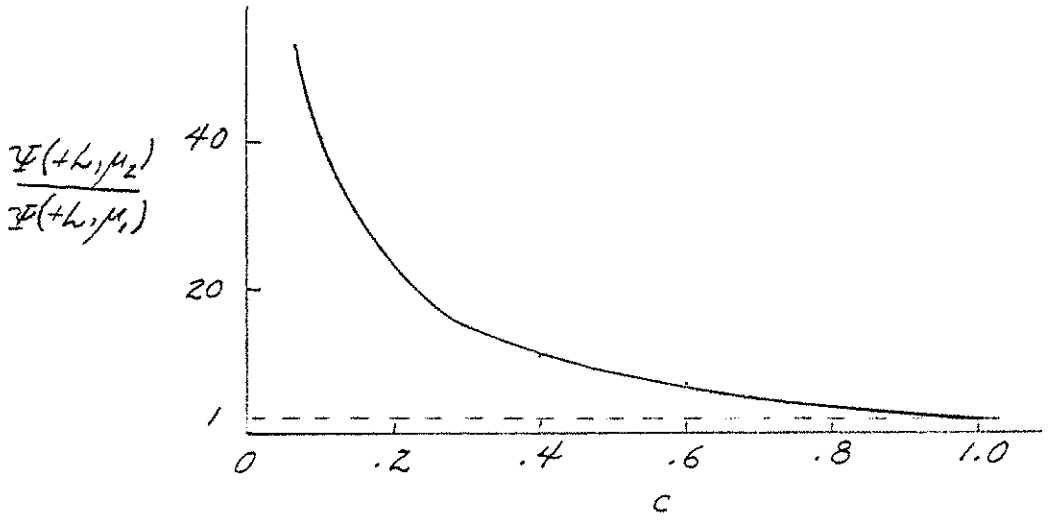
$$\Phi(x,\mu_1) = A\ \Psi(+L,\mu_1)e^{-x/L}$$

$$\Phi(x,\mu_2) = A\ \Psi(+L,\mu_2)e^{-x/L}$$

A description of interest is the flux "angular spectrum" which can be expressed by the ratio $\Phi(x,\mu_2)/\Phi(x,\mu_1)$, i.e.,

$$\frac{\Phi(x,\mu_2)}{\Phi(x,\mu_1)} = \frac{\Psi(+L,\mu_2)}{\Psi(+L,\mu_1)} = \frac{c/2}{(1-c/2) - \sqrt{1-c}}$$

which is surprisingly independent of the choice of μ-quadrature (i.e., μ_2). However, as expected, the illustrated graph of the angular spectrum is generally



greater than unity, approaching unity as $c \to 1$ and approaching unbounded value as $c \to 0$ (which would yield no radiation in the μ_1-direction).

To this point in this discussion, the discrete ordinates method has been presented as based on transformation of the direction-of-travel variable, μ, to discrete form leaving the position variable, x, in continuous form. The motivation for such a presentation is primarily for comparison with previously discussed analytical resolution approaches. We now proceed to the equation forms which are usually numerically resolved with the aid of digital computers, i.e., a discrete treatment of both μ and x.

Discrete ordinates method with discrete position variable--

The radiation flux, evaluated at discrete values of both direction-of-travel and position, takes on the indexed form $\Phi(x_m,\mu_n)$ which is reminiscent of the radiation flux moments Φ_{nm}. As is the motivation in the development of the moments method, the full discretization of the flux specification is performed with the purpose of developing a strictly algebraic set of relations which can then be resolved by digital computation procedures.

The operation applied to the x-variable which must be transformed to a discrete form appears in the "flow term," $\mu\, d\Phi/dx$. In discrete terms, a possible formulation is

$$\frac{d\Phi(x,\mu_n)}{dx} \rightarrow \frac{\Phi(x_{m+1},\mu_n) - \Phi(x_m,\mu_n)}{x_{m+1} - x_m}$$

and the discrete ordinates equation can be expressed in the form

$$\mu_n \frac{\Phi(x_{m+1},\mu_n) - \Phi(x_m,\mu_n)}{x_{m+1} - x_m} + \Sigma_t \bar{\Phi}(x_m,\mu_n) = \frac{c\Sigma_t}{2} \sum_{n'=1}^{N} w_{n'} \bar{\Phi}(x_m,\mu_{n'}) + \bar{s}(x_m,\mu_n)$$

$$\text{for } n = 1,2,3,\ldots,N;\ m = 1,2,3,\ldots,M-1$$

The notation $\bar{\Phi}(x_m,\mu_n)$ indicates that it is appropriate to perform an averaging process over the x-interval x_m to x_{m+1} in expressing such terms. For example, presuming that $\Phi(x,\mu_n)$ is approximately linear in x over the interval $x_m \leq x \leq x_{m+1}$ would indicate

$$\bar{\Phi}(x_m,\mu_n) = \frac{\Phi(x_{m+1},\mu_n) + \Phi(x_m,\mu_n)}{2}$$

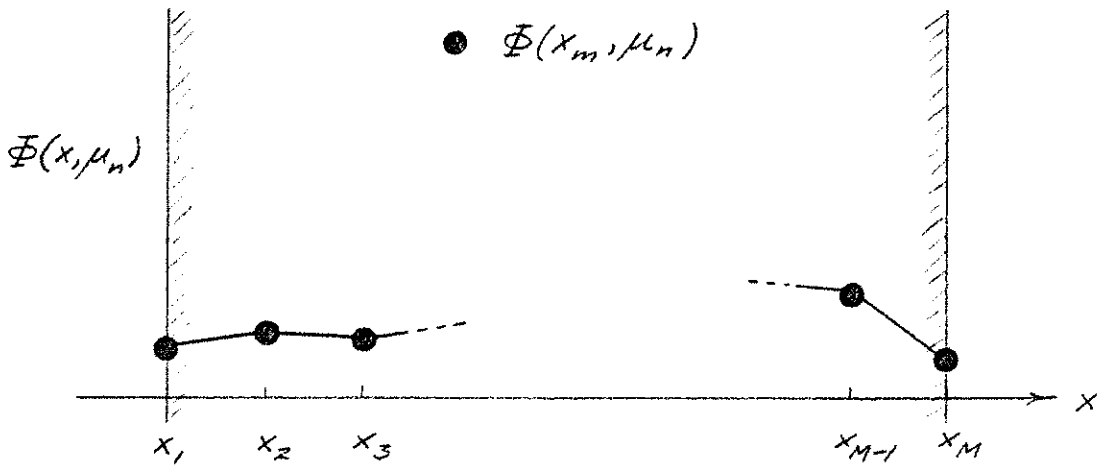
It is unnecessary to make any assumptions regarding $\bar{s}$, that is the averaging process for radiation source terms since, $s(x,\mu)$ is presumed to be a given function and the evaluation of $\bar{s}(x_m,\mu_n)$ should proceed via

$$\bar{s}(x_m,\mu_n) = \frac{\int_{x_m}^{x_{m+1}} s(x,\mu_n)\,dx}{x_{m+1} - x_m}$$

The discretized transport equation has been reduced to the form of N(M-1) linear, coupled, algebraic equations in the NM unknowns

$$\{\Phi(x_m,\mu_n);\ n = 1,2,\ldots,N;\quad m = 1,2,\ldots,M\}$$

For each discrete direction-of-travel, μ_n, the radiation flux is illustrated



As indicated, the positions x_1 and x_M are usually associated with actual physical boundaries (they are always associated with boundary conditions). The incoming radiation flux at the boundaries generate boundary conditions for the discrete flux of the form

$$\Phi(x_1,\mu_n) = \Psi_n(x_1), \quad n = N' + 1,\ldots,N$$

$$\Phi(x_M,\mu_n) = \Psi_n(x_M), \quad n = 1,2,\ldots,N'$$

where the $\Psi_n(x_1)$ and $\Psi_n(x_M)$ are either given incident flux conditions or are derivable from fluxes other than those in the above boundary sets, and $N' < N$ is determined by the largest value of n such that $\mu_n < 0$ (i.e., μ_1 through $\mu_{N'}$ are negative and $\mu_{N'+1}$ through μ_N are positive). With the N boundary conditions specified there is a total of NM equations in the NM unknown $\Phi(x_m,\mu_n)$ and solution should be possible.

A solution strategy for the discretized equation--

Since the flux induced emission (including scattering) and radiation sources are employed in the same manner in the iterative solution strategy outlined here, use the notation

$$Q_{nm} = \frac{c\Sigma_t}{4} \sum_{n'=1}^{N} w_{n'}[\Phi_{n',m+1} + \Phi_{n',m}] + \bar{s}_{nm}$$

and

$$\Phi_{nm} = \Phi(x_m, \mu_n)$$

which should not be confused with the same notation used earlier in these notes for the radiation flux moments (page 3-17). The discretized transport equation, rewritten in these terms, is

$$\mu_n \frac{\Phi_{n,m+1} - \Phi_{nm}}{\Delta x_m} + \frac{\Sigma_t}{2}(\Phi_{n,m+1} + \Phi_{nm}) = Q_{nm}$$

$$\text{for } n = 1,2,\ldots,N; \quad m = 1,2,\ldots,M-1$$

where $\Delta x_m = x_{m+1} - x_m$, and the boundary conditions become

$$\Phi_{n,1} = \Psi_n(x_1), \quad n = N/2 + 1,\ldots,N$$

$$\Phi_{n,M} = \Psi_n(x_M), \quad n = 1,2,\ldots,N/2$$

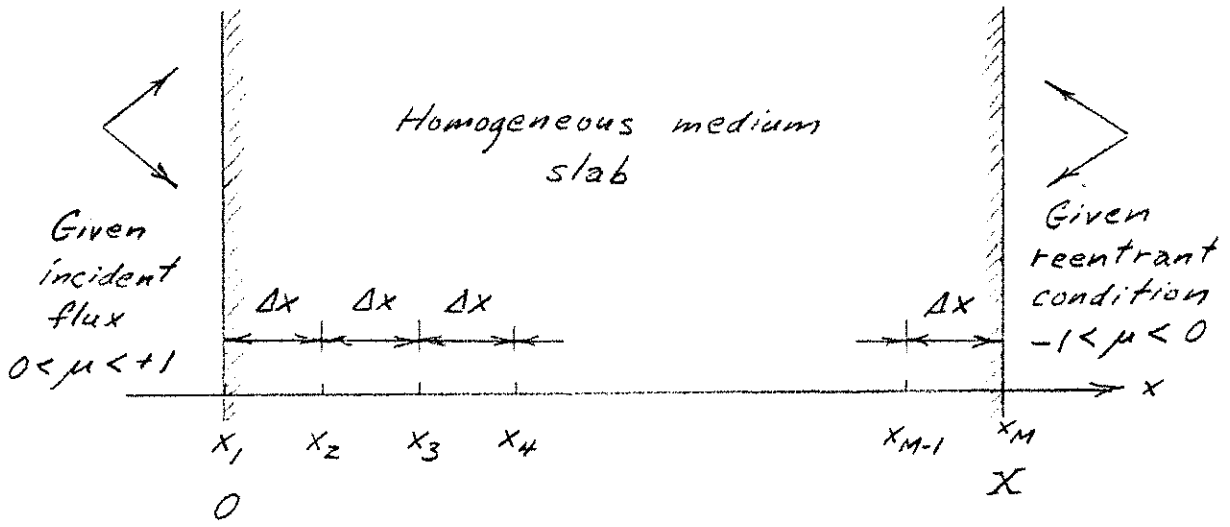
where for obvious symmetry advantages the quadrature set $\{\mu_n\}$ is chosen such that N is an even number and $\mu_1 = -\mu_N$, $\mu_2 = -\mu_{N-1}, \ldots, \mu_{N/2} = -\mu_{N/2+1}$. Two forms of the discretized equation are useful, viz.

$$\Phi_{n,m+1} = \frac{1 - \Sigma_t \Delta x_m/2\mu_n}{1 + \Sigma_t \Delta x_m/2\mu_n} \Phi_{nm} + \frac{Q_{nm}}{\Sigma_t/2 + \mu_n/\Delta x_m}$$

$$\Phi_{nm} = \frac{1 + \Sigma_t \Delta x_m/2\mu_n}{1 - \Sigma_t \Delta x_m/2\mu_n} \Phi_{n,m+1} + \frac{Q_{nm}}{\Sigma_t/2 - \mu_n/\Delta x_m}$$

To describe the particular solution strategy presented here, it is useful to detail a problem which is, at least, specified by a given class of boundary conditions. To this end, consider the problem of a slab of uniform material

illuminated with a given radiation flux on the face x = 0 and occupying the region $0 \leqq x \leqq X$. At the face x = X, a specific reentrant (or, non-reentrant) flux condition is imposed. The general problem and specification of position



mesh points (with uniform spacing $\Delta x = X/(M-1)$) is illustrated. With the previously mentioned condition of N even and a symmetric μ-gradrature set, the boundary values at x = 0 can be expressed as

$$\Phi_{n1} = \Psi_n, \quad n = N/2+1,\ldots,N$$

where $\{\Psi_n;\ n = N/2+1,\ldots,N\}$ describes the illumination radiation flux. The boundary condition at x = X is described when it is required in this formulation of a solution strategy.

The starting point (or, zeroth-order interation) of the solution is to select (guess) a set $\{Q_{nm};\ n = 1,2,\ldots,N;\ \ m = 1,2,\ldots,M-1\}$. To signify the iteration index, denote this set $\{Q_{nm}(0)\}$. Actually, it is presumed that the $\bar{s}_{nm}$ contribution to Q_{nm} is given and thus the selection is for the remaining radiation emission term (e.g., a possible guess is $Q_{nm}(0) = \bar{s}_{nm} + K$). The iteration strategy is accomplished as follows:

1. Use the "forward progressing" form of the discretized transport equation, i.e.,

$$\Phi_{n,m+1} = \frac{1 - \Sigma_t \Delta x/2\mu_n}{1 + \Sigma_t \Delta x/2\mu_n} \Phi_{nm} + \frac{Q_{nm}(0)}{\Sigma_t/2 + \mu_n/\Delta x}$$

$$\text{for } n = N/2 + 1,\ldots,N; \quad m = 1,2,\ldots,M-1$$

Denote the results of this calculation $\Phi_{nm}(1)$ signifying the results of the first iteration (note, only for the forward directions $\mu_n > 0$).

2. The last calculation of step 1 determine

$$\Phi_{nM}(1), \quad n = N/2+1,\ldots,N$$

which are the emerging (transmitted) radiation fluxes of the first iteration, forward calculation. The boundary conditions at x = X are applied to these flux values. For example, if an operator α describes the reflection properties of the space in the region x > X, then

$$\Phi_{nM}(1) = \alpha[\{\Phi_{N+1-n,M}(1)\}], \quad n = 1,2,\ldots,N/2$$

which provides an "effective illumination" on the slab face at x = X for continuation of the first iteration calculation.

3. Use the "backward progressing" form of the discretized transport equation, i.e.,

$$\Phi_{nm} = \frac{1 + \Sigma_t \Delta x/2\mu_n}{1 - \Sigma_t \Delta x/2\mu_n} \Phi_{n,m+1} + \frac{Q_{nm}(0)}{\Sigma_t/2 - \mu_n/\Delta x}$$

$$\text{for } n = 1,2,\ldots,N/2; \quad m = M-1, M-2,\ldots,1$$

Denote the results of this calculation $\Phi_{nm}(1)$ which completes the first

iteration flux results by supplying the components n = 1,2...,N/2 (i.e., $\mu_n < 0$) at each position x_m. The values of $\Phi_{nM}(1)$ for n = 1,2,...,N/2 are determined in step 2 and the $Q_{nm}(0)$ have already been selected (guessed).

4. The second iteration begins with determining an updated value for the set $\{Q_{nm}\}$, i.e., with obvious notation

$$Q_{nm}(1) = \bar{s}_{nm} + \frac{c\Sigma_t}{4} \sum_{n'=1}^{N} w_{n'} [\Phi_{n',m+1}(1) + \Phi_{n',m}(1)]$$

Steps 1 through 3 are then applied to generate the set $\{\Phi_{nm}(2);\ n = 1,2,...,N;\ m = 1,2,...,M\}$, and, the iterative strategy is established.

Illustrative examples of the "albedo" operator, α, are helpful in understanding the role of boundary conditions at x = X in the iterative process. Three relevant cases are:

A. A non-reentrant surface at x = X, i.e., the condition that $\Phi_{nM} = 0$ for n = 1,2,...,N/2 independent of the iteration. For this case α is just the zero operator.

B. "Specular" reflection at x = X is described by requiring that the emerging flux Φ_{nM} for $(N/2 + 1) \leq n \leq N$ only acts a source for the symmetric guadrature direction μ_{N+1-n}. Thus, independent of the iteration, the set of relations

$$\Phi_{nM} = \alpha_n \Phi_{N+L-n,M} \quad \text{for } n = 1,2,...,N/2$$

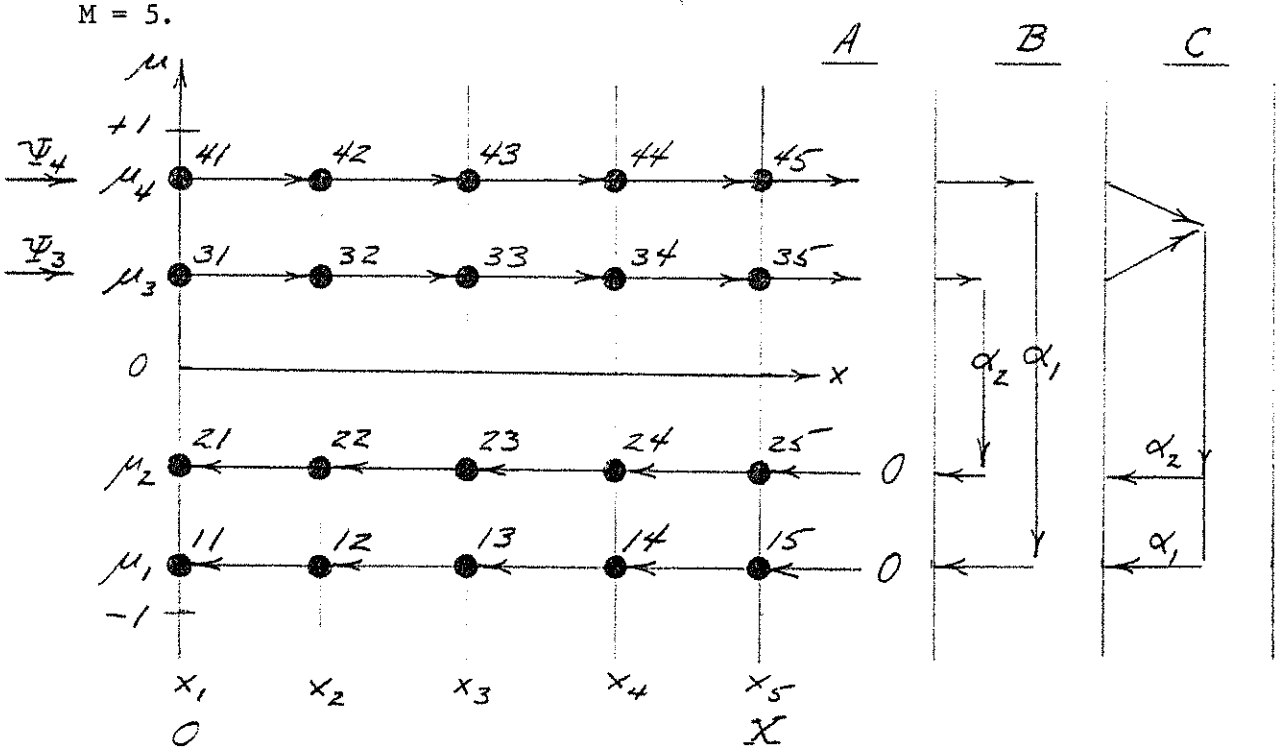
with each $\alpha_n < 1$, describes the reflection at the surface x = X.

C. "Diffuse" reflection at x = X is described by requiring that the emerging flux Φ_{nM} for $(N/2+1) \leq n \leq N$ acts as a source of equal intensity for all the reentrant directions (i.e., μ_n, n = 1,2,...,N/2). Thus, independent of the iteration, the set of relations

$$\Phi_{nM} = \alpha_n \sum_{n'=1}^{N/2} \Phi_{N+1-n',M} \quad \text{for } n = 1,2,\ldots,N/2$$

with each $\alpha_n < 1$, describes the reflection at the surface x = X.

The solution strategy progression of calculation is illustrated for the three boundary condition cases at x = X for the particular choice N = 4 and M = 5.



Approach 2. The Monte Carlo method:

The method outlined in these notes (pages 3-4 through 3-6) under the title "orders-of-scattering" suggests another numerical approach to solution of the transport equation. Recall that the successive scattering method is based on initially calculating the uncollided flux, $\Phi_0(\underline{r})$, by a convolution of the free-flight Green's function, $G_0(\underline{r},\underline{r}')$, with the source density, $s(\underline{r}')$. This result provides a means of calculating the first-scattering density, i.e., $\Sigma_s\Phi_0(\underline{r})$, which, in turn, provides a source for the once-collided radiation flux, $\Phi_1(\underline{r})$, which is calculated by a convolution of $G_0(\underline{r},\underline{r}')$ with $\Sigma_s\Phi_0(\underline{r}')$. The process is continued to determine the twice-collided flux, $\Phi_2(\underline{r})$, the thrice-collided flux, $\Phi_3(\underline{r})$, etc. The total radiation flux, $\Phi(\underline{r})$, is given by

$$\Phi(\underline{r}) = \sum_{m=0}^{M} \Phi_m(\underline{r})$$

where the value of M for valid truncation of the sum depends on the value of c. This method of determining $\Phi(\underline{r})$ is based on progressively following the expected trajectory histories of particles as they "migrate" through a medium from their point of "origin" at a source. The Monte Carlo numerical approach is based on a similar tracing of the path-histories of particles, but, in contrast to the orders-of-scattering method, the point-of-view is to simulate the statistical interaction sequence by a numerical analog experiment.

Suppose that we have the means to generate random numbers, ξ, in the range $0 \leq \xi \leq 1$. Another way to express this is that the probability of choosing ξ in the interval $d\xi$ about ξ is independent of the value of ξ, i.e., if

$P(\xi)d\xi$ = the probability of choosing the value of the number ξ in the range ξ to $\xi + d\xi$,

then, $P(\xi) = 1$ for $0 \leq \xi \leq 1$. In order to use our random number generator for the purpose of simulating radiation travel and interaction, relations must be developed which couple the statistical aspects of the physical process to the probability distribution $P(\xi)$. As an example, consider the free-flight travel of a particle in a given direction in a homogeneous medium from a point which we arbitrarily designate as the origin of distance coordinate r. If

$p(r)dr$ = the probability that a particle will suffer the first collision (after leaving r = 0) in the distance interval r to r + dr,

then, it has been often used in these notes, that $p(r)dr = \Sigma_t \exp(-\Sigma_t r)dr$. We would like to find the transformation $r(\xi)$, i.e. $\xi \rightarrow r$, such that $P(\xi)$ generates $p(r)$. Thus,

$$P(\xi) = p(r)\left|\frac{dr}{d\xi}\right| = 1$$

for $0 \leq \xi \leq 1$ and $r \geq 0$

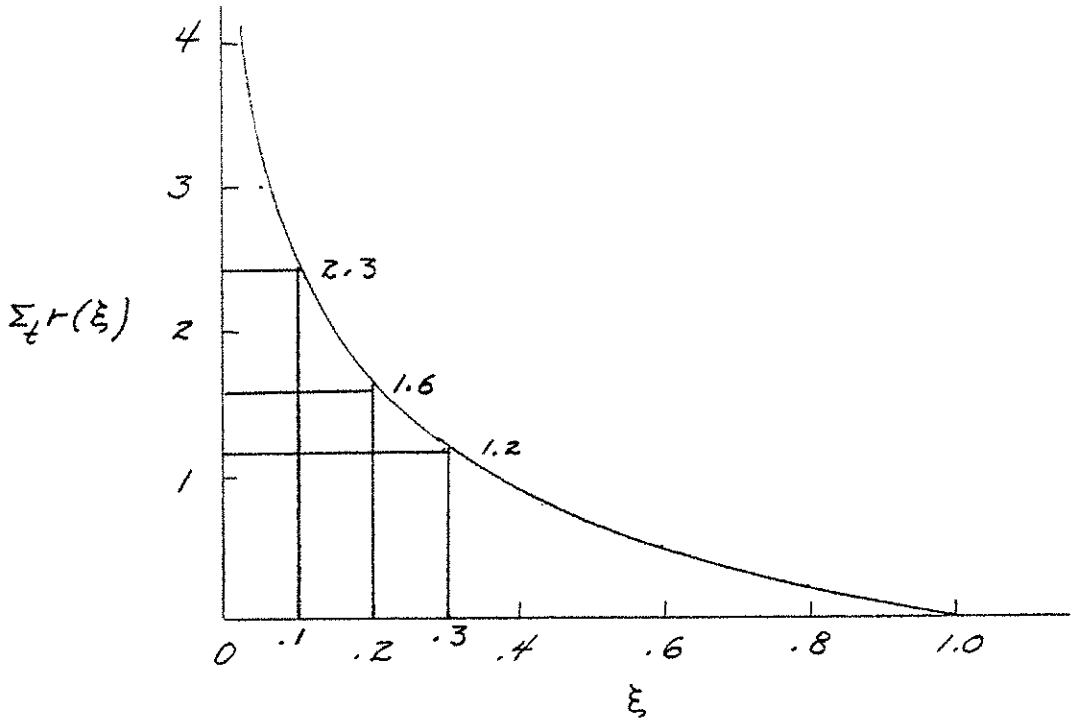
Whence,

$$\left|\frac{d\xi}{dr}\right| = p(r) = \Sigma_t \exp(-\Sigma_t r)$$

$$\xi(r) = - \exp(-\Sigma_t r)$$

$$\Sigma_t r(\xi) = - \ell n \xi$$

Similar to the discussions on page 1-8 of these notes, a graph of $\Sigma_t r(\xi)$ illustrates the idea of using a random number generator to simulate a physical process (in this case, free-flight transport). Note that random



numbers in the range $0 < \xi < 0.1$ yield values of free-flight distance, r, in the range $-\ell n\ 0.1 = 2.3 < \Sigma_t r < \infty$; random numbers in $0.1 < \xi < 0.2$ generate $1.6 < \Sigma_t r < 2.3$; random numbers in $0.2 < \xi < 0.3$ generate $1.2 < \Sigma_t r < 1.6$; etc. Since $P(\xi)$ is a constant, the first-collision density, which is proportional to the uncollided particle flux, is maximum at $r = 0$ and monotonically decreases with increasing r, viz. the decreasing exponential function $\exp(-\Sigma_t r)$.

Expanding these ideas to describe particle emission direction probability densities, consider the case of isotropic emission, i.e.,

$$p(\mu,\phi)d\mu d\phi = \frac{1}{4\pi}\, d\mu d\phi = \frac{1}{2}\, d\mu\, \frac{1}{2\pi}\, d\phi$$

where $\mu = \cos\theta$ is the polar scattering angle direction cosine ($-1 < \mu < +1$), ϕ is the azimuthal scattering angle ($0 < \phi < 2\pi$), and identification of $1/2$ with $d\mu$ and $1/2\pi$ with $d\phi$ is justified by the part of the normalization which comes from each variable, i.e.,

$$p(\mu)d\mu = \frac{1}{2}\, d\mu$$

$$q(\phi)d\phi = \frac{1}{2\pi}\, d\phi$$

$$p(\mu,\phi) = p(\mu)q(\phi)$$

We require the transformations $\mu(\xi)$, i.e., $\xi \to \mu$, and $\phi(\eta)$, i.e., $\eta \to \phi$, which yield the direction-of-emission distributions, $p(\mu)$ and $q(\phi)$, from the random numbers ξ and η. Note that

$$P(\xi,\eta) = p(\mu,\phi)\left|J\left(\frac{\mu,\phi}{\xi,\eta}\right)\right| = 1$$

is simplified to

$$P(\xi) = p(\mu)\left|\frac{d\mu}{d\xi}\right| = 1$$

$$Q(\eta) = q(\phi)\left|\frac{d\phi}{d\eta}\right| = 1$$

since μ and ϕ are independent descriptors of particle emission. Whence,

$$\left|\frac{d\xi}{d\mu}\right| = p(\mu) = \frac{1}{2}$$

$$\xi(\mu) = \frac{1}{2}\,(\mu + 1)$$

$$\mu(\xi) = 2\xi - 1$$

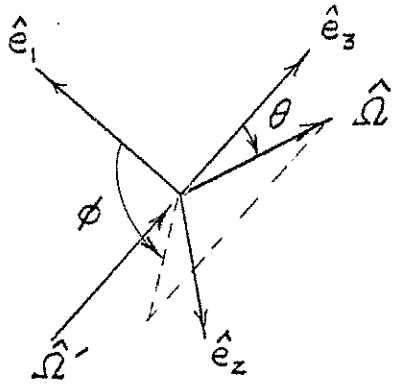
and,

$$\left|\frac{d\eta}{d\phi}\right| = q(\phi) = \frac{1}{2\pi}$$

$$\eta(\phi) = \frac{1}{2\pi}\,\phi$$

$$\phi(\eta) = 2\pi\eta$$

In terms of the illustrated coordinates (with bases vectors $\hat{e}_1$, $\hat{e}_2$, $\hat{e}_3$) which relate pre-collision direction-of-travel, $\hat{\Omega}'$, with emission direction, $\hat{\Omega}$,

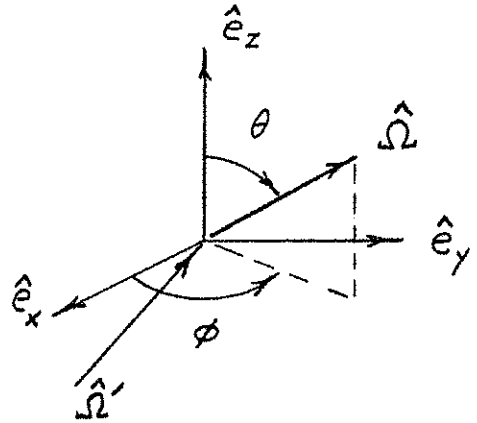


$$\Omega_1 = \sin\theta\cos\phi$$

$$\Omega_2 = \sin\theta\sin\phi$$

$$\Omega_3 = \cos\theta$$

and the direction cosines of a particle emitted from a collision are established. The values of $\theta = \arccos\mu$ and ϕ are generated from the respective random variables ξ and η via the transformations $\mu(\xi)$ and $\phi(\eta)$. It should be noted that for the case of isotropic emission (and, only for that case) the coordinate bases set $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ may be chosen with a fixed relation to location coordinates, $\underline{r}$. For example, using the illustrated conventional relation between



$$\Omega_x = \sin\theta\cos\phi$$

$$\Omega_y = \sin\theta\sin\phi$$

$$\Omega_z = \cos\theta$$

Cartesian location coordinates (x,y,z) and spherical polar direction coordinates

(θ,ϕ), the emission direction, $\hat{\Omega}$, has the indicated components.

Point source emission directional dependence, $s(\mu,\phi)$, also yields transformations between random variables and direction cosines. For sources, the coordinate bases set is always chosen with a fixed relation to location coordinates, $\underline{r}$, e.g., $(\hat{e}_x,\hat{e}_y,\hat{e}_z)$ as indicated in the illustration for isotropic emission.

At each collision a decision must be made as to what particular interaction type occurred. Suppose that there are I interaction types possible indexed by i = 1,2,..., I, and described by the cross sections Σ_i. The probability that a collision (which has occurred) is of the i-type is

$$p_i = \Sigma_i/\Sigma_t \quad \text{where } \Sigma_t = \sum_{i=1}^{I} \Sigma_i$$

The transformation of random variable, ξ, to interaction type, i, is relatively easily accomplished. With the definition of random variable limits

$$\xi(i) = \sum_{j=1}^{i} p_j$$

the random variable range $0 \leq \xi \leq \xi(1)$ indicates that a 1-type interaction occurred; the range $\xi(1) \leq \xi \leq \xi(2)$ indicates a 2-type interaction;...and the range $\xi(I-1) \leq \xi \leq 1$ indicates a I-type interaction.

Application of Numerical Methods

It is significantly more tedius to detail application of numerical resolution techniques than is the case for strictly analytical approaches. Not only in the demonstration of validity, but also in just obtaining anything but trivial results there is usually a requirement of extensive calculation. This can be reasonably accomplished only on digital computers.

Use of the discrete ordinates approach will be focused on the calculation of a homogeneous, half-space reflection coefficient and the procedures and

results may be compared with the P_N-approximation application to the same problem. The Monte Carlo approach will be discussed as applied to the determination of the radiation flux generated by a point, isotropic source in an infinite, homogeneous medium.

Reflection coefficient of a half-space:

Consider, once more, the problem of a radiation flux illuminating the plane surface of a homogeneous half-space with a prescribed angular description,

$$\Phi(0,\mu) = \Psi(\mu) \text{ for } 0 < \mu < +1$$

The specific example of the discrete ordinates method discussed in these notes on pages 3-42 through 3-44 (i.e., $N = 2$, $\mu_1 = -\mu_2$, $w_1 = w_2 = 1$) can be applied to the determination of the reflection coefficient. Using discretization of only the μ-variable, the radiation flux for positive x is given by

$$\Phi(x,\mu_1) = A\,\Psi(+L,\mu_1)e^{-x/L}$$

$$\Phi(x,\mu_2) = A\,\Psi(+L,\mu_2)e^{-x/L}$$

where

$$L = +\frac{\mu_2}{\Sigma_t\sqrt{1-c}}$$

and, the discrete angular-dependence ratio $\Phi(x,\mu_2)/\Phi(x,\mu_1)$ is given by

$$\frac{\Psi(+L,\mu_2)}{\Psi(+L,\mu_1)} = \frac{c/2}{(1-c/2) - \sqrt{1-c}}$$

As is the case of the P_1-approximation approach to this problem (pages 3-20 through 3-24) we usually face the situation of not being able to exactly meet the illumination boundary condition with the required general solution form obtained for the approximation. For the P_1-approximation it required

the fortuity of a special linear μ-dependence to exaxtly meet incident boundary values. Here, only the "monodirectional" illumination case of

$$\Psi(\mu) = C\ \delta(\mu-\mu_2)$$

yields point-wise agreement between incident flux and required solution form. The alternative, practical approach of employing intuitive relations between the given $\Psi(\mu)$ and the required form for $\Phi(0,\mu)$ can, again, be applied, e.g.,

$$J_+(0) = 2\pi\mu_2\Phi(0,\mu_2) = 2\pi \int_0^{+1} \mu\Psi(\mu)d\mu = I$$

That is, the equivalent of the current condition suggested for the P_1-approximation.

Using the arbitrary normalization $\Psi(+L,\mu_1) = 1$, the present general solution form, and the incident current condition,

$$J_+(0) = \frac{2\pi\mu_2\ Ac/2}{(1-c/2) - \sqrt{1-c}} = I$$

and, the radiation flux for $x > 0$ is given by

$$\Phi(x,\mu_1) = \frac{(1-c/2) - \sqrt{1-c}}{\pi c\mu_2}\ I\ e^{-x/L}$$

$$\Phi(x,\mu_2) = \frac{1}{2\pi\mu_2}\ I\ e^{-x/L}$$

Moreover, the reflected radiation current at the medium surface, $J_-(0)$, is then given by

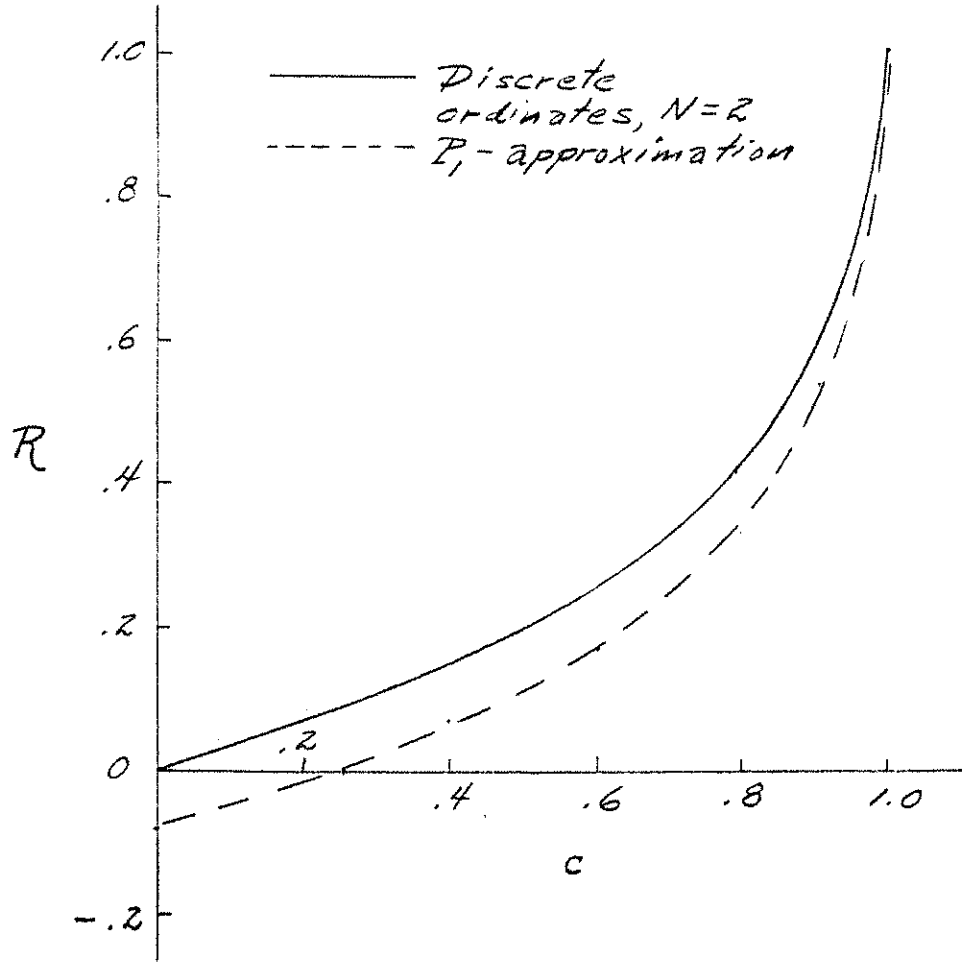
$$J_-(0) = -2\pi\mu_1\Phi(0,\mu_1) = \frac{(1-c/2) - \sqrt{1-c}}{c/2}\ I$$

where the condition $\mu_1 = -\mu_2$ has been applied. The reflection coefficient is thus

$$R = \frac{J_-(0)}{I} = \frac{(1-c/2) - \sqrt{1-c}}{c/2}$$

It should be noted that this result for R is independent of the particular incident flux boundary condition chosen to determine the radiation flux. This is analogous to the same situation found in the P_1-approximation (and, the P_2-approximation) where only one useful eigenfunction allowed little flexibility in solution form. It is, perhaps, surprising to find here that R is independent of the choice of μ_2 (or, equivalently, L).

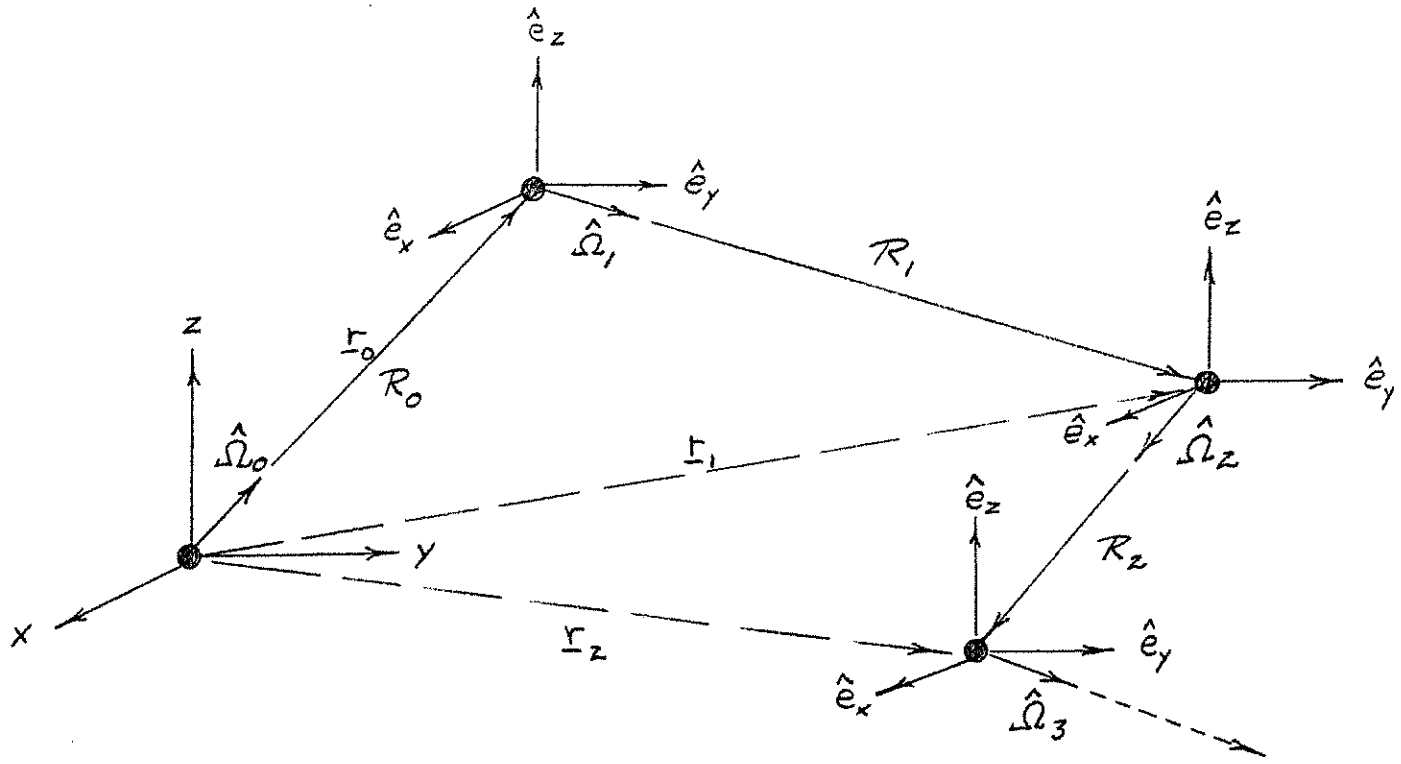
The illustrated curves of R as a function of c for the P_1-approximation and the present discrete ordinates approach provide a comparison between the two methods for this type of problem. The complete breakdown of the P_1-approximation for low vlaues of c is expected and is briefly predicted in the discussion on page 3-24.



Radiation flux from a point source:

Demonstration of a complete Monte Carlo approach to solution of a given physical problem requires extensive numerical calculation. Such is considered outside the scope of these lecture notes. To indicate the steps required in an application, an outline of the sequential procedure is presented here. For the sake of notational simplicity, the simple problem of determining the radiation flux resulting from a point, isotropic source in a homogeneous, infinite medium characterized by the two interactions, capture (nonproductive absorption) and isotropic scattering, is presented.

The sequence of decisions required to perform a Monte Carlo simulation of the point source problem is illustrated by the indication of a possible trajectory emanating from the source location which is chosen to be at the origin of $\underline{r}$-coordinates, i.e., point 0. With reference to the illustration, the Monte Carlo approach steps follow:



1. Two random numbers are generated, say ξ_0 and η_0, which establish the emission direction, $\hat{\Omega}_0$, via the transformations derived on pages 3-54 and 3-55. Specifically, $\mu_0 = 2\,\xi_0 - 1$ and $\phi_0 = 2\pi\eta_0$. Note that the fineness of the mesh describing emission directions, $\hat{\Omega}_0$, depends on the number of significant digits retained in the specification of the random numbers, e.g., random numbers generated as 0.00 to 1.00 yields 101 possibilities for μ_0 and 101 possibilities for ϕ_0, whereas 0.000 to 1.000 yields 1,001 choices for μ_0 and ϕ_0.
2. One random number is generated, say Ξ_0, which establishes the first free-flight distance-of-travel, R_o, via the transformation derived on page 3-53. Specifically, $\Sigma_t R_0 = -\ln \Xi_0$. Note that the location of the first collision, $\underline{r}_0$, is easily determined by the relations $x_0 = R_0 \sin\theta_0 \cos\phi_0$, $y_0 = R_0 \sin\theta_0 \sin\phi_0$, and $z_0 = R_0 \cos\theta_0$ (where $\theta_0 = \arccos\mu_0$).
3. One random number is generated, say χ_0, which establishes the type of the first interaction. Using the notation discussed on page 3-56, let $\chi(1)$ represent the ratio Σ_s/Σ_t (rounded off to the number of significant digits in the random number generator). Then, following the ideas expressed on page 3-56, if $\chi_0 \leqq \chi(1)$ the collision is a scattering and we proceed to step 4; if $\chi_0 > \chi(1)$ the collision is a capture and the simulated history of the first emitted particle is terminated (indicating a return to step 1 and emission of the next particle). In either case, the collision is recorded in a manner that both $\underline{r}_0$ and $\hat{\Omega}_0$ can be recalled. Note that after all the simulated particle trajectories have been completed, the sum of all the collisions which occurred in a volume $\Delta^3 r_0$ about $\underline{r}_0$ with pre-collision direction-of-travel in $\Delta^2\Omega_0$ about $\hat{\Omega}_0$ will establish the radiation

flux at $(\underline{r}_0,\hat{\Omega}_0)$ via, $\Sigma_t\Phi(\underline{r}_o,\hat{\Omega}_0)$ is proportional to the collision sum.

4. Two random numbers are generated, say ξ_1 and η_1, which establishes the first-scattering direction, $\hat{\Omega}_1$, via the transformations $\mu_1 = 2\xi_1 - 1$ and $\phi_1 = 2\pi\eta_1$.

5. One random number is generated, say Ξ_1, which establishes the second free-flight distance-of-travel, R_1, via the transformation $\Sigma_t R_1 = -\ell n\Xi_1$. The location of the second collision, $\underline{r}_1$, is determined by the relations $x_1 = x_0 + R_1\sin\theta_1\cos\phi_1$, $y_1 = y_0 + R_1\sin\theta_1\sin\phi_1$, and $z_1 = z_0 + R_1\cos\theta_1$ (where $\theta_1 = \arccos\mu_1$). Note that the simplicity of these expressions is a consequence of the presumption of isotropic scattering.

6. One random number is generated, say χ_1, which establishes the type of the second interaction. Specifically, if $\chi_1 \leqq \chi(1)$ the collision is a scattering and we proceed to step 7; if $\chi_1 \geqq \chi(1)$ the collision is a capture and the simulated history of the particle is terminated (indicating a return to step 1 and emission of the next particle). Again, in either case, the collision is recorded such that $\underline{r}_1$ and $\hat{\Omega}_1$ can be recalled.

7. Steps 4 through 6 are repeated requiring random numbers ξ_2 and η_2 to establish $\hat{\Omega}_2$, random number Ξ_2 to establish R_2, and random number χ_2 to establish the interaction type for the third collision. The location of the third collision, $\underline{r}_2$, is determined by the relations $x_2 = x_1 + R_2\sin\theta_2\cos\phi_2$, $y_2 = y_1 + R_2\sin\theta_2\sin\phi_2$, and $z_2 = z_1 + R_2\cos\theta_2$.

Thus, the Monte Carlo simulation proceeds following each emitted particle through its "life history" which terminates when the particle experiences a capture collision. As indicated previously, the radiation flux is determined

(after a large number of particle histories have been generated) by the relation

$\Sigma_t \Phi(\underline{r},\hat{\Omega})\Delta^3 r \Delta^2 \Omega$ is proportional to the sum of recorded collisions which occurred in $\Delta^3 r$ about $\underline{r}$ with pre-collision direction-of-travel in $\Delta^2\Omega$ about $\hat{\Omega}$.

Generalization of the ideas to more realistic problems is straight-forward but usually algebraically complicated and tedious. Since many particle histories are required to generate useful information, the computational costs (use of a digital computer) is usually high. Several strategies are employed to emphasize the radiation of particular interest in a given problem.

PARTICLE ENERGY SPECTRUM RELATIONS

Classical Equilibrium Distributions

Consideration of the E-dependence of particle distributions can proceed directly from the transport equation and such will be accomplished later in this section. Energy spectrum formulation is often more difficult to visualize than configuration spatial distributions--thus, let us begin this discussion with some of the more directly addressed problems. One of these is the derivation of thermodynamic equilibrium particle distributions. For the moment define "equilibrium" for a particle distribution as:

1) Steady state, i.e., t-independence

2) Uniformity, i.e., $\underline{r}$-independence

3) Isotropic motion of particles, i.e., $\hat{\Omega}$-independence.

Whence, with this definition, $n(\underline{r},\underline{v},t) \rightarrow n(v)$.

Maxwell-Boltzmann distribution:

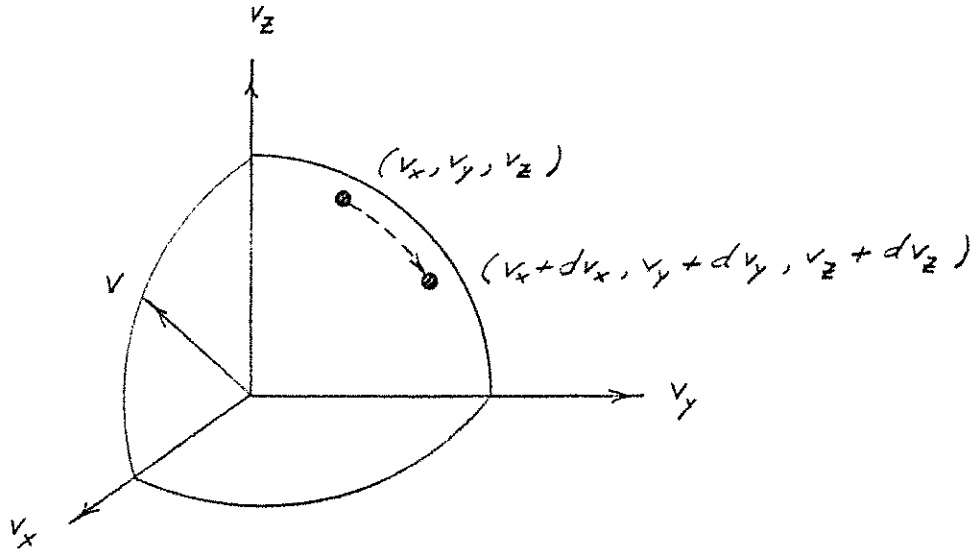
The method employed here is based on a variational technique used in Maxwell's original derivation. Use Cartesian $\underline{v}$-coordinates, i.e., $\underline{v} = (v_x, v_y, v_z)$ and let $dn = \frac{\partial n}{\partial v_x} dv_x + \frac{\partial n}{\partial v_y} dv_y + \frac{\partial n}{\partial v_z} dv_z$

Assuming that $n(v)$ is separable in the form $n(v) = n_x(v_x)n_y(v_y)n_z(v_z)$ yields

$$\frac{dn}{n} = \frac{1}{n_x}\frac{dn_x}{dv_x} + \frac{1}{n_y}\frac{dn_y}{dv_y} dv_y + \frac{1}{n_z}\frac{dn_z}{dv_z} dv_z$$

Consider a special change in $\underline{v}$ such that v is a constant, i.e.,

$$v_x^2 + v_y^2 + v_z^2 = v^2 = \text{constant}$$



For such a change in $\underline{v}$,

1. $dn = 0$ since $n = n(v)$
2. $2v_x dv_x + 2v_y dv_y + 2v_z dv_z = 2vdv = 0$

Note that only two of the dv_i are arbitrary (i.e., independent). With this change in $\underline{v}$,

$$\frac{1}{n_x}\frac{dn_x}{dn_x}\,dv_x + \frac{1}{n_y}\frac{dn_y}{dv_y}\,dv_y + \frac{1}{n_z}\frac{dn_z}{dv_z}\,dv_z = 0 \quad \text{and}$$

$2\alpha v_x dv_x + 2\alpha v_y dv_y + 2\alpha v_z dv_z = 0$ for an arbitrary constant α. Whence,

$$(\frac{1}{n_x}\frac{dn_x}{dv_x} + 2\alpha v_x)dv_x + (\frac{1}{n_y}\frac{dn_y}{dv_y} + 2\alpha v_y)dv_y + (\frac{1}{n_z}\frac{dn_z}{dv_z} + 2\alpha v_z)dv_z = 0$$

Choose α such that one of the $\frac{1}{n_i}\frac{dn_i}{dv_i} + 2\alpha v_i = 0$ and let the remaining two dv_i be arbitrary, e.g., choose α such that $\frac{1}{n_x}\frac{dn_x}{dv_x} + 2\alpha v_x = 0$ and let dv_y and dv_z be arbitrary differential variations. The implication is that $\frac{1}{n_i}\frac{dn_i}{dv_i} + 2\alpha v_i = 0$, $i = x,y,z$, and thus, $n_i(v_i) = C_i \exp[-\alpha v_i^2]$. Finally,

$n(v) = n_x(v_x)n_y(v_y)n_z(v_z) = Ce^{-\alpha v^2}$ in Cartesian $\underline{v}$-space coordinates.

Evaluation of the constant C --

$N = \int n(\underline{v})\, d^3v$ here becomes

$$N = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} Ce[-\alpha(v_x^2 + v_y^2 + v_z^2)]\, dv_x dv_y dv_z \quad \text{implies } C = \left(\frac{\alpha}{\pi}\right)^{3/2} N$$

Have used the gamma function defined by

$$\Gamma(x) = \int_0^\infty u^{x-1} e^{-u}\, du, \quad x > 0$$

and the properties

$$\Gamma(x) = (x-1)\Gamma(x-1)$$

$$\Gamma(m) = (m-1)! \quad m = \text{integer} \geq 1$$

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi}$$

The classical equilibrium distribution is therefore given by

$$n(\underline{v}) = \left(\frac{\alpha}{\pi}\right)^{3/2} Ne^{-\alpha v^2}$$

Quasi-equilibrium classical distribution --

If $n(\underline{r},\underline{v},t)$ is a "slowly varying" function of $(\underline{r},t)$, then

$$N(\underline{r},\underline{v},t) \approx \left(\frac{\alpha}{\pi}\right)^{3/2} N(\underline{r},t)\, e^{-\alpha v^2}$$

Recall that this result is in Cartesian $\underline{v}$-space and thus might more appropriately be written

$$n(\underline{r},v_x,v_y,v_z,t) = \left(\frac{\alpha}{\pi}\right)^{3/2} N(\underline{r},t)\, \exp[-\alpha(v_x^2 + v_y^2 + v_z^2)]$$

In spherical polar $\underline{v}$-space coordinates, (v,θ,ϕ),

$$n'(v,\theta,\phi) = v^2 \sin\theta \; n(v_x,v_y,v_z)$$

Whence,

$$n'(\underline{r},v,\theta,\phi,t) = \left(\frac{\alpha}{\pi}\right)^{3/2} N(\underline{r},t) v^2 \sin\theta e^{-\alpha v^2}$$

Particle speed distribution:

$$n_1(v) = \int_0^{\pi} \int_0^{2\pi} n'(v,\theta) \; d\theta d\phi$$

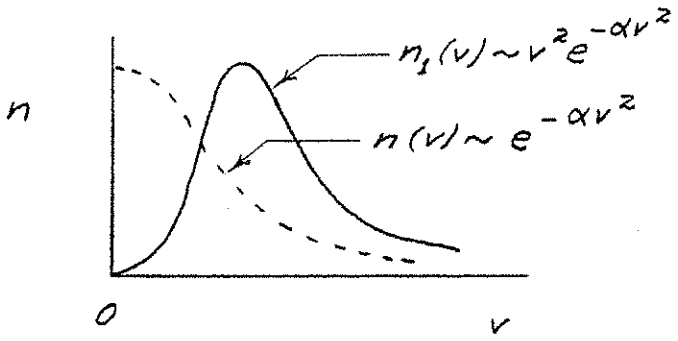
i.e.,

$$n_1(v) = \left(\frac{\alpha}{\pi}\right)^{3/2} N v^2 e^{-\alpha v^2} \int_0^{\pi} \int_0^{2\pi} \sin\theta d\theta d\phi$$

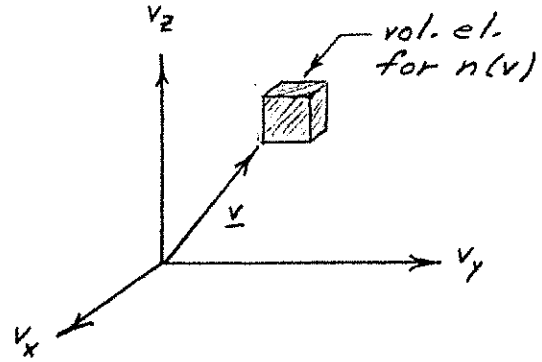
Note that

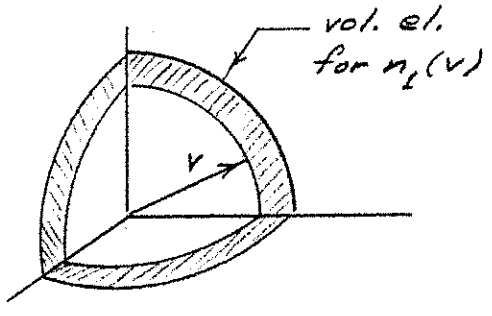
$$\int_0^{\pi} \int_0^{2\pi} \sin\theta d\theta d\phi = \int d^2\Omega = 4\pi$$

$$n_1(v) = 4\pi^{-1/2} \; \alpha^{3/2} \; N v^2 e^{-\alpha v^2}$$



Considering the relevant volume element for each case helps explain the different spectrum appearance.





Moments of the speed distribution --

$$\bar{v} = \frac{1}{N} \int_0^\infty v n_1(v)\,dv = \frac{2}{(\pi\alpha)^{1/2}}$$

$$\bar{E} = \frac{1}{N} \int_0^\infty \tfrac{1}{2}mv\, n_1(v)\,dv = \frac{3}{4}\,\frac{m}{\alpha}$$

Note that this relation will occur later in these notes as an identification of the constant α, i.e.,

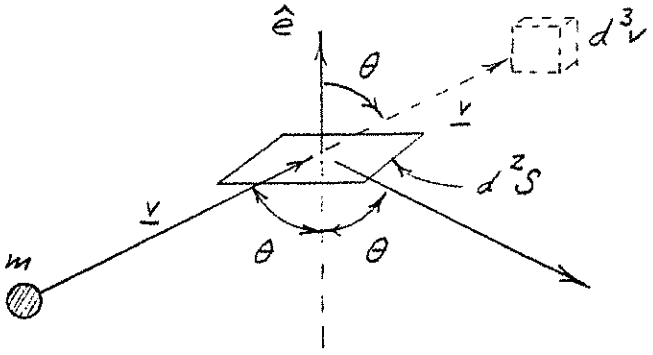
$$\alpha = \frac{3}{4}\,\frac{m}{\bar{E}}$$

Particle energy spectrum:

$$n'(E) = n_1[v(E)]\,\frac{dv}{dE}$$

$$= 4\left(\frac{\alpha}{m}\right)^{3/2}\left(\frac{2E}{\pi}\right)^{1/2} Ne^{-2\alpha E/m}$$

Particle pressure:



Rate at which particles in d^3v strike d^2S, as in the derivation of particle current relations, is given by $n(\underline{v})d^3v\ \underline{v}\cdot\hat{e}d^2S$

However, here assume that particles do not pass through d^2S but are instead reflected. Presuming "specular reflection" (as illustrated), the particle momentum change in the surface collision is $-2mv\cos\theta\hat{e}$, i.e.,

$$2m\underline{v}\cdot\hat{e}\ \ (-\hat{e}).$$

The magnitude of the force on d^2S is

$$2m(\underline{v}\cdot\hat{e})^2\, n(\underline{v})d^3v d^2S.$$

Thus, with p representing the pressure

$$p = \int_{\underline{v}\cdot\hat{e}>0} 2m(\underline{v}\cdot\hat{e})^2 n(\underline{v}) d^3v$$

Case of an isotropic distribution --

$$p = 2m \int_{\underline{v}\cdot\hat{e}>0} (\underline{v}\cdot\hat{e})^2 \, n(v) d^3v$$

where $n(v)$ is expressed in Cartesian $\underline{v}$-coordinates. With the integration expressed in spherical, polar coordinates ($\hat{e}$ as the polar axis),

$$p = 2m \int_0^{\infty} \int_0^{\pi/2} \int_0^{2\pi} (v\cos\theta)^2 n(v) v^2 \sin\theta \, dv \, d\theta \, d\phi$$

$$= \frac{m}{3} \int_0^{\infty} v^2 n_1(v) dv$$

$$= \frac{mN}{3} \overline{v^2} = \frac{2}{3} N\overline{E}$$

In particular, for the case of a classical equilibrium distribution

$$p = \frac{2}{3} N \left(\frac{3m}{4\alpha}\right) = \frac{Nm}{2\alpha}$$

Moreover, the "perfect gas law," or equation of state is $p = NkT$, where the Boltzmann constant is

$$k = 1.38 \times 10^{-16} \text{ erg/°K}$$

$$= 8.62 \times 10^{-5} \text{ ev/°K}$$

and T is the "absolute temperature" of the particle distribution (in °K). Whence,

$$\alpha = \frac{m}{2kT}$$

and, as a function of T,

$$n(v_x,v_y,v_z) = N\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-mv^2/2kT}$$

$$n'(v,\theta,\phi) = N\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 \sin\theta e^{-mv^2/2kT}$$

$$n_1(v) = N\left(\frac{m}{2\pi kT}\right)^{3/2} 4\pi v^2 e^{-mv^2/2kT}$$

$$n'(E) = N\left(\frac{1}{2kT}\right)^{3/2} 4\left(\frac{2}{\pi}\right)^{1/2} E^{1/2} e^{-E/kT}$$

Elementary Quantum Statistics

The classical equilibrium distribution is actually a limiting case (the classical limit) of more fundamental particle distributions. Because the energy states and energy exchanges in interactions for individual particles are of such small magnitude, the effects of the quantum (discrete) nature of energy exchange must be taken into account. In these lectures a heuristic derivation of such quantum effects and the resulting particle distributions are presented.

Quantization rules:

Wilson-Sommerfeld conditions --

Consider an independent set of coordinates x_i which specify the configuration of a system. If the forces acting on the system are conservative, then can define a set of generalized momenta p_i by

$$p_i = \frac{\partial}{\partial \dot{x}_i} E(\underline{x},\dot{\underline{x}})$$

where E is the system kinetic energy and $\dot{x}_i = \frac{\partial}{\partial t} x_i$. Moreover, if the system configuration is periodic (i.e., x_i and p_i are cyclical) then the "allowed" trajectories must satisfy a quantization rule $\oint p_i dx_i = \alpha_i h$ where the integration is over a complete cycle of motion, α_i is an integer, and Planck's

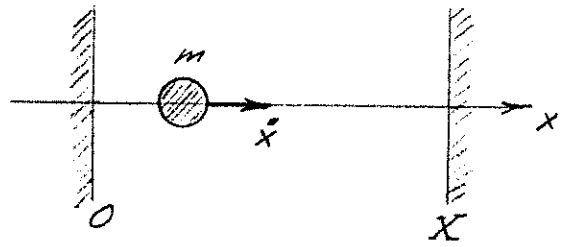
constant is

$$h = 6.63 \times 10^{-27} \text{ erg-sec}$$

$$= 4.14 \times 10^{-15} \text{ ev-sec.}$$

Examples --

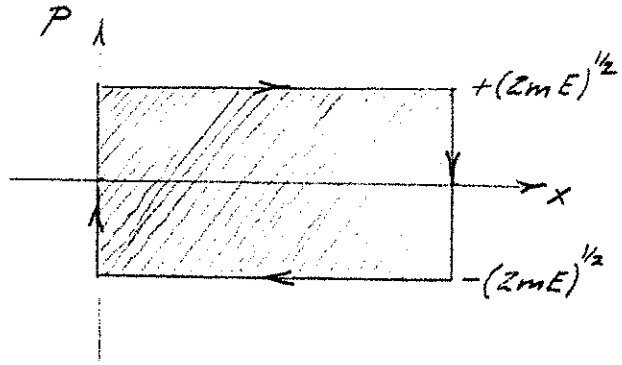
1. One-dimensional motion of particles between elastic walls.



$$E = \frac{1}{2}m\dot{x}^2$$

Implies $p = m\dot{x}$

Implies $E = \frac{p^2}{2m}$



Periodic trajectory $p = p(x)$ is as illustrated. The quantization implies that the shaded area (enclosed by the trajectory) is αh,

i.e.,

$$2(2mE)^{1/2} X = \alpha h$$

Thus, the permitted kinetic energy states of the particle are given by

$$E = \frac{\alpha^2 h^2}{8mX^2} \qquad \alpha = 0,1,2,...$$

Energy state separation is given by

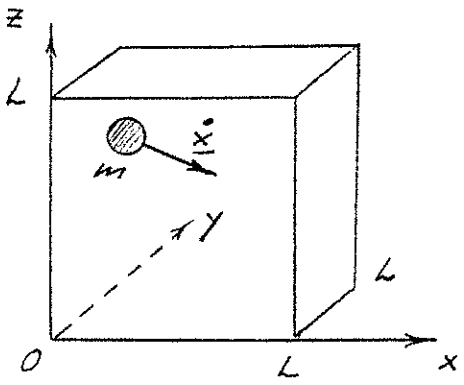
$$\Delta E = E_{\alpha+1} - E_\alpha = \frac{(2\alpha + 1)h^2}{8mX^2} \approx \frac{dE}{d\alpha} = \frac{2\alpha h^2}{8mX^2}$$

Note that the classical limit of continuously distributed allowed energy

states is approached if either m or X is "large." Of more significance,

$$\frac{\Delta E}{E} \sim \frac{1}{\alpha} \to 0 \qquad \text{as} \quad \alpha \to \infty.$$

2. Three-dimensional motion of particles in an elastic box.



$\underline{x} = (x, y.z)$

$\dot{\underline{x}} = (\dot{x}, \dot{y}, \dot{z})$

$E = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$

Implies $p_x = m\dot{x}$, $p_y = m\dot{y}$

$p_z = m\dot{z}$

Quantization rule implies that

$$p_x = \frac{\alpha_x h}{2L}, \quad p_y = \frac{\alpha_y h}{2L}, \quad p_z = \frac{\alpha_z h}{2L}$$

Whence,

$$E_{\alpha_x \alpha_y \alpha_z} = \frac{(\alpha_x^2 + \alpha_y^2 + \alpha_z^2)h^2}{8mL^2}$$

$\alpha_x = 0, 1, 2, \ldots$

$\alpha_y = 0, 1, 2, \ldots$

$\alpha_z = 0, 1, 2, \ldots$

Particle spin --

In order for quantum mechanical arguments to yield meaningful predictions when applied to particle groups, it is required that certain particle types have an intrinsic angular momentum of fixed magnitude. This magnitude can have the values

$$[s(s+1)\ (\frac{h}{2\pi})^2]^{1/2}$$

where s = 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, ... is termed the particle "spin."

particle	spin
electron	$\frac{1}{2}$
proton	$\frac{1}{2}$
neutron	$\frac{1}{2}$
photon	1
(nuclei, ions, atoms molecules odd no. of elects., prots., neuts.)	$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, ...
(nuclei, ions, atoms, molecules even no. of elects., prots., neuts.,)	0, 1, 2, 3, ...

Spin states --

There is a "quantum number" associated with the spin orientation and this number can take on only 2s + 1 values (except for a photon where there are only 2 possible spin states with s = 1). An energy state is specified by trajectory quantum numbers and spin quantum numbers (e.g., for non-interacting particles in a box α_x, α_y, α_z are trajectory quantum numbers and for each set there are 2s + 1 possible spin states).

Pauli exclusion principle --

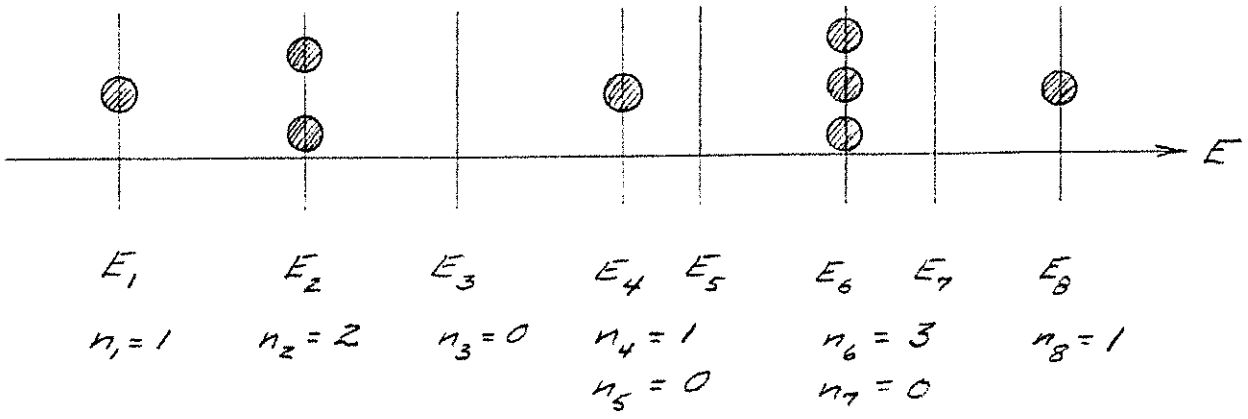
No two particles with half-odd-integer values of spin, s, can be in the same energy state (e.g., for non-interacting half-odd, integer spin particles in a box there are at most 2s + 1 particles with the same values of α_x, α_y, α_z).

Thermodynamic probability:

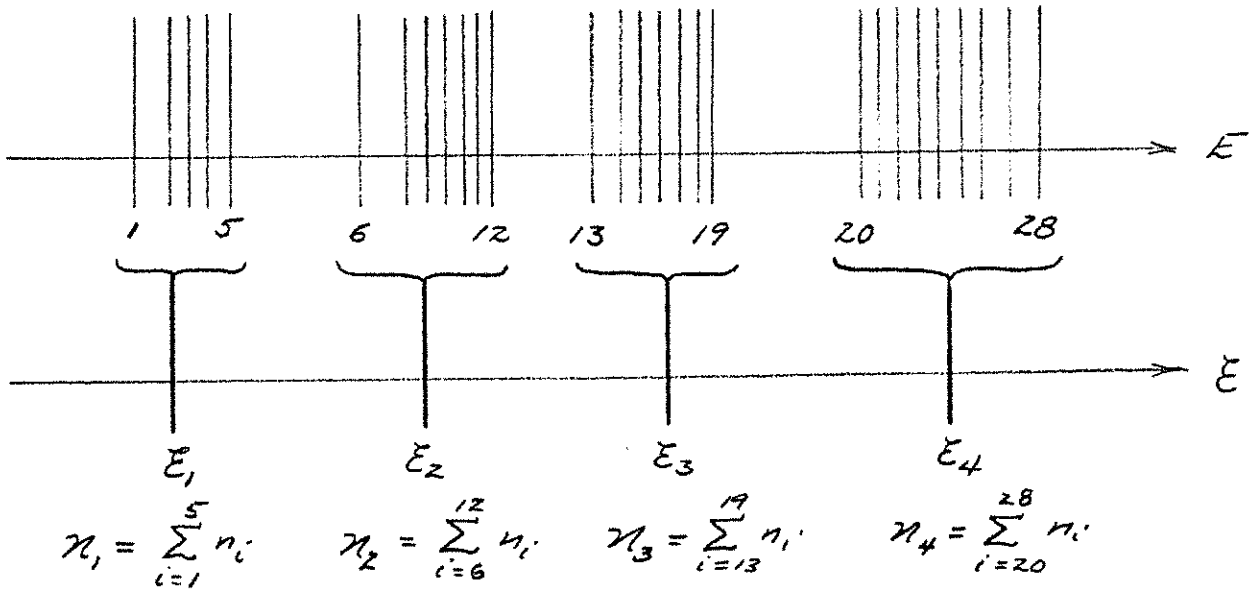
Particle distribution in energy --

Denote the permitted energy states of a system of particles by the set $\{E_i \quad i = 1, 2, 3, \ldots\}$ and the particle population corresponding to each

state by $\{n_i \quad i = 1, 2, 3, \ldots\}$



Recalling the results for particles in a box of side L, $E_\alpha = \frac{\alpha^2 h^2}{8mL^2}$ and $\Delta E_\alpha = \frac{\alpha\, h^2}{4mL^2}$. For L = 1 cm., and m = 10^{-24} gram (ca. nucleon mass), $\Delta E_\alpha = 0(10^{-17})\alpha$ ev. Presuming that following energy exchanges of such small magnitude is not of interest in the particle distribution problem, a method of conglomerating individual energy states into groups of more significant energy separation is considered. In the "macrostate" description, the particle occupation population is the sum of the actual energy state occupation numbers, n_i, over each conglomerate, e.g.,



The marcostate is described by the set $\{E_i, N_i \quad i = 1, 2, 3, \ldots\}$. Note that each macrostate is generated by many possible "microstates" which are described by the set $\{E_i, n_i \quad i = 1, 2, 3, \ldots\}$.

Ergodic hypothesis --

Every microstate (consistent with any restraints on the particle system) is equally probable. Restraints on the particle system are such conditions as a fixed total number of particles, or a fixed total particle kinetic energy.

Particle distribution in macrostates --

With every microstate presumed equally probable, the relative probability of finding the occupation number N_i in the macrostate E_i is proportional to the number of microstate occupation possibilities consistent with (N_i, E_i). Let $w(N_i)$ represent this number of possibilities. The "thermodynamic probability" of an occupation complexion is defined as

$$W(\{N_i\}) = \prod_i w(N_i).$$

Role of restraints --

As an example, consider the case where the total particle population and total particle kinetic energy are fixed values. Then, certainly the range of possibilities for $\{N_i, E_i\}$ is restricted by the constraints

$$\sum_i N_i = N = \text{total population}$$

$$\sum_i N_i E_i = N\bar{E} = \text{total kinetic energy}$$

if there are further dynamic constraints, they must also be included.

Expected particle distribution:

The "expected" particle distribution is given by that occupation complexion $\{N_i\}$ which maximized $W(\{N_i\})$ consistent with the relevant restraints on the system. Equivalent, and more convenient to apply, is the maximization of $\ln W(\{N_i\})$.

In order to accomplish the determination of $w(N_i)$ and thereby $W(\{N_i\})$, denote the number of microstate energy levels $\{E_j\}$ in the i^{th} macrostate level (i.e., at E_i) by M_i. The counting procedure employed to evaluate $w(N_i)$ depends on the set of restraints on the particle system as well as a presumption on whether or not particles are distinguishable (i.e., in principle, can be labelled). Accordingly, different forms for the particle statistics emerge. In these lectures three forms are developed:

1. Fermi-Dirac statistics.
    a. indistinguishable particles.
    b. half-odd-integer spin.
    c. N fixed.
    d. $N\overline{E}$ fixed.
2. Bose-Einstein statistics.
    a. indistinguishable particles.
    b. integer spin.
    c. N fixed.
    d. $N\overline{E}$ fixed.
3. Boltzmann statistics.
    a. distinguishable particles.
    b. integer spin, or exclusion volume of particle occupancy.
    c. N fixed.
    d. $N\overline{E}$ fixed.

Fermi-Dirac statistics:

A "Fermi gas" is a collection of particles with the properties

1. they are indistinguishable (i.e., even in principle they cannot be labelled.)
2. half-odd integer spin,
3. fixed total population N,

4. fixed total kinetic energy $N\bar{E}$,

5. contained in a box of volume V.

Note that E_i here includes spin orientation, e.g., for s = 1/2, E_1 has E_* and s "up," E_2 has E_* and s "down."

By the Pauli exclusion principle, the microstate occupation numbers, n_i, must be either 0 or 1. Thus,

$$w(N_i) = \frac{M_i!}{(M_i-N_i)!N_i!}$$

and

$$W(\{N_i\}) = \prod_i \frac{M_i!}{(M_i-N_i)!N_i!}$$

Whence,

$$\ell n\ W(\{N_i\}) = \sum_i [\ell nM_i! - \ell n(M_i-N_i)! - \ell nN_i!]$$

and using Stirling's approximation (i.e., $\ell nM! \approx M\ell nM - M$ for large M),

$$\ell nW(\{N_i\}) \approx \sum_i [M_i \ell nM_i - (M_i-N_i)\ell n(M_i-N_i) - N_i \ell nN_i]$$

which is to be maximized subject to the restraints

$$\sum_i N_i = N \text{ and } \sum_i N_i E_i = N\bar{E}$$

Employing the method of Lagrange multipliers, maximize the function

$$F(\{N_i\}, \gamma, \beta) = \ell n\ W(\{N_i\}) + \gamma(\sum_i N_i - N) - \beta(\sum_i N_i E_i - N\bar{E})$$

Note that

$$\frac{\partial F}{\partial N_i} = 0 \text{ implies } \ell n\ (\frac{M_i}{N_i} - 1) + \gamma - \beta E_i = 0$$

if the approximation for $\ell n\ W(\{N_i\})$ above is used.

Whence,

$$\frac{N_i}{M_i} = [\exp[(\beta E_i - \gamma)] + 1]^{-1}$$

Moreover, if this result is presumed to generate an approximate average occupation complexion for the M_i microstates, then

$$n_i \approx [\exp[\beta E_i - \gamma] + 1]^{-1}$$

In quantum-number-space (i.e., $\underline{\alpha}$-space),

$$n_{\underline{\alpha}} = \frac{2s + 1}{\exp[\beta E_{\underline{\alpha}} - \gamma] + 1}$$

Where s is the particle spin and it is presumed that $E_{\underline{\alpha}}$ is spin-orientation-independent.

Let $n(\underline{\alpha})d^3\alpha$ represent the expected particle density in $\underline{r}$-space and population in $d^3\alpha$ volume element of $\underline{\alpha}$-space. Presuming that the particles are in a cubical box (of side L),

$$n(\underline{\alpha}) = \frac{1}{L^3} \frac{2s + 1}{\exp[\beta E_{\underline{\alpha}} - \gamma] + 1}$$

Where

$$E_{\underline{\alpha}} = \frac{(\underline{\alpha} \cdot \underline{\alpha})h^2}{8mL^2} = \frac{\vec{\alpha}h^2}{8mL^2}$$

Employing spherical polar coordinates in $\underline{\alpha}$-space (α, θ, ϕ)

$$n_1(\alpha) - \int_0^{\pi/2} \int_0^{\pi/2} n(\underline{\alpha})\, \alpha^2 \sin\theta d\theta d\phi$$

$$n_1(\alpha) = \frac{\pi\alpha^2}{2L^3} (2s + 1) \left[e^{-\gamma} \exp\left(\frac{\beta\alpha^2h^2}{8mL^2}\right) + 1\right]^{-1}$$

Note that only the first octant of $\underline{\alpha}$-space is covered since

$$\alpha_x = 0, 1, 2, \ldots, \quad \alpha_y = 0, 1, 2, \ldots, \quad \alpha_z = 0, 1, 2, \ldots$$

In terms of particle kinetic energy and speed,

$$n'(E) = n_1(\alpha(E)) \left|\frac{d\alpha}{dE}\right|$$

$$= 4\pi \frac{(2m^3)^{1/2}}{h^3} (2s + 1) \left(\frac{E^{1/2}}{\exp[\beta E - \gamma] + 1}\right)$$

$$n_1(v) = n'(E(v)) \left|\frac{dE}{dv}\right|$$

$$= 4\pi\left(\frac{m}{h}\right)^3 (2s + 1) \frac{v}{e^{-\gamma}\exp(\beta \tfrac{1}{2} mv^2) + 1}$$

Since $n(\underline{\alpha})$ is "isotropic" in $\underline{\alpha}$-space, $n(\underline{v})$ must be isotropic in $\underline{v}$-space. Thus, in 6-dimensional Cartesian $(\underline{r},\underline{v})$-space,

$$n(\underline{r},\underline{v},t) = \frac{1}{4\pi v^2} n_1(v)$$

$$= \left(\frac{m}{h}\right)^3 (2s + 1) [e^{-\gamma}\exp(\beta \tfrac{1}{2} mv^2) + 1]^{-1}$$

It remains to identify the constants β and γ. The restraint conditions must be used, i.e., in the present terms,

$$\int n(\underline{r},\underline{v},t)\, d^3v = \int_0^\infty n_1(v)\, dv = N$$

and

$$\int \tfrac{1}{2} mv^2 n(\underline{r},\underline{v},t)\, d^3v = \int_0^\infty \tfrac{1}{2} mv^2 n_1(v)\, dv = N\overline{E}$$

The classical limit --

If for each macrostate $N_i \ll M_i$, i.e., a very "dilute" occupation complexion, then

$$w(N_i) = \frac{M_i!}{(M_i - N_i)! N_i!}$$

$$= \frac{M_i(M_i-1)(M_i-2)\ldots(M_i - N_i + 1)}{N_i!}$$

$$\approx \frac{M_i^{N_i}}{N_i!}$$

and

$$W(\{N_i\}) \simeq \prod_i \frac{M_i^{N_i}}{N_i!}$$

Presuming that N_i is still large enough to use Stirling's approximation,

$$\ell n W(\{N_i\}) \simeq \sum_i N_i (\ell n M_i - \ell n N_i + 1)$$

and maximizing $\ell n\ W\ (\{N_i\})$ subject to the restraints $\sum_i N_i = N$ and $\sum_i N_i E_i = N\bar{E}$ yields the result

$$\frac{N_i}{M_i} = \exp[\gamma - \beta E_i]$$

Whence, $n_i = \exp[\gamma - \beta E_i]$, or $n(\underline{r},\underline{v},t) = (\frac{m}{h})^3\ (2s + 1)\ e^{\gamma} e^{-\beta \frac{1}{2} mv^2}$ in Cartesian $(\underline{r},\underline{v})$-space. Note that this result is the classical equilibrium distribution, i.e., $n(\underline{r},\underline{v},t) \sim e^{-\beta \frac{1}{2} mv^2}$, and that this classical limit is achieved by requiring $N_i << M_i$. Such a condition is developed if

1. N and L are fixed and $\bar{E}$ is increased, i.e., N_i is decreased holding M_i fixed, or
2. N and $\bar{E}$ are fixed and M or L is increased, i.e., M_i is increased holding N_i fixed.

Moreover, comparison with the classical equilibrium result yields the identifications

$$\beta = \frac{1}{kT}$$

and

$$(\frac{m}{h})^3\ (2s + 1)e^{\gamma} = N(\frac{m}{2\pi kT})^{3/2}$$

The identification of β is valid even for the case $N_i = 0(M_i)$, however, the identification of γ is only valid in the classical limit.

Fermi energy:

Defining μ, the Fermi energy, by

$$\mu = \gamma kT$$

the Fermi-Dirac energy distribution is

$$n'(E) = C \frac{E^{1/2}}{e^{(E-\mu)/kT} + 1}$$

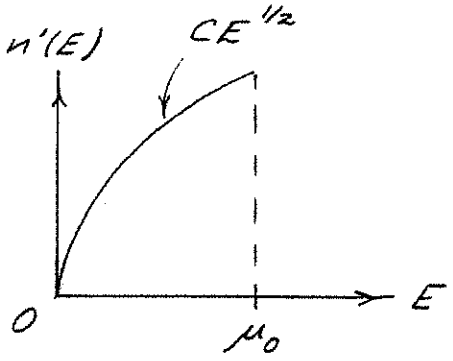
where $C = 4\pi \frac{(2m^3)^{1/2}}{h^3} (2s + 1)$.

$\mu = \mu(T)$ is determined from the restraint on particle populations, i.e.,

$$\int_0^\infty n'(E)dE = N$$

Consider the case of $T \to 0$ and denote $\mu(0) = \mu_0$. The result is

$$n'(E) = \begin{cases} CE^{\frac{1}{2}} \text{ for } E < \mu_0 \\ 0 \text{ for } E > \mu_0 \end{cases}$$

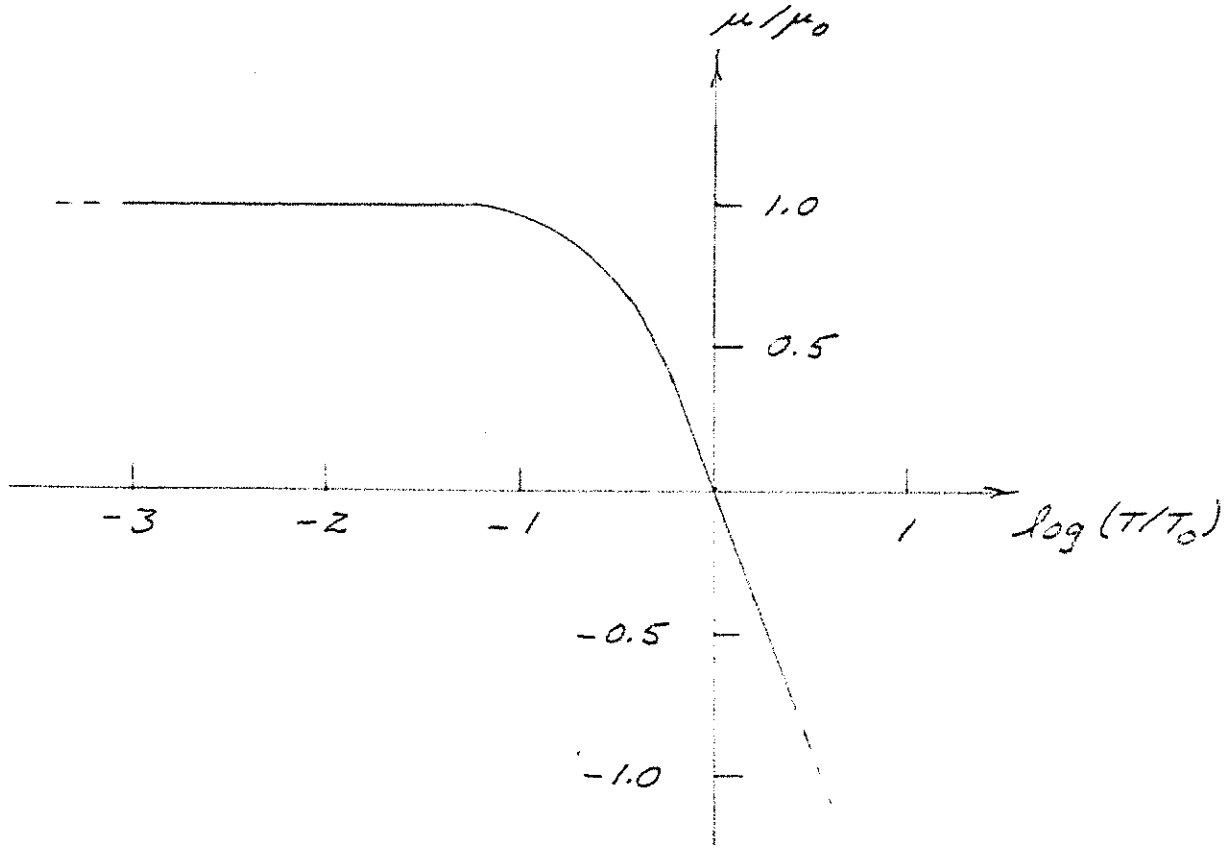


$$N = \int_0^\infty n'(E)dE = \frac{2}{3} C\mu_0^{3/2}$$

Whence,

$$\mu_0 = \frac{h^2}{2m} \left[\frac{3N}{4\pi(2s + 1)}\right]^{2/3}$$

For the more general case, i.e., $T \neq 0$, numerical solution of $N = \int_0^\infty n'(E)dE$ yields the results



Where $\mu(T_0) = 0$ and $kT_0 = 3.37\ \mu_0$

For example --

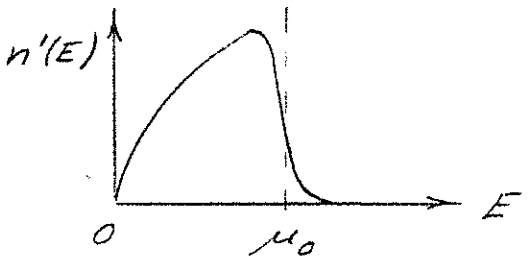
Gas	m	N	μ_0	T_0
Molecular (at STP)	10^{-24} g	10^{19} cc^{-1}	10^{-5} ev	0.1°K
Electrons (in metal)	10^{-27}	10^{23}	10	10^{+5}

i.e., for a molecular gas at STP, $T >> T_0$ and $-\frac{\mu}{\mu_0} >> 1$ which imply that

$$n'(E) \simeq Ce^{\mu/kT} E^{\frac{1}{2}} e^{-E/kT}$$

which is the classical equilibrium distribution. In contrast, for electrons

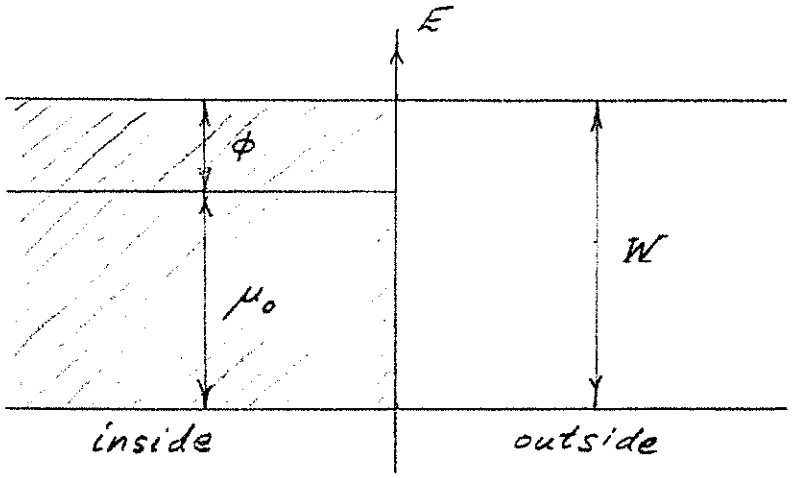
in a metal, $T \ll T_0$ and $\mu \simeq \mu_o$ which imply that $n'(E)$ is like the T = 0 Fermi distribution,



For T = 0 (100°K) the electron distribution is as illustrated.

Thermionic emission of electrons:

Consider an electron gas in a metal with T = 0 (100°K). Suppose that the "wall" potential retaining the electrons in the "box" is such that an electron with E > W hitting the metal surface does escape from the metal volume. The "work function" of the metal is defined as $\phi = W - \mu_0$.



$$J_+ = \int_{(\frac{2W}{m})^{\frac{1}{2}}}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} v_x n(\underline{v}) dv_x dv_y dv_z$$

where

$$n(\underline{v}) = (\frac{m}{h})^3 (2s + 1) \{\exp[(\tfrac{1}{2}mv^2 - \mu)/kT] + 1\}^{-1}$$

is the outgoing electron current at the metal surface. Using $s = \frac{1}{2}$, $\mu \simeq \mu_o$, and noting that $v_x > (\frac{2W}{m})^{\frac{1}{2}}$ implies $(\frac{1}{2}mv^2 - \mu_o) >> kT$ for $\phi = 0(\mu_o)$, the result is

$$n(\underline{v}) \approx 2(\frac{m}{h})^3 \exp[\mu_o/kT]\ e^{-mv^2/2kT}$$

for $v_x > (\frac{2W}{m})^{\frac{1}{2}}$,

whence,

$$J_+ \approx \frac{4\pi m}{h^3}\ (kT)^2\ e^{-\phi/kT}$$

and the emitted electric current density is given by

$$I_+ = eJ_+ \approx 120\ T^2 e^{-\phi/kT} \text{amp/cm}^2$$

where $e = 1.5 \times 10^{-19}$ coulomb. This is the Richardson-Dushman relation for thermionic emission.

Bose-Einstein statistics:

A "Bose gas" is a collection of particles with the properties

1. They are indistinguishable,
2. integer spin,
3. fixed population, N,
4. fixed kinetic energy, $N\overline{E}$,
5. contained in box of volume V.

There are no limits (other than the N and $N\overline{E}$ constraints) on the microstate occupation numbers, n_i. In order to determine $w(N_i)$ consider a sequence of N_i periods (1) and $M_i - 1$ commas (,), e.g.,

. . . , . . , , . , . . . , .

which represents the microstate complexion $n_1 = 3$, $n_2 = 2$, $n_3 = 0$, $n_4 = 1$, $n_5 = 3$, . . . There are $(N_i + M_i - 1)!$ permutations of the periods and commas of which $N_i!$ permutations of the periods and $(M_i - 1)!$ permutations of the

commas do not lead to different energy state occupations. Thus,

$$w(N_i) = \frac{(N_i + M_i - 1)!}{N_i!\ (M_i - 1)!}$$

and

$$W(\{N_i\}) = \prod_i \frac{(N_i + M_i - 1)!}{N_i!\ (M_i - 1)!}$$

Using Stirling's approximation, and maximizing $\ln W(\{N_i\})$ subject to the restraints $\sum_i N_i = N$ and $\sum_i N_i E_i = N\bar{E}$ yields

$$\frac{N_i}{M_i} = [\exp(\beta E_i - \gamma) - 1]^{-1}$$

Whence,

$$n_i = [\exp(\beta E_i - \gamma) - 1]^{-1}$$

and, with the identifications

$$\beta = 1/kT \text{ and } \gamma = \mu/kT,$$

$$n_i = \{\exp[(E_i - \mu)/kT] - 1\}^{-1}$$

If the restraint $\sum_i N_i = N$ is removed (i.e., when particles can be created or destroyed, then the parameter γ would not be introduced and the result is

$$n_i = \{\exp(E_i/kT) - 1\}^{-1}$$

Photons in a cavity --

An electromagnetic wave of frequency ν and velocity c can be considered to be photon particles of energy $h\nu$ and momentum $h\nu/c$ with spin 1. There are two possible spin states associated with a photon (not the usual $2s + 1$) corresponding to the two possible directions of wave polarization. The wave intensity is determined by the number of photons, and photons are easily created

and destroyed thereby generating a variable particle population problem.

Consider photons in a unit volume cubical box with perfectly reflecting walls, i.e.,

$$\vec{p}^2 = (\alpha_x^2 + \alpha_y^2 + \alpha_z^2)\ h^2/4$$

or,

$$(h\nu)^2 = c^2(\alpha_x^2 + \alpha_y^2 + \alpha_z^2)\ h^2/4$$

$$E_{\underline{\alpha}} = h\nu_{\underline{\alpha}} = \tfrac{1}{2}\alpha hc$$

Bose-Einstein statistics with a variable particle population apply, i.e.,

$$n_{\underline{\alpha}} = 2\ [\exp(h\nu_{\underline{\alpha}}/kT) - 1]^{-1}$$

$$\nu_{\underline{\alpha}} = \tfrac{1}{2}\alpha c$$

Whence,

$$n_1(\alpha) = \frac{\pi\alpha^2}{\exp[h\nu_\alpha/kT] - 1}$$

and

$$n_1(\nu) = n_1[\alpha(\nu)]\ \left|\frac{d\alpha}{d\nu}\right|$$

$$= \frac{8\pi\nu^2/c^3}{e^{h\nu/kT} - 1}$$

The photon energy density is

$$\int_0^\infty h\nu n_1(\nu)\ d\nu = \frac{8\pi^5(kT)^4}{15c^3h^3}$$

and the photon energy current per unit area is

$$\int_0^\infty h\nu \tfrac{1}{4} n_1(\nu)\ c\,d\nu = \frac{2\pi^5(kT)^4}{15c^2h^3}$$

A "black body" is an object which absorbs all incident radiant energy. Consider a black body placed in the box containing photons. When at equilibrium with the radiation in the box, the black body is at temperature T, and it is emitting radiant energy at the rate of photon energy absorption, i.e., per unit area, the radiation rate is

$$\sigma T^4 \text{ with } = \frac{2\pi^5 k^4}{15 c^2 h^3}$$

which is the Stefan-Boltzmann radiation law and σ is the Stefan constant.

Boltzmann statistics:

Consider a collection of N distinguishable particles in the sense that the labels 1, 2, 3,...,N can be meaningfully assigned to the particles (e.g., the atoms in a solid lattice). A microstate is no longer specified by merely the occupation numbers $\{n_i\}$. Rather, it is now important to specify, in addition, where each labelled particle is in energy space. Presuming integer spin particles, or exclusive volume of occupancy for each particle, there are M_i possible microstate occupancies for each of the N_i particles in the ith macrostate. Whence,

$$w(N_i) = M_i^{N_i}$$

Note that if $W(\{N_i\})$ is taken as $\prod_i w(N_i)$, as used previously, then the interchange of labelled particles between different macrostates is not counted as yielding separate and distinct particle occupation complexions. Consider a macrostate occupation complexion $\{N_i\}$ to be represented by a series of integers (the labelled particles) and commas (the separation between macrostate energy levels), e.g.,

1 2 3 4 , 5 6 , 7 8 9 , , 10 11 ,

For this case, $N_1 = 4$, with particles 1,2,3,4, $N_2 = 2$, with particles 5,6, $N_3 = 3$, with particles 7,8,9, $N_4 = 0$ . . . There are N! permutations of the integers,

however, permutations of the integers within a macrostate has already been included in $w(N_i)$. Thus, there are

$$\frac{N!}{\prod_i N_i!}$$

meaningful permutations of labelled particles with a given macrostate occupation complexion $\{N_i\}$, and

$$W(\{N_i\}) = \frac{N!}{\prod_i N_i!} \prod_i w(N_i)$$

i.e.,

$$W(\{N_i\}) = N! \prod_i \frac{M_i^{N_i}}{N_i!}$$

Maximizing $\ell nW(\{N_i\})$ subject to the restraints $\sum_i N_i = N$ and $\sum_i N_i E_i = N\bar{E}$ yields

$$\frac{N_i}{M_i} = \exp[\gamma - \beta E_i]$$

and

$$n_i = \exp[\gamma - \beta E_i]$$

Identifying $\beta = 1/kT$ and using $\sum_i n_i = N$ gives the Boltzmann (quantum statistics) distribution

$$n_i = N \frac{\exp[-E_i/kT]}{\sum_i \exp[-E_i/kT]}$$

Energy-Dependent Transport Relations

As mentioned in the first paragraph of this section of these lecture notes, the E-dependence of particle distributions can be included in the formulation of the Boltzmann transport equation. So far in these notes, the derivations of relations describing particle transport were restricted to the presumption of monoenergetic radiation (pages 3-7 through 3-11). However, the arguments presented in the derivation of the monoenergetic equation (page 3-10) are easily extended to the E-dependent case with the changes

$$v \rightarrow v(E)$$

$$\Phi(\underline{r},\hat{\Omega},t) \rightarrow \Phi(\underline{r},\hat{\Omega},E,t)$$

$$s(\underline{r}\,\hat{\Omega},t) \rightarrow s(\underline{r},\hat{\Omega},E,t)$$

$$c\int_{4\pi} d^2\Omega' f(\hat{\Omega}' \rightarrow \hat{\Omega}) \rightarrow \int_{4\pi}\int_{0}^{\infty} d^2\Omega' dE' f(\hat{\Omega}',E' \rightarrow \hat{\Omega},E)$$

The emission distribution, f, has been redefined such that

> $f(\hat{\Omega}',E' \rightarrow \hat{\Omega},E)d^2\Omega dE$ = the expected number of particles emitted in the increment $d^2\Omega dE$ about $(\hat{\Omega},E)$ due to a collision involving a particle with pre-collision variables $(\hat{\Omega}',E')$. Note that the total number of particles emitted per collision (c) in the mono-energetic version is now included in the requirements for f such that f is no longer normalized as a probability distribution.

In these terms, the E-dependent Boltzmann transport equation is

$$\frac{1}{v(E)}\frac{\partial}{\partial t}\Phi(\underline{r},\hat{\Omega},E,t) = -\hat{\Omega}\cdot\nabla\Phi(\underline{r},\hat{\Omega},E,t) - \Sigma_t(\underline{r},E,t)\Phi(\underline{r},\hat{\Omega},E,t)$$
$$+\int_{4\pi}\int_{0}^{\infty}\Sigma_t(\underline{r},E',t)f(\underline{r},t;\hat{\Omega}',E' \rightarrow \hat{\Omega},E)\Phi(\underline{r},\hat{\Omega}',E',t)d^2\hat{\Omega}'dE' + s(\underline{r},\hat{\Omega},E,t)$$

The solution complications introduced by describing the actual energy exchanges, which do, in fact, take place in most situations of interest, are certainly extensive. We shall approach the resolution of the E-dependent equation in a manner similar to that used for the monoenergetic relation, i.e., with simplifying presumptions which yield relatively easy to express notation and algebra.

A conservation relation (the E-spectral equation):

Consider the operation $\int d^2\Omega$ applied to the E-dependent transport equation. Term-by-term the results are

$$\int \frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(\underline{r},\hat{\Omega},E,t)d^2\Omega = \frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(\underline{r},E,t)$$

$$\int \hat{\Omega}\cdot\nabla\Phi(\underline{r},\hat{\Omega},E,t)d^2\Omega = \nabla\cdot\underline{J}(\underline{r},E,t)$$

$$\int \Sigma_t(\underline{r},E,t)\Phi(\underline{r},\hat{\Omega},E,t)d^2\Omega = \Sigma_t(\underline{r},E,t)\Phi(\underline{r},E,t)$$

$$\int_{4\pi}\int_{4\pi}\int_0^\infty \Sigma_t(\underline{r},E',t)f(\underline{r},t;\hat{\Omega}',E' \rightarrow \hat{\Omega},E)\Phi(\underline{r},\hat{\Omega}',E',t)d^2\Omega d^2\Omega' dE'$$

$$= \int_0^\infty \Sigma_t(\underline{r},E;,t)f(\underline{r},t;E' \rightarrow E)\Phi(\underline{r},E',t)dE'$$

$$\int s(\underline{r},\hat{\Omega},E,t)d^2\Omega = s(\underline{r},E,t)$$

where,

$\Phi(\underline{r},E,t) = \int \Phi(\underline{r},\hat{\Omega},E,t)d^2\Omega$ = the angular-integrated radiation flux at $(\underline{r},E,t)$ which is also termed the flux E-spectrum at $(\underline{r},t)$,

$\underline{J}(\underline{r},E,t) = \int \hat{\Omega}\Phi(\underline{r},\hat{\Omega},E,t)d^2\Omega$ = the radiation current vector for particles of energy E at $(\underline{r},t)$,

$f(E' \to E) = \int f(\hat{\Omega}', E' \to \hat{\Omega}, E) d^2\Omega$ = the collision transfer of energy description which has been presumed to be Ω'-independent,

$s(\underline{r}, E, t) = \int s(\underline{r}, \hat{\Omega}, E) d^2\Omega$ = the angular-integrated radiation source density.

Whence, the E-spectral equation

$$\frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(\underline{r}, E, t) = - \nabla \cdot \underline{J}(\underline{r}, E, t) - \Sigma_t(\underline{r}, E, t) \Phi(\underline{r}, E, t)$$

$$+ \int_0^\infty \Sigma_t(\underline{r}, E', t) f(\underline{r}, t, E' \to E) \Phi(\underline{r}, E', t) dE' + s(\underline{r}, E, t)$$

Thermodynamic equilibrium spectrum--

In the derivation of the classical equilibrium particle distribution (page 4-1), "equilibrium" was defined by the restrictions:

1) Steady state, i.e, t-independent

2) Uniformity, i.e., $\underline{r}$-independence

3) Isotropic motion, i.e., $\hat{\Omega}$-independence.

To these we here add the presumptions of:

4) No radiation absorption, i.e., $\Sigma_a = 0$, or $\Sigma_t = \Sigma_s$

5) No radiation sources, i.e., $s = 0$.

The E-spectral equation becomes a relation describing thermodynamic equilibrium, i.e.,

$$\Sigma_s(E) \Phi(E) = \int_0^\infty \Sigma_s(E') f(E' \to E) \Phi(E') dE'$$

With reference to page 4-7 of these notes, we already have a solution of this equation, viz.

$$\Phi(E) = AEe^{-E/kT}$$

This should seem intriguing since we have not as yet specified $\Sigma_s(E)$ and $f(E' \rightarrow E)$. The puzzle is understood by considering as a trial property for $\Phi(E)$

$$\Sigma_s(E')f(E' \rightarrow E)\Phi(E') = \Sigma_s(E)f(E \rightarrow E')\Phi(E)$$

This reciprocity (or symmetry) relation is termed the "principle of detailed balance." Its physical significance will be addressed in a moment. Here, note that substitution into the spectral equation yields

$$\Sigma_s(E)\Phi(E) = \Sigma_s(E)\Phi(E) \int_0^\infty f(E \rightarrow E')dE'$$

Moreover, since the only allowed interaction is scattering, each collision results in the emission of a single particle, viz.

$$\int_0^\infty f(E \rightarrow E')dE' = 1$$

for this case. Thus, the principle of detailed balance is an acceptable property for the solution to possess. In fact, it is a required property.

The physical meaning of the principle of detailed balance is easily illuminated by considering

$$[\Sigma_s(E')\Phi(E')dE'][f(E' \rightarrow E)dE]$$

$$= [\Sigma_s(E)\Phi(E)dE][f(E \rightarrow E')dE']$$

which is obtained directly from the definition of the principle. The left-hand-side of the relation is a specification of the transfer rate of radiation from increment dE' at E' to dE at E. The right-hand-side is the transfer rate from dE at E to dE'at E'. The principle is thus a statement that in a thermodynamic equilibrium state each energy increment has a balance

of energy transfered to and received from each other energy increment. In this equilibrium state, the particles and targets must be distributed in energy such that the principle of detailed balance is maintained. This is, indeed, a property which the product $\Sigma_s(E')f(E' \rightarrow E)$ satisfies in the multi-scattering process which establishes the particle and target E-spectrums.

It is important to realize that all the presumptions are required to yield a thermodynamic equilibrium condition. The particle moderation problem (considered next) is a good example of a situation where the equation to be resolved appears to be the equilibrium condition but results are clearly very different.

Moderation spectrum--

A particle moderation problem is defined to be such that

$$f(E' \rightarrow E) = 0 \text{ for } E > E'$$

i.e., particles must lose energy in a collision. In order to achieve a steady state situation is a moderation problem, it is required to have radiation sources at some energy (usually high E) and radiation absorption at some energy (usually low E). To be specific, and to emphasize the comment made at the end of the discussion on equilibrium, consider the moderation case where all radiation sources have energy greater than E_0 and all radiation absorption occurs at energies below E_1 with $E_1 < E_0$. The E-spectral equation for a steady state, uniform, isotropic motion problem is identical to the thermodynamic equilibrium equation--with one important exception, i.e., $E_1 < E < E_0$ is required. Specifically,

$$\Sigma_s(E)\Phi(E) = \int_E^\infty \Sigma_s(E')f(E' \rightarrow E)\Phi(E')dE'$$

$$\text{for } E_1 < E < E_0$$

where the lower limit of the integral reflects the moderation restriction applied to f.

The moderation of fission neutrons by protons is a basic process in many thermal (spectrum) nuclear reactors. In this case $E_0 > 100$ Kev and $E_1 < 1$ ev. The scattering interactions are elastic with isotropic emission in the collision center-of-mass coordinate system. These kinematic and emission distribution conditions yield

$$f(E' \to E) = \frac{1}{E'}, \quad \text{for } 0 < E < E'$$

and the required $f(E' \to E) = 0$ for $E > E'$. The moderation spectral equation becomes

$$\Sigma_s(E)\Phi(E) = \int_E^\infty \Sigma_s(E') \frac{1}{E'} \Phi(E')dE'$$

$$\text{for } E_1 < E < E_0$$

which has the solution $\Phi(E) = A/E\Sigma_s(E)$ for E in the restricted range. This is not a classical equilibrium distribution and the principle of detailed balance is certainly not followed for $E_1 < E < E_0$ (since only moderation occurs). The equilibrium restriction of no sources or absorptions was relaxed and the solution is non-equilibrium.

Plane symmetry problems:

In order to pursue more non-equilibrium radiation transport problems and maintain a reasonably simple notation and algebra, consider restriction to plane symmetry problems in homogeneous, steady state media. The transport equation is

$$\frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(x,\mu,E,t) = -\mu \frac{\partial}{\partial x} \Phi(x,\mu,E,t) - \Sigma_t(E)\Phi(x,\mu,E,t)$$

$$+ \int_{4\pi} \int_0^\infty \Sigma_t(E') f(\hat{\Omega}', E' \to \hat{\Omega}, E) \Phi(x,\mu',E',t) d^2\Omega' dE' + s(x,\mu,E,t)$$

wherein the integral term must clearly be reducible to a form which does not involve the direction components ϕ or ϕ'. An often encountered case which leads directly to such a reduction is

$$f(\hat{\Omega}',E' \rightarrow \hat{\Omega},E) = f(\hat{\Omega}'\cdot\hat{\Omega},E' \rightarrow E)$$

i.e., the case of azimuthally symmetric emission (about the pre-collision direction, $\hat{\Omega}'$). Employing the usual form of Legendre polynomial expansion, i.e.,

$$f(\Omega'\cdot\Omega,E' \rightarrow E) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} f_\ell(E' \rightarrow E)P_\ell(\hat{\Omega}'\cdot\hat{\Omega})$$

and the spherical harmonics addition theorem, i.e.,

$$P_\ell(\hat{\Omega}'\cdot\hat{\Omega}) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{-\ell} Y_{\ell m}(\mu',\phi')Y_{\ell m}{}^*(\mu,\phi)$$

it is not difficult to show that

$$\int_{4\pi} \int_0^{\infty} \Sigma_t(E')f(\hat{\Omega}'\cdot\hat{\Omega},E' \rightarrow E)\Phi(x,\mu',E',t)d^2\Omega'dE'$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \int_0^{\infty} dE'\Sigma_t(E')f_\ell(E' \rightarrow E) \int_{-1}^{+1} P_\ell(\mu')\Phi(x,\mu',E',t)d\mu'$$

which demonstrates (for the case of emission azimuthal symmetry) the expected elimination of the ϕ and ϕ' variables.

The E-dependent, plane symmetry transport equation can thus be expressed as

$$\frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(x,\mu,E,t) = -\mu\frac{\partial}{\partial x} \Phi(x,\mu,E,t) - \Sigma_t(E)\Phi(x,\mu,E,t)$$

$$+ \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \int_0^{\infty} dE'\Sigma_t(E')f_\ell(E' \rightarrow E) \int_{-1}^{+1} P_\ell(\mu')\Phi(x,\mu',E',t)d\mu'$$

$$+ s(x,\mu,E,t)$$

and, the orthogonality of the Legendre polynomials can be employed to yield the E-spectral equation

$$\frac{1}{v(E)} \frac{\partial}{\partial t} \Phi(x,E,t) = - \frac{\partial}{\partial x} J_x(x,E,t) - \Sigma_t(E)\Phi(x,E,t)$$

$$+ \int_0^\infty \Sigma_t(E')f_0(E' \to E)\Phi(x,E',t)dE' + s(x,E,t)$$

It should be noted that the definition

$$f(E' \to E) = \int f(\hat{\Omega}',E' \to \hat{\Omega},E)d^2\Omega$$

used in previous discussions of the E-spectral equation, and the Legendre polynomial expansion of the emission distribution yield the identification

$$f_0(E' \to E) = f(E' \to E)$$

Whence, the principle of detailed balance takes the form

$$\Sigma_s(E')f_0(E' \to E)\Phi(E') = \Sigma_s(E)f_0(E \to E')\Phi(E)$$

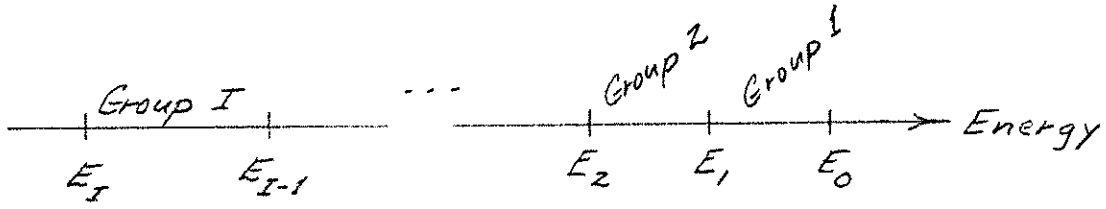
These comments are included to indicate the particular physical significance of the emission expansion coefficient $f_0(E' \to E)$.

Multigroup transport formulation:

For the purpose of introducing the E-multigroup method of reducing the transport equation to more easily resolved terms, consider the E-spectral equation for a plane symmetry, steady state, uniform radiation problem, i.e.,

$$\Sigma_t(E)\Phi(E) = \int_0^\infty \Sigma_t(E')f_0(E' \to E)\Phi(E')dE' + s(E)$$

Divide the energy range of interest into I contiguous intervals indexed as illustrated and define



$$\Phi_i = \int_{E_i}^{E_{i-1}} \Phi(E)dE \text{ for } i = 1,2,\ldots, I$$

The radiation with energy in the interval E_i to E_{i-1} is termed group i radiation, and Φ_i is termed the group i radiation flux.

The operation $\int_{E_i}^{E_{i-1}} dE$ applied to the spectral equation yields

$$\Sigma_{ti}\Phi_i = \int_0^{E_o} \Sigma_0(E' \to i)\Phi(E')dE' + s_i$$

where,

$$\Sigma_{ti} = \frac{1}{\Phi_i} \int_{E_i}^{E_{i-1}} \Sigma_t(E)\Phi(E)dE$$

is the group i total cross section (a flux-weighted average over the group energy interval),

$$\Sigma_0(E' \to i) = \Sigma_t(E') \int_{E_i}^{E_{i-1}} f_0(E' \to E)dE$$

is the cross section for transfer (by radiation interaction caused emission) from energy E' to energy group i, and

$$s_i = \int_{E_i}^{E_{i-1}} s(E)dE$$

is the radiation source emitted in group i. To use consistent dependent variables, the integral term in the group spectral equation should be reexpressed

according to

$$\int_0^{E_o} \Sigma_o(E' \to i)\Phi(E')dE' = \sum_{j=1}^{I} \Sigma_o(j \to i)\Phi_j$$

where the group-to-group transfer cross section, $\Sigma_o(j \to i)$, is defined by

$$\Sigma_o(j \to i) = \frac{1}{\Phi_j} \int_{E_j}^{E_{j-1}} \Sigma_o(E' \to i)\Phi(E')dE'$$

Note that these definitions are such that $\Sigma_o(j \to i)\Phi_j$ is the transfer rate density of radiation with energy in group j to radiation with energy in group i due to interactions (not sources).

If the group i radiation "removal" cross section is defined by $\Sigma_{ri} = \Sigma_{ti} - \Sigma_o(i \to i)$, the usual form of the group spectral equation is obtained, i.e.,

$$\Sigma_{ri}\Phi_i = \sum_{j \neq i}^{I} \Sigma_o(j \to i)\Phi_j + s_i$$

$$\text{for } i = 1,2,\ldots,I$$

This relation could be used to study E-spectrum problems and properties. Note, for example, that the group equivalent of the principle of detailed balance is

$$\Sigma_o(j \to i)\Phi_j = \Sigma_o(i \to j)\Phi_i$$

if scattering is the only mode of radiation energy transfer and $\{\Phi_i\}$ is the thermodynamic equilibrium group spectrum. In these notes the derivation of the group spectral equation is intended to merely be an introduction to the derivation and use of the more-complicated group transport equation.

Multigroup transport equation--

Consider the E-dependent transport euqation for a plane symmetry, steady state problem, i.e.,

$$\mu \frac{\partial}{\partial x} \Phi(x,\mu,E) + \Sigma_t(E)\Phi(x,\mu,E)$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \int_0^\infty dE' \Sigma_t(E') f_\ell(E' \to E) \int_{-1}^{+1} P_\ell(\mu')\Phi(x,\mu',E')d\mu'$$

$$+ s(x,\mu,E)$$

Applying the operation $\int_{E_i}^{E_{i-1}} dE$, and the definitions of variables and parameters used in the discussion of the multigroup spectral equation, yields the E-multigroup transport equation, i.e.,

$$\mu \frac{\partial}{\partial x} \Phi_i(x,\mu) + \Sigma_{ti} \Phi_i(x,\mu)$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \sum_{j=1}^{I} \Sigma_\ell(j \to i) \int_{-1}^{+1} P_\ell(\mu')\Phi_j(x,\mu')d\mu' + s_i(x,\mu)$$

where, direct extension of the definition of $\Sigma_o(j \to i)$ is employed in the definition

$$\Sigma_\ell(j \to i) = \frac{1}{\Phi_j} \int_{E_j}^{E_{j-1}} dE' \Phi(E') \Sigma_t(E') \int_{E_i}^{E_{i-1}} f_\ell(E' \to E) dE$$

The example of isotropic emission (i.e., $\Sigma_\ell(j \to i) = \Sigma_o(j \to i)\delta_{\ell o}$) is somewhat academic since usually emission direction is correlated with energy exchange (through the kinematics relations). However, because of the resulting simplifications in algebraic manipulations, the isotropic emission case will be the example chosen (in these notes) for further amplification.

If post-collision radiation emission is isotropic, the multigroup transport equation reduces to the form

$$\mu \frac{\partial}{\partial x} \Phi_i(x,\mu) + \Sigma_{ti} \Phi_i(x,\mu) = \frac{1}{2} \sum_{j=1}^{I} \Sigma_0(j\to i) \int_{-1}^{+1} \Phi_j(x,\mu')d\mu' + s_i(x,\mu)$$

$$\text{for } i = 1,2,\ldots,I$$

The structure of each member of this set of I equations is identical to that of the monoenergetic transport equation. The set is, however, coupled through the energy transfer term by the group transfer cross sections $\Sigma_0(j\to i)$, and the monoenergetic flux, $\Phi(x,\mu)$, is replaced by an "I-dimension vector" flux form $\{\Phi_i(x,\mu);\ i = 1,2,\ldots,I\}$.

In order to illustrate how the solution approaches, which were applied to the monoenergetic equation, can be directly extended to solution of the multigroup equation set, we shall here consider details of the P_N-approximation method.

Solution by a P_N-approximation--

Following the P_N-approximation procedure as applied to the solution of the monoenergetic radiation transport equation, employ the expression

$$\Phi_i(x,\mu) = \sum_{n=0}^{N} \frac{2n+1}{4\pi} \Phi_{i,n}(x)\ P_n(\mu)$$

in the I-group equation set, the relevant Legendre polynomial recurrence relation, and the linear independence of the Legendre polynomials to obtain

$$n \frac{d}{dx} \Phi_{i,n-1}(x) + (n+1) \frac{d}{dx} \Phi_{i,n+1}(x) + (2n+1) \Sigma_{ti} \Phi_{i,n}(x)$$

$$= \sum_{j=1}^{I} \Sigma_0(j\to i) \Phi_{j,n}(x) \delta_{no} + (2n+1) s_{i,n}(x)$$

$$\text{for } n = 0,1,2\ldots,N \text{ and } i = 1,2,\ldots,I$$

In the coupled set of (N+1)I linear, first-order differential equations $s_{i,n}(x)$ is defined by a Legendre polynomial expansion of the source in group i in a manner identical to the flux expansion coefficients, $\Phi_{i,n}(x)$ and in equations indexed with n = N, $\Phi_{i,N+1}(x)$ is set equal to zero.

It is useful to reexpress the set of equations as

$$\frac{d}{dx}\ \Phi_{i,1}(x) + \Sigma_{ri}\Phi_{i,0}(x) - \sum_{j=1}^{I} \Sigma_0(j\to i)\Phi_{j,0}(x) = s_{i,0}(x)$$

and, for n > 0,

$$n\,\frac{d}{dx}\,\Phi_{i,n-1}(x) + (n+1)\,\frac{d}{dx}\,\Phi_{i,n+1}(x) + (2n+1)\Sigma_{ti}\,\Phi_{i,n}(x) = {}^{(2n+1)}s_{i,n}(x)$$

The collision-induced radiation transfer-into-group-i term appears only in the n = 0 equations because of the presumption of isotropic emission.

In order to continue this comparison of the E-multigroup solution approach and the monoenergetic technique, consider the homogeneous (s = 0) form of the transport equation with the purpose of determining eigenvalues and eigenfunctions. With the $s_{i,n}(x) = 0$ the equation set is translationally invariant with respect to x suggesting solutions of the form

$$\Phi_{i,n}(x) = \Psi_{i,n}(\ell)e^{-x/\ell}$$

The transport equation set becomes

$$\Psi_{i,1}(\ell) - \ell\Sigma_{ri}\ \Psi_{i,0}(\ell) + \sum_{j\neq i}^{I} \ell\Sigma_0(j\to i)\Psi_{j,0}(\ell) = 0$$

and, for n > 0,

$$n\ \Psi_{i,n-1}(\ell) + (n+1)\Psi_{i,n+1}(\ell) - (2n+1)\,\ell\Sigma_{ti}\ \Psi_{i,n}(\ell) = 0$$

for i = 1,2,...,I and n = 0,1,2,...,N with $\Psi_{i,N+1}(\ell) = 0$ in the n = N equation.

An example; two-group, diffusion analysis--

The example of I = 2 and N = 1 yields a two-group, P_1-approximation which is the simplest version of an energy-dependent diffusion approximation. For this example there are four equations in the four unknowns $\Psi_{10}(\ell)$, $\Psi_{11}(\ell)$, $\Psi_{20}(\ell)$ and $\Psi_{21}(\ell)$. They are

$$\Psi_{11}(\ell) - \Sigma_{r1}\Psi_{10}(\ell) + \Sigma_0(2\to1)\Psi_{20}(\ell) = 0$$

$$\Psi_{10}(\ell) - 3\ell\Sigma_{t1}\Psi_{11}(\ell) = 0$$

$$\Psi_{21}(\ell) - \ell\Sigma_{r2}\Psi_{20}(\ell) + \ell\Sigma_0(1\to2)\Psi_{10}(\ell) = 0$$

$$\Psi_{20}(\ell) - 3\ell\Sigma_{t2}\Psi_{21}(\ell) = 0$$

Note that the second and fourth equations constitute the two-group version of Fick's Law of Diffusion. Non-trivial solution of the $\Psi_{i,n}(\ell)$ implies the secular equation which can be manipulated to the form

$$[\Sigma_{r1}\Sigma_{r2} - \Sigma_0(1\to2)\Sigma_0(2\to1)]\ell^4 - [D_1\Sigma_{r2} + D_2\Sigma_{r1}]\ell^2 + D_1D_2 = 0$$

where $D_1 = 1/3\Sigma_{t1}$ and $D_2 = 1/3\Sigma_{t2}$ are the respective diffusion coefficients for group 1 and group 2 radiation. Whence, the four eigenvalues $\ell = \pm L_+$ and $\ell = \pm L_-$ where

$$L_\pm = \frac{D_1\Sigma_{r2} + D_2\Sigma_{r1}}{2[\Sigma_{r1}\Sigma_{r2} - \Sigma_0(1\to2)\Sigma_0(2\to1)]} \left\{ 1 \pm \left[1 - \frac{4D_1D_2[\Sigma_{r1}\Sigma_{r2} - \Sigma_0(1\to2)\Sigma_0(2\to1)]}{[D_1\Sigma_{r2} + D_2\Sigma_{r1}]^2} \right]^{1/2} \right\}$$

If either $\Sigma_0(1\to2) = 0$ or $\Sigma_0(2\to1) = 0$, then it is more direct to rewrite the secular equation which can then be reduced to the form

$$(\Sigma_{r1}\ell^2 - D_1)(\Sigma_{r2}\ell^2 - D_2) = 0$$

Whence, in these cases, the four eigenvalues

$$\ell = \pm L_1 \text{ and } \ell = \pm L_2$$

where

$$L_1 = + \left[\frac{D_1}{\Sigma_{r1}}\right]^{1/2} \text{ and } L_2 = + \left[\frac{D_2}{\Sigma_{r2}}\right]^{1/2}$$

are the respective "unclupled" diffusion lengths for group 1 and group 2 radiation (and should not be confused with the same notation used for asymptotic eigenvalues in monoenergetic P_N-approximations, N = 1 and N = 2).

Eigenfunctions and general solution forms vary significantly in expression and physical interpretation according to the group transfer cross sections. There are three cases and they are described here on an individual basis.

Case 1: $\Sigma_0(1\to2) = \Sigma_0(2\to1) = 0$.

In this case the two energy groups are totally uncoupled and radiation transport is described by two monoenergetic relations. General flux solutions can be expressed as

$$\Phi_1(x,\mu) = A_1\left[1 + 3\frac{\Psi_{11}(+L_1)}{\Psi_{10}(+L_1)}\mu\right]e^{-x/L_1} + C_1\left[1 + 3\frac{\Psi_{11}(-L_1)}{\Psi_{10}(-L_1)}\mu\right]e^{+x/L_1}$$

$$\Phi_2(x,\mu) = A_2\left[1 + 3\frac{\Psi_{21}(+L_2)}{\Psi_{20}(+L_2)}\mu\right]e^{-x/L_2} + C_2\left[1 + 3\frac{\Psi_{21}(-L_2)}{\Psi_{20}(-L_2)}\mu\right]e^{+x/L_2}$$

The eigenfunction ratios follow from the individual group expressions for Fick's Law, i.e.,

$$\frac{\Psi_{11}(\pm L_1)}{\Psi_{10}(\pm L_1)} = \pm \frac{1}{3L_1\Sigma_{t1}} \quad \text{and} \quad \frac{\Psi_{21}(\pm L_2)}{\Psi_{20}(\pm L_2)} = \pm \frac{1}{3L_2\Sigma_{t2}}$$

There is little need to further discuss the meaning of these solutions since they represent merely the superposition of two independent monoenergetic problems and thereby introduce no new physical concepts when compared to our previous monoenergetic radiation transport discussions.

Case 2: $\Sigma_0(1\to2) \neq 0$ and $\Sigma_0(2\to1) \neq 0$.

The opposite extreme relative to case 1, this case has complete coupling of the two radiation groups, i.e., transfer up in energy and transfer down in energy. General flux solutions take on the more complicated form

$$\begin{aligned}
\Phi_1(x,\mu) &= A_{1+} + \left[1 + 3\frac{\Psi_{11}(+L_+)}{\Psi_{10}(+L_+)}\mu\right]e^{-x/L_+} \\
&\quad + C_{1+}\left[1 + 3\frac{\Psi_{11}(-L_+)}{\Psi_{10}(-L_+)}\mu\right]e^{+x/L_+} \\
&\quad + A_{1-}\left[1 + 3\frac{\Psi_{11}(+L_-)}{\Psi_{10}(+L_-)}\mu\right]e^{-x/L_-} \\
&\quad + C_{1-}\left[1 + 3\frac{\Psi_{11}(-L_-)}{\Psi_{10}(-L_-)}\mu\right]e^{+x/L_-} \\
\Phi_2(x,\mu) &= A_{2+}\left[1 + 3\frac{\Psi_{21}(+L_+)}{\Psi_{20}(+L_+)}\mu\right]e^{-x/L_+} \\
&\quad + C_{2+}\left[1 + 3\frac{\Psi_{21}(-L_+)}{\Psi_{20}(-L_+)}\mu\right]e^{-x/L_+} \\
&\quad + A_{2-}\left[1 + 3\frac{\Psi_{21}(+L_-)}{\Psi_{20}(+L_-)}\mu\right]e^{-x/L_-} \\
&\quad + C_{2-}\left[1 + 3\frac{\psi_{21}(-L_-)}{\psi_{20}(-L_-)}\mu\right]e^{+x/L_-}
\end{aligned}$$

As in case 1, the relevant eigenfunction ratios are determined by using the two-group form of Fick's Law, viz.

$$\frac{\Psi_{11}(\pm L_+)}{\Psi_{10}(\pm L_+)} = \pm \frac{1}{3L_+\Sigma_{t1}} \quad \text{and} \quad \frac{\Psi_{11}(L_-)}{\Psi_{10}(L_-)} = \pm \frac{1}{3L_-\Sigma_{t1}}$$

$$\frac{\Psi_{21}(\pm L_+)}{\Psi_{20}(\pm L_+)} = \pm \frac{1}{3L_+\Sigma_{t2}} \quad \text{and} \quad \frac{\Psi_{21}(\pm L_-)}{\Psi_{20}(\pm L_-)} = \pm \frac{1}{3L_-\Sigma_{t2}}$$

Each energy group experiences influence from the other group (through the two nonzero transfer cross sections). Thus, the eigenvalues and eigenfunction ratios all carry parameter descriptions from both groups. There are no solutions which are strictly monoenergetic in character.

It appears that there are too many arbitrary coefficients in the general solution form (A_{1+}, C_{1+}, A_{1-}, C_{1-}, A_{2+}, C_{2+}, A_{2-}, C_{2-}). In analogy with monoenergetic diffusion results we expect two coefficients for each group allowing the satisfaction of two boundary conditions for each group. This yields a total of four coefficients rather than the apparent eight. However, substitution of the general solution form in the i = 1, n = 0 equation and in the i = 2, n = 0 equation gives relations between A_{1+} and A_{2+}, C_{1+} and C_{2+}, A_{1-} and A_{2-}, and C_{1-} and C_{2-}. Thus, there are actually available only the expected four arbitrary coefficients to meet boundary condition requirements for both groups.

Case 3: $\Sigma_0(1\to2) \neq 0$ but $\Sigma_0(2\to1) = 0$, or $\Sigma_0(2\to1) \neq 0$ but $\Sigma_0(1\to2) = 0$.

The two possibilities lead to the same character of solution. Here, consider the usual relevant case of $\Sigma_0(1\to2) \neq 0$ but $\Sigma_0(2\to1) = 0$. In this case, the i = 1 equations do not depend on the i = 2 solutions, but the i = 2 equations do depend on the i = 1 solutions. As in case 1, the eigenvalues are L_1 and L_2. General solutions take on the form

$$\Phi_1(x,\mu) = A_1\left[1 + 3\frac{\Psi_{11}(+L_1)}{\Psi_{10}(+L_1)}\mu\right]e^{-x/L_1}$$

$$+ C_1\left[1 + 3\frac{\Psi_{11}(-L_1)}{\Psi_{10}(-L_1)}\mu\right]e^{+x/L_1}$$

$$\Phi_2(x,\mu) = A_{22}\left[1 + 3\frac{\Psi_{21}(+L_2)}{\Psi_{20}(+L_2)}\mu\right]e^{-x/L_2}$$

$$+ C_{22}\left[1 + 3\frac{\Psi_{21}(-L_2)}{\Psi_{20}(-L_2)}\mu\right]e^{+x/L_2}$$

$$+ A_{21}\left[1 + 3\frac{\Psi_{21}(+L_1)}{\Psi_{20}(+L_1)}\mu\right]e^{-x/L_1}$$

$$+ C_{21}\left[1 + 3\frac{\Psi_{21}(-L_1)}{\Psi_{20}(-L_1)}\mu\right]e^{+x/L_1}$$

The relevant eigenfunction ratios are again found by using the two-group Fick's Law.

The group 1 radiation flux is independent of the group 2 flux (since $\Sigma_0(2\to1) = 0$) and thus the solution form is the expected monoenergetic form with parameters descriptive of group 1 alone. The group 2 flux is dependent on the group 1 flux (since $\Sigma_0(1\to2) \neq 0$) and thus the solution form is not monoenergetic in form and parameters descriptive of both groups appear.

As in case 2, it appears that there are too many arbitrary coefficients (A_1, C_1, A_{22}, C_{22}, A_{21}, C_{21}). In order to satisfy boundary conditions we again expect only four coefficients. In this case, substitution of the general solution form in the i = 2, n = 0 equation yields relations between A_1 and A_{21}, and C_1 and C_{21}. Thus, again there are actually available only the expected four coefficients to meet boundary condition requirements for both groups.

ABSTRACT

The mathematical formulation of a new approach to the homogenization of certain types of heterogeneous media (such as a regular array of holes in a scattering media) for the purpose of neutron diffusion calculations is developed in this Report. The new method is based on the inclusion of an angular-dependent mean free path in the theory of neutron transport. In the present effort, calculations are restricted to media with plane symmetry and monoenergetic neutron theory is employed.

It is found that a neutron-flux based theory and a collision-density based theory can lead to significantly different results when low-order approximations, such as diffusion theory, are employed in the solution of the transport equation. For the case of isotropic scattering, the normal mode technique is found applicable and closed-form, exact solutions are determined.

There is little existing experimental work in the description of neutron distribution in such anisotropic media. It is therefore difficult to evaluate the results of the new theory. The interpretation of physical and numerical (Monte Carlo) experiments could be approached directly with the new techniques.

I. INTRODUCTION

This Report develops the mathematical formulation of a new method of treating neutron diffusion in certain types of heterogeneous media. The heterogeneity of immediate concern, and toward which this work is directed, is that of a regular array of vacuum channels (such as a square lattice of cylindrical holes) in an otherwise homogeneous medium. The general procedure; with modification of details, should be applicable to other types of heterogeneity. However, a requirement which should be imposed is that the heterogeneity results in two characteristic directions. For example, in the case of a regular array of vacuum channels, the two characteristic directions are parallel and perpendicular to the channel axis.

Probably the most important considerations of neutron diffusion in media with holes are those of Behrens (Ref. 1). However, all previous work, including that in Ref. 1, is devoted to the determination of the effects of heterogeneity on specific parameters relevant to neutron diffusion, rather than to a formulation of a general method from which various descriptions of the neutron distribution can be determined. The general problem may be stated along these lines: in media with heterogeneity, such as the type considered here, it is clear that a "simple homogenization" of the medium for neutron diffusion calculations is not a valid representation. A simple homogenization is defined as the process of reducing the medium cross sections

merely by the ratio of material volume to material-plus-vacuum volume. The streaming of neutrons in the vacuum channels leads to a spreading of the neutrons in the longitudinal direction (parallel to channel axis) which is larger than that in the transverse direction (perpendicular to channel axis). Thus, not only is the simple homogenization questionable for omnidirectional parameter calculation, but also the anisotropic effects are completely subdued. Of course, the reason for considering homogenization of the medium is the existence of an "arsenal" of possible mathematical attacks for such problems.

The new approach to homogenization, which will be developed here, is based on the reasoning that neutrons traveling with a large component of their velocity in the longitudinal direction probably travel further between collisions, on the average, than those traveling with a large component of velocity in the transverse direction. Let this effect be introduced into the neutron transport equation for the homogenized medium by allowing the mean free path to be angular-dependent. Clearly, by so doing, a mathematical fiction will be utilized since the mean free path, as used in neutron transport calculations, is a local parameter. This concept is certainly no more confusing than the idea of medium homogenization. It should be stressed that a total cross section which varies according to the direction of neutron travel, and not merely the usual scattering directional dependence, is being imposed.

All considerations will be based on the idealization of monoenergetic neutron transport. Although time-dependent equations will be developed, most of the analysis will be devoted to the calculation of stationary states. For the purpose of completeness, the mathematical formulation will be developed along several lines. Specifically: both the neutron flux and collison density will be considered as dependent variables; the familiar P_N and double-P_N approximations, as well as the moment decomposition will be applied; and it will be demonstrated that, for the case of isotropic scattering, the normal mode procedure, recently used for the solution of several types of neutron transport problems, is applicable and yields exact, closed-form solutions.

The major part of this work is directed toward the mathematical formulation and physical interpretation of the new theory. A section, however, will be devoted to brief remarks relevant to application. There is meager experimental data available for lattices of the type considered. It will therefore be difficult to evaluate the present theory. These considerations will yield a well-defined, albeit not well-substantiated, route to solution of problems involving neutron diffusion in media pierced by vacuum channels.

II. MATHEMATICAL FORMULATION

It would seem that application of these ideas to finite media dictates the use of non-separable position-angle-dependent mean free paths. The inclusion of position-dependence leads to gross difficulties which we have as yet not resolved. It will be assumed that the mean free path in the homogenized medium depends only on the angle between the neutron velocity and the direction of the position variable. In all calculations plane symmetry is assumed, with the position variable either along the longitudinal or transverse direction.

A. The Neutron-Flux Equation

The monoenergetic neutron transport equation for homogeneous media with plane symmetry may be written as

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(x,\mu,t)+\mu\frac{\partial}{\partial x}\psi(x,\mu,t)+\sigma(\mu)\psi(x,\mu,t)$$

$$=c\int\sigma(\mu')f(\Omega\cdot\Omega')\psi(x,\mu',t)\,d\Omega'+S(x,\mu,t) \qquad (1)$$

where $\psi(x, \mu, t)$ is the neutron flux distribution as a function of position x, direction cosine of neutron travel relative to x-direction μ, and time t; v is neutron speed; $\sigma(\mu)$ is the angular-dependent total cross section; c is the mean number of secondary neutrons which emanate from a neutron–nucleus collision; $f(\Omega \cdot \Omega')$ is the normalized distribution in Ω, the neutron post-collision direction of travel, of secondary neutrons produced by collision of a primary neutron with pre-collision direction Ω'; and $S(x, \mu, t)$ is the rate of neutron introduction from sources which are independent of the neutron distribution. Although c and f are not necessarily descriptive of a non-multiplying medium, the terms scattering probability for c and scattering distribution for f will be used to avoid stilted discourse. An expansion of the scattering distribution in terms of Legendre polynomials $\{P_n(\Omega \cdot \Omega')\}$ will be employed, i.e.,

$$f(\Omega \cdot \Omega') = \sum_n \frac{2n+1}{4\pi} f_n P_n(\Omega \cdot \Omega') \tag{2}$$

and the spherical harmonics addition theorem (Ref. 2, p. 143) to eliminate the azimuthal direction dependence appearing in the integral in Eq. (1). The result is

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(x, \mu, t) + \mu\frac{\partial}{\partial x}\psi(x, \mu, t) + \sigma(\mu)\psi(x, \mu, t) = \frac{c}{2}\sum_n (2n+1) f_n P_n(\mu) \int_{-1}^{+1} P_n(\mu')\sigma(\mu')\psi(x, \mu', t)\, d\mu' + S(x, \mu, t) \tag{3}$$

In order to proceed with a general discussion of the properties of Eq. (3) a more specific representation of $\sigma(\mu)$ is required. It is supposed, with little loss in relevant generality, that

$$\sigma(\mu) = \sum_n \sigma_n P_n(\mu) \tag{4}$$

The sets $\{\psi_n(x, t)\}$ and $\{S_n(x, t)\}$ are further defined by

$$\psi_n(x, t) = \int_{-1}^{+1} P_n(\mu)\psi(x, \mu, t)\, d\mu \tag{5a}$$

$$S_n(x, t) = \int_{-1}^{+1} P_n(\mu) S(x, \mu, t)\, d\mu \tag{5b}$$

Equations (5a and b) specify the respective expansion coefficients in Legendre polynomial expansions of the neutron flux and source density, e.g.

$$\psi(x, \mu, t) = \sum_n \frac{2n+1}{2}\psi_n(x, t) P_n(\mu) \tag{6}$$

In these terms, integration of Eq. (3) over the interval $\mu \in (-1, +1)$ yields the relation

$$\frac{1}{v}\frac{\partial \psi_0}{\partial t} + \frac{\partial \psi_1}{\partial x} + (1 - c)\sum_n \sigma_n \psi_n = S_0 \tag{7}$$

Eq. (7) is the continuity equation for neutron motion. The only term which appears in an unfamiliar form is that which expresses the total neutron interaction rate. Clearly,

$$\sum_n \sigma_n \psi_n(x, t) = \int_{-1}^{+1} \sigma(\mu)\psi(x, \mu, t)\, d\mu \tag{8}$$

A further, familiar, reduction of the transport equation can be made in terms of the sets $\{\psi_n\}$, $\{S_n\}$, and $\{\sigma_n\}$. Using the recurrence relation for Legendre polynomials (Ref. 2, p. 32),

$$(2n+1)\mu P_n(\mu) = n P_{n-1}(\mu) + (n+1) P_{n+1}(\mu) \tag{9}$$

yields the set of coupled differential equations

$$\frac{1}{v}\frac{\partial}{\partial t}\psi_n(x, t) + \frac{n}{2n+1}\frac{\partial}{\partial x}\psi_{n-1}(x, t) + \frac{n+1}{2n+1}\frac{\partial}{\partial x}\psi_{n+1}(x, t) + \sum_{l, m}(2l+1)\sigma_m A_{lmn}(1 - cf_n)\psi_l(x, t) = S_n(x, t) \tag{10}$$

The set $\{A_{lmn}\}$ is defined by

$$A_{lmn} = \frac{1}{2}\int_{-1}^{+1} P_l(\mu) P_m(\mu) P_n(\mu)\, d\mu \tag{11}$$

and has the following properties (Ref. 2, p. 87):

1. The order of the indices is unimportant.
2. $A_{lmn} = 0$ if the sum of any two of the indices is less than the third.
3. $A_{lmn} = 0$ if $l + m + n$ is odd.
4. When $A_{lmn} \neq 0$, i.e., avoiding (2) and (3),

$$A_{lmn} = \left(\frac{1}{l+m+n+1}\right)\left(\frac{(1)(3)\cdots(l+m-n-1)}{(2)(4)\cdots(l+m-n)}\right) \times \left(\frac{(1)(3)\cdots(l+n-m-1)}{(2)(4)\cdots(l+n-m)}\right) \times \left(\frac{(1)(3)\cdots(n+m-l-1)}{(2)(4)\cdots(n+m-l)}\right) \times \left(\frac{(2)(4)\cdots(l+m+n)}{(1)(3)\cdots(l+m+n-1)}\right) \tag{12}$$

It is from Eq. (10) that the various approximations to the transport equation are derived. Before proceeding with detailed examination of some approximations, re-examine Eq. (3). A simpler integral term is obtained if the dependent variable is changed to the neutron collision density

$$F(x, \mu, t) = \sigma(\mu)\,\psi(x, \mu, t).$$

B. The Collision-Density Equation

Reformulating Eq. (3) in terms of the collision density, $F(x, \mu, t)$, and the mean free path, $\lambda(\mu) = 1/\sigma(\mu)$,

$$\frac{\lambda(\mu)}{v}\frac{\partial}{\partial t}F(x, \mu, t) + \mu\lambda(\mu)\frac{\partial}{\partial x}F(x, \mu, t) + F(x, \mu, t) = \frac{c}{2}\sum_n (2n+1) f_n P_n(\mu) \times \int_{-1}^{+1} P_n(\mu')\,F(x, \mu', t)\,d\mu' + S(x, \mu, t) \tag{13}$$

With the sets $\{F_n(x, t)\}$ and $\{\lambda_n\}$ defined by

$$F(x, \mu, t) = \sum_n \frac{2n+1}{2} F_n(x, t)\,P_n(\mu) \tag{14a}$$

$$\lambda(\mu) = \sum_n \lambda_n P_n(\mu) \tag{14b}$$

the set of coupled differential equations [cf., Eq. (10)] is obtained,

$$\sum_{l,m} (2l+1) A_{lmn}\frac{\lambda_m}{v}\frac{\partial}{\partial t}F_l(x, t) + \frac{n}{2n+1}\sum_{l,m} (2l+1) A_{lm,\,n-1}\lambda_m \frac{\partial}{\partial x}F_l(x, t) + \frac{n+1}{2n+1}\sum_{l,m} (2l+1) A_{lm,\,n+1}\lambda_m \frac{\partial}{\partial x}F_l(x, t) + (1 - cf_n) F_n(x, t) = S_n(x, t) \tag{15}$$

Note that if $\lambda_n = 0$ for $n > 0$, i.e., the familiar case of an angle-independent mean free path, then Eq. (15), with the aid of the properties of $\{A_{lmn}\}$, reduces to

$$\frac{\lambda_0}{v}\frac{\partial F_n}{\partial t} + \frac{n\lambda_0}{2n+1}\frac{\partial F_{n-1}}{\partial t} + \frac{(n+1)\lambda_0}{2n+1}\frac{\partial F_{n+1}}{\partial t} + (1 - cf_n) F_n = S_n \tag{16}$$

which is the expected result. Note further that the $n = 0$ member of Eq. (15) yields the continuity equation

$$\sum_m \lambda_m \frac{\partial F_m}{\partial t} + \sum_{l,m} (2l+1)\lambda_m A_{lm1}\frac{\partial F_l}{\partial x} + (1 - c) F_0 = S_0 \tag{17}$$

In recognizing Eq. (17) as the continuity equation, use is made of the easily derived relations

$$\psi_0(x, t) = \sum_n \lambda_n F_n(x, t) \tag{18a}$$

$$\psi_1(x, t) = \sum_{m,n} (2n+1)\lambda_m A_{nm1} F_n(x, t) \tag{18b}$$

In the remainder of this work the case of a stationary state is assumed. In most cases this assumption merely leads to simpler algebra and notation and is actually not a requirement for the determination of a solution. The P_N-approximation and double-P_N-approximation, as applied to both flux and collision density expansions, will be discussed and the moment decomposition for both flux and collision density will be considered. Finally, in greater depth, the case of isotropic scattering using the collision density as dependent variable will be covered.

C. The P_N-Approximation

The P_N-approximation based on a flux expansion, or collision density expansion, is defined by the requirements that in Eq. (10), or Eq. (15), $\psi_n(x) = 0$ for $n > N$, or $F_n(x) = 0$ for $n > N$, and the equations labelled by $n > N$ are discarded. Thus, in a P_N-approximation, $N + 1$ coupled differential equations are obtained with the $N + 1$ dependent variables $\psi_n(x)$, $n = 0, 1, \cdots, N$, or $F_n(x)$, $n = 0, 1, \cdots, N$. For example, the P_0-approximation based on the flux expansion gives the single relation

$$\sigma_0(1 - c)\,\psi_0(x) = 0 \tag{19}$$

which has the implication $c = 1$ for non-trivial ψ_0. This is a familiar result. The P_0-approximation based on a collision density expansion gives the unusual relation

$$\frac{\lambda_1}{3}\frac{dF_0}{dx} + (1 - c) F_0(x) = 0 \tag{20}$$

After this present brief comment considerations will be restricted to the case of $\lambda(\mu)$ a symmetric function of μ on the interval $\mu \in (-1, +1)$, and, in that case $\lambda_1 = 0$. For the moment, suppose that $\lambda_1 \neq 0$. To be specific, suppose that $\lambda_1 > 0$. According to Eq. (20), the implication is that

$dF_0/dx < 0$ which indicates a neutron flow in the $+x$-direction. The question which must be posed is: can F be μ-independent (consistent with P_0-approximation) and yet have $\psi(x, \mu)$ represent a neutron flow in $+x$-direction (i.e., ψ increase with μ)? Clearly the answer is in the affirmative since, if $\lambda(\mu)$ increases with μ (implied by $\lambda_1 > 0$), then the ratio ψ/λ can be μ-independent if ψ also increases with μ. In all following considerations assume that $\lambda(\mu)$, and thus $\sigma(\mu)$, is a symmetric function of μ. Thus it will always be required that $\lambda_n = 0$, and $\sigma_n = 0$, for n odd.

The P_1-approximation (i.e., diffusion theory) based on a flux expansion gives the two equations

$$\frac{d\psi_1}{dx} + (1 - c)\,\sigma_0\psi_0(x) = S_0(x) \tag{21a}$$

$$\frac{1}{3}\frac{d\psi_0}{dx} + (1 - cf_1)\left(\sigma_0 + \frac{2}{5}\sigma_2\right)\psi_1(x) = S_1(x) \tag{21b}$$

If it is further assumed that all neutron sources are isotropic such that $S_n(x) = 0$ for $n > 0$, then Eqs. (21a and b) combine to give the usual diffusion theory relations

$$-D\frac{d^2\psi_0}{dx^2} + \sigma'\psi_0(x) = S_0(x) \tag{22a}$$

$$\psi_1(x) = -D\frac{d\psi_0}{dx} \tag{22b}$$

with diffusion coefficient D, and "absorption" cross section σ', given by

$$D = \frac{1}{3(1 - cf_1)\left(\sigma_0 + \frac{2\sigma_2}{5}\right)} \tag{23a}$$

$$\sigma' = (1 - c)\,\sigma_0 \tag{23b}$$

It should be noted that only σ_0 and σ_2 enter into the diffusion theory parameters. The $\sigma(\mu)$ expansion was not truncated at a quadratic in order to obtain Eqs. (23a and b). In passing, it is also worth noting, had time-dependence been included, that the P_1-approximation would have given the "telegraphist's equation." The added assumption that $\partial\psi_1/v\partial t << \partial\psi_0/\partial x$ results in the form of the familiar time-dependent diffusion theory with D and σ' again given by Eqs. (23a and b).

The P_1-approximation based on a collision density expansion gives the two equations

$$\left(\lambda_0 + \frac{2}{5}\lambda_2\right)\frac{dF_1}{dx} + (1 - c)\,F_0(x) = S_0(x) \tag{24a}$$

$$\frac{1}{3}\left(\lambda_0 + \frac{2}{5}\lambda_2\right)\frac{dF_0}{dx} + (1 - cf_1)\,F_1(x) = S_1(x) \tag{24b}$$

In the case of isotropic sources, Eqs. (24a and b) combine to give

$$-D'\frac{d^2F_0}{dx^2} + (1 - c)\,F_0(x) = S_0(x) \tag{25a}$$

$$F_1(x) = -\frac{D'}{\left(\lambda_0 + \frac{2\lambda_2}{5}\right)}\frac{dF_0}{dx} \tag{25b}$$

where the "diffusion coefficient" is

$$D' = \frac{\left(\lambda_0 + \frac{2\lambda_2}{5}\right)^2}{3(1 - cf_1)} \tag{26}$$

As is the case in the flux-based diffusion theory, a quadratic truncation of $\lambda(\mu)$ is not necessary to obtain the results given in Eqs. (25 and 26).

The usual result of exponential spatial decline away from sources in infinite media is found for flux and collision density. The "period" of the exponential, the diffusion length L, is given by

$$L_\psi^2 = \frac{1}{3\sigma_0(1 - c)(1 - cf_1)\left(\sigma_0 + \frac{2\sigma_2}{5}\right)} \tag{27}$$

based on a flux expansion, and

$$L_F^2 = \frac{\left(\lambda_0 + \frac{2\lambda_2}{5}\right)^2}{3(1 - c)(1 - cf_1)} \tag{28}$$

based on a collision density expansion. The dissimilar results obtained from a P_0-approximation based on flux and collision density expansions have been pointed out. The divergence of results for the P_1-approximation can be illustrated by considering the ratio L_ψ/L_F for a given problem. Suppose that $\lambda(\mu)$ is actually an even quadratic, i.e., $\lambda_n = 0$ for $n = 1$ and $n > 2$. The corresponding

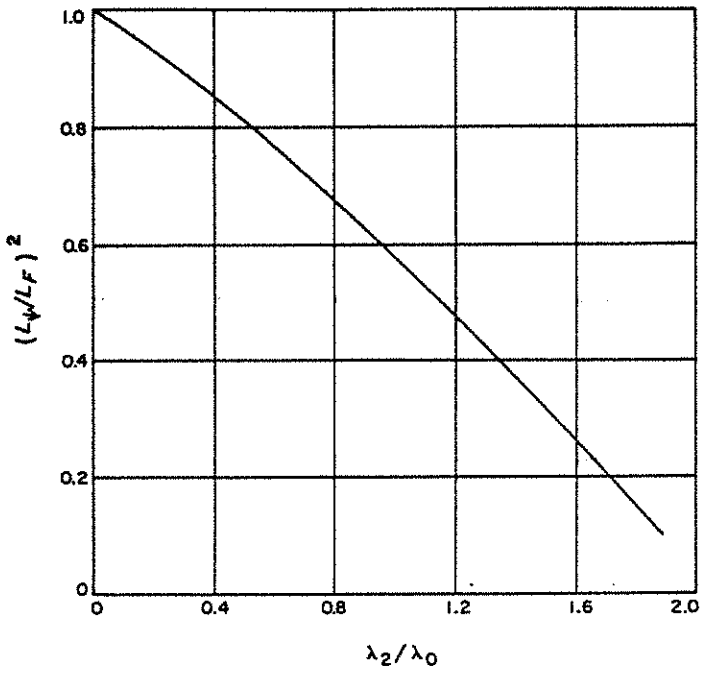


Fig. 1. The ratio of diffusion lengths as calculated by a neutron flux based and collision density based P_1-approximation for the case of an even quadratic mean free path, $\lambda(\mu) = \lambda_0 + \lambda_2 P_2(\mu)$

$\sigma(\mu)$ is not a quadratic, but only σ_0 and σ_2 need be computed since these coefficients determine L_ψ. In Fig. 1 the results are displayed for the range $\lambda_2/\lambda_0 \in (0, 2)$. Clearly, the flux and collision density based expansions can lead to significantly different results.

It should be expected that the two diffusion theories give different results. Note that whereas the ψ-approximation yields an accurate representation for neutron current $\psi_1(x)$ but an inaccurate (truncated) representation for collision density, the F-approximation results in an accurate representation for total interaction rate $F_0(x)$ but an inaccurate representation for current. For several reasons it will seem that the collision density expansion is favored in this work. However, these reasons are mainly of an algebraic character and it should not be construed that the F-formulation is, in all cases, superior.

Approximations of higher order than P_1 are accomplished following the usual general prescriptions. The added complications due to the angular-dependence of the mean free path place no restrictions on the formalism. Higher order approximations lessen the differences exhibited by the ψ and F-formulations.

D. The Double-P_N-Approximation

The double-P_N-approximation is derived from Yvon's method whereby the angular-dependence of the neutron flux, or collision density, is decomposed into contributions from $+x$-directed and from $-x$-directed neutrons. In order to simplify notation, let us consider the case of a stationary state in a medium characterized by isotropic scattering. The plane symmetry, monoenergetic neutron transport equation, Eq. (3), is then

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \sigma(\mu)\psi(x,\mu) = \frac{c}{2} \times \int_{-1}^{+1} \sigma(\mu')\psi(x,\mu')\,d\mu' + S(x,\mu) \tag{29}$$

Use the half-angle-range expansions

$$\psi(x,\mu) = \sum_n (2n+1)\,\psi_n^+(x)\,P_n(2\mu-1), \mu > 0 \tag{30a}$$

$$= \sum_n (2n+1)\,\psi_n^-(x)\,P_n(2\mu+1), \mu < 0 \tag{30b}$$

$$S(x,\mu) = \sum_n (2n+1)\,S_n^+(x)\,P_n(2\mu-1), \mu > 0 \tag{30c}$$

$$= \sum_n (2n+1)\,S_n^-(x)\,P_n(2\mu+1), \mu < 0 \tag{30d}$$

$$\sigma(\mu) = \sum_n \sigma_n^+ P_n(2\mu-1), \mu > 0 \tag{30e}$$

$$= \sum_n \sigma_n^- P_n(2\mu+1), \mu < 0 \tag{30f}$$

to obtain the set of coupled differential equations

$$\frac{n}{2n+1}\frac{d\psi_{n-1}^\pm}{dx} + \frac{n+1}{2n+1}\frac{d\psi_{n+1}^\pm}{dx} \pm \frac{d\psi_n^\pm}{dx} + 2\sum_{l,m}(2l+1)\,A_{lmn}\,\sigma_m^\pm\,\psi_l^\pm = c\delta_{no}\sum_l(\sigma_l^-\psi_l^- + \sigma_l^+\psi_l^+) + 2S_n^\pm \tag{31}$$

The double-P_N-approximation is defined by the requirement $\psi_n^\pm(x) = 0$ for $n > N$ and the equations labelled by $n > N$ are discarded.

The same analysis is followed for the collision density based approximation. Thus, with the definitions

$$F(x,\mu) = \sum_n (2n+1)\, F_n^+(x)\, P_n(2\mu - 1), \mu > 0 \tag{32a}$$

$$= \sum_n (2n+1)\, F_n^-(x)\, P_n(2\mu + 1), \mu < 0 \tag{32b}$$

$$\lambda(\mu) = \sum_n \lambda_n^+ P_n(2\mu - 1), \mu > 0 \tag{32c}$$

$$= \sum_n \lambda_n^- P_n(2\mu + 1), \mu < 0^- \tag{32a}$$

the transport equation is obtained in the form

$$\frac{n}{2n+1} \sum_{l,m} (2l+1)\, \lambda_m^{\pm} A_{lm,n-1} \frac{dF_l^{\mp}}{dx} + \frac{n+1}{2n+1} \sum_{l,m} (2l+1)\, \lambda_m^{\pm} A_{m,n+1} \frac{dF_l^{\mp}}{dx} \pm \sum_{l,m} (2l+1)\, \lambda_m^{\pm} A_{lmn} \frac{dF_l^{\mp}}{dx} + 2F_n^{\pm} = c\delta_{n_0}(F_0^+ + F_0^-) + 2S_n^{\pm} \tag{33}$$

The collision density double-P_N-approximation is defined as in the ψ-formulation.

In addition to the usefulness of Yvon's method in the solution of problems where accurate representation of source or free boundaries are required, there is an added flexibility for the angular-dependence of the mean free path. Thus, $\lambda(\mu)$ may have one form for $\mu > 0$ determined by the set $\{\lambda_n^+\}$, or $\{\sigma_n^+\}$, and another form for $\mu < 0$ following the set $\{\lambda_n^-\}$, or $\{\sigma_n^-\}$. For example, by using these methods a symmetric $\lambda(\mu)$ which varies linearly with μ for $\mu > 0$ and $\mu < 0$ can be expressed by using only two terms in each $\lambda(\mu)$ expansion, i.e., set $\lambda_0^+ = \lambda_0^-, \lambda_1^+ = -\lambda_1^-$, and $\lambda_n^{\pm} = 0$ for n > 1.

E. A Moment Decomposition

In the usual theory of neutron transport through homogeneous media, it is well-know that any space-angle moment of the neutron distribution can be found even though the distribution itself is unknown. In fact, an important method of determining the neutron distribution is the construction of a likely flux shape from a finite set of moments. Let us now consider a moment decomposition for the case of an angular-dependent mean free path where, as in our previous considerations, two formulations will be examined, i.e., with ψ and F as dependent variable.

We define the neutron flux and source moments by

$$\psi_n^j = \int_{-\infty}^{+\infty} x^j \psi_n(x)\, dx \tag{34a}$$

$$S_n^j = \int_{-\infty}^{+\infty} x^j S_n(x)\, dx \tag{34b}$$

Assume that the medium is of infinite extent. Multiplication of the stationary state form of Eq. (10) by x^j and integration over $x \epsilon (-\infty, +\infty)$ yields the set of algebraic moment relations

$$\sum_{l,m} (2l+1)\, \sigma_m A_{lmn}(1 - cf_n)\, \psi_l^j = S_n^j + \frac{j}{2n+1} \times \left[n\psi_{n-1}^{j-1} + (n+1)\, \psi_{n+1}^{j-1} \right] \tag{35}$$

With the collision density moments similarly defined, i.e.,

$$F_n^j = \int_{-\infty}^{+\infty} x^j F_n(x)\, dx \tag{36}$$

and performing similar operations on the stationary state form of Eq. (15), the result is a set of algebraic equations relating the collision density moments, i.e.,

$$(1 - cf_n)\, F_n^j = S_n^j + \frac{jn}{2n+1} \sum_{l,m} (2l+1)\, \lambda_m A_{lm,n-1}\, F_l^{j-1} + \frac{j(n+1)}{2n+1} \sum_{l,m} (2l+1)\, \lambda_m A_{lm,n+1}\, F_l^{j-1} \tag{37}$$

The moments of the neutron distribution resulting from a unit, plane, isotropic source (at $x = 0$) are easily interpretable in terms of important macroscopic parameters. For this source, $S_n^j = \delta_{n0}\delta_{j0}$. Consider calculation of flux moments first and then contrast this result with the method applied to collision density moments. For the sake of definiteness, assume that $\sigma(\mu)$ is an even M degree polynomial in μ. With $\sigma(\mu)$ an even function, it is clear that $\psi_n^j = 0$ for $j + n$ odd. An examination of Eq. (35), using the properties of the set $\{A_{lmn}\}$, indicates that with $M \neq 0$ and $n + j$ even, ψ_n^j depends on $\psi_{n-1}^{j-1}, \psi_{n+1}^{j-1}, \psi_{|n-M|}^j, \psi_{|n-M|+2}^j, \cdots, \psi_{n+M-2}^j, \psi_{n+M}^j$. Thus, ψ_n^j can not be determined without employing a truncation on the set $\{\psi_n(x)\}$. This is, of course, the simplification used in a P_N-approximation and would not yield exact moments. The familiar case of $M = 0$ poses no such difficulties and one can readily find the exact moments.

In considering the collision density moments, assume that $\lambda(\mu)$ is an even M degree polynomial in μ. It follows that $F_n^j = 0$ for $n + j$ odd. It is also possible to show, from Eq. (37) and the properties of $\{A_{lmn}\}$, that $F_n^j = 0$ for $n > j(M+1)$ and therefore, with finite M, any collision density moment can be calculated exactly. For example, for the case of $M = 2$

$$\langle x^2 \rangle = \frac{F_0^2}{F_0^0} = 2L_P^2 + \frac{18}{175}\frac{\lambda_2^2}{(1-c)(1-cf_3)} \tag{38}$$

where $\langle x^2 \rangle$ is the mean value of x^2 and L_P is the diffusion length as calculated by a collision density based P_1-approximation. Note that the result of Eq. (38) is unlike that found in the angle-independent mean free path case. In that case $M = 0$ and the second spatial moment is given correctly by diffusion theory, i.e., $\langle x^2 \rangle = 2L^2$ both in the exact calculation and in diffusion theory.

In passing, note that the set $\{\psi_n^j\}$ can be found from the set $\{F_n^j\}$ via the easily derived relation

$$\psi_n^j = \sum_{l,m} (2l+1)\lambda_m A_{lmn} F_l^j \tag{39}$$

The result of Eq. (39) does not contradict the earlier assertion regarding the problem of finding the flux moments. When the determination of the $\{\psi_n^j\}$ is approached directly by Eq. (35), it is the total cross section which is considered to be an M-degree polynomial in μ. When $\{\psi_n^j\}$ is found using $\{F_n^j\}$ as in Eq. (39), the mean free path is assumed to be an M-degree polynomial in μ.

F. The Case of Isotropic Scattering

The stationary state form of Eq. (13) with the additional assumption of isotropic scattering gives the collision density equation

$$\mu\lambda(\mu)\frac{\partial}{\partial x}F(x,\mu) + F(x,\mu) = \frac{c}{2}\int_{-1}^{+1} F(x,\mu')\,d\mu' + S(x,\mu) \tag{40}$$

In this case of isotropic scattering an angle variable change is suggested. Specifically, define the angle variable $u = \mu\lambda(\mu)/\lambda(1)$, measure x in units of $\lambda(1)$, and change dependent variable to $F(x,u) = g(u)F(x,\mu)$ with $g(u) = |d\mu/du|$. With the source density change $S(x,u) = g(u)S(x,\mu)$, Eq. (40) takes the form

$$u\frac{\partial}{\partial x}F(x,u) + F(x,u) = \frac{c}{2}g(u)\int_{-1}^{+1} F(x,u')\,du' + S(x,u) \tag{41}$$

Various aspects of the solution of Eq. (41) will be considered.

1. Legendre Polynomial Expansion

Following the procedure used in the derivation of Eq. (10), the coupled differential equation form of the transport equation

$$\frac{n}{2n+1}\frac{dF_{n-1}}{dx} + \frac{n+1}{2n+1}\frac{dF_{n+1}}{dx} + F_n(x) = \frac{cg_n}{2n+1}F_0(x) + S_n(x) \tag{42}$$

is obtained where the Legendre polynomial expansions are used:

$$F(x,u) = \sum_n \frac{2n+1}{2} F_n(x) P_n(u) \tag{43a}$$

$$S(x,u) = \sum_n \frac{2n+1}{2} S_n(x) P_n(u) \tag{43b}$$

$$g(u) = \sum_n g_n P_n(u) \tag{43c}$$

It should be noted that the requirement of a symmetric $\lambda(\mu)$ imposes the condition that $g_n = 0$ for n odd.

The idea of a P_N-approximation is equally well-applied here. For example, the P_1-approximation (diffusion theory) takes the usual form [cf., Eq. (25)]

$$-\frac{1}{3}\frac{d^2F_0}{dx^2} + (1 - cg_0)F_0 = S_0 \tag{44a}$$

$$F_1 = -\frac{1}{3}\frac{dF_0}{dx} \tag{44b}$$

where only isotropic sources are allowed.

2. Moment Decomposition

With the collision density and source moments defined in the usual manner [i.e., by Eq. (34)], Eq. (42) can be transformed to the algebraic set

$$F_n^j = S_n^j + \frac{cg_n}{2n+1}F_n^j + \frac{j}{2n+1}\left[nF_{n-1}^{j-1} + (n+1)F_{n+1}^{j-1}\right] \tag{45}$$

It has been assumed that $\lambda(\mu)$ is symmetric which implies that $g(u)$ is symmetric. We also find that $F_n^j = 0$ for

$j + n$ odd, and, for odd n, F_n^j depends only on F_{n-1}^{j-1} and F_{n+1}^{j-1}. Furthermore there is the interesting property that the spatial moment F_0^j depends only on the set of moments $\{F_n^i, n + i \leqq j\}$. Therefore, the calculations of a low-order spatial moment require the specification of a small number of the g_n and the prior determination of a small number of other moments.

As an example, calculate by these methods the second spatial moment of the neutron distribution resulting from a unit, plane, isotropic source (at $x = 0$). In this case $S_n^j = \delta_{n0}\delta_{j0}$. The moments F_0^0 F_2^0, and F_1^1 are easily determined and are the only values required in the calculation of F_0^2. For the normalized second spatial moment [cf., Eq. (38)],

$$\langle x^2 \rangle = \frac{F_0^2}{F_0^0} = \frac{2}{3}\frac{1 + \dfrac{2cg_2}{5}}{1 - cg_0} \tag{46}$$

3. Normal Mode Expansion

The recently developed normal mode technique (Ref. 3) will be applied to the problem of determining the exact and asymptotic solution of Eq. (41). In so doing there is generated an interesting mathematical problem the details of which are considered in Appendix B. Consider the homogeneous form of Eq. (41), i.e., $S = 0$. Translational invariance suggests the "ansatz"

$$F(x, u) = \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) \tag{47}$$

where the separation variable ν is allowed to be complex. The integral equation

$$(\nu - u)\,\phi(\nu, u) = \frac{c}{2}\,\nu\, g(u) \int_{-1}^{+1} \phi(\nu, u')\, du' \tag{48}$$

is thereby obtained. Adopting the usual normalization,

$$\int_{-1}^{+1} \phi(\nu, u)\, du = 1 \tag{49}$$

If solutions of Eq. (48) are allowed to be distributions (in the sense of L. Schwartz, Ref. 4), then

$$\phi(\nu, u) = \frac{c}{2}\frac{\nu g(u)}{\nu - u} + \Lambda(\nu)\,\delta(\nu - u) \tag{50}$$

Assume that $g(u)$ satisfies a Holder condition (Ref. 5, p. 11) on the interval of the real line $u \in (-1, +1)$. Any singular integrals which might appear are then of the Cauchy type and their evaluation is defined as the Cauchy principal value (Ref. 5, p. 26).

The normalization required of $\phi(\nu, u)$, i.e., Eq. (49), leads to a specification of allowed discrete values of ν in the region of the ν-complex-plane excluding the line $(-1, +1)$, and to a specification of the function $\Lambda(\nu)$ for $\nu \in (-1, +1)$. To aid in the analysis of these results, define the Cauchy integral, $G(\nu)$, by

$$G(\nu) = \frac{1}{2\pi i}\int_{-1}^{+1} \frac{g(u)}{u - \nu}\, du \tag{51}$$

With $\nu \notin (-1, +1)$, Eq. (49) gives

$$1 + i\pi c\nu G(\nu) = 0 \tag{52}$$

which has a set of roots which are distinct. With $\nu \in (-1, +1)$, Eq. (49) yields an explicit formula for the function $\Lambda(\nu)$ and no restrictions are placed on allowed values of ν. We find

$$\Lambda(\nu) = 1 + i\pi c\nu G(\nu) \tag{53}$$

Thus, if the definition of $\Lambda(\nu)$ is extended, as expressed in Eq. (53), to the entire ν-plane, the zeroes of $\Lambda(\nu)$ determine the set of allowed distinct values of ν. Since $g(u)$ is symmetric, $G(-\nu) = -G(\nu)$, whence, $\Lambda(\nu)$ is an even function of ν. The zeroes of $\Lambda(\nu)$, therefore, appear in pairs which are labeled $\pm\nu_j$.

A set of functions of the angle variable u indexed by ν, $\{\phi(\nu, u)\}$ have been found. There is a discrete indexed set with $\nu \notin (-1, +1)$ and members characterized by

$$\phi(\pm\nu_j, u) = \frac{c}{2}\frac{\nu_j g(u)}{\nu_j \mp u} \tag{54}$$

and, a continuous indexed set with $\nu \in (-1, +1)$ and of form given by Eq. (50). The function $\Lambda(\nu)$, which appears in $\phi(\nu,u)$ for $\nu \in (-1, +1)$, is given by Eq. (53). Furthermore, the zeroes of $\Lambda(\nu)$ for $\nu \notin (-1, +1)$ establish the set of discrete indices $\{\pm\nu_j\}$.

If we assume that $g(u) \neq 0$ for $u \in (-1, +1)$, Eq. (48), with the normalization of Eq. (49), may be written in the form

$$\left[1 - \frac{u}{\nu}\right]\frac{\phi(\nu, u)}{g(u)} = \frac{c}{2} \tag{55}$$

Multiply Eq. (55) with index ν by $\phi(\nu', u)$ and subtract the result from Eq. (55) with index ν' multiplied by $\phi(\nu, u)$. Employing Eq. (49) and integrating over $u \epsilon (-1, +1)$

$$\left[\frac{1}{\nu} - \frac{1}{\nu'}\right] \int_{-1}^{+1} \frac{u}{g(u)} \phi(\nu, u) \phi(\nu', u)\, du = 0 \qquad (56)$$

There is clearly no degeneracy and thus Eq. (56) may be rewritten as the orthogonality relation

$$\int_{-1}^{+1} \frac{u}{g(u)} \phi(\nu, u) \phi(\nu', u)\, du = 0 \text{ for } \nu \neq \nu' \qquad (57)$$

The nature of the orthogonality relation including the case $\nu = \nu'$ depends on whether ν is a member of the discrete index set or belongs to the continuum. If ν is a discrete index, then

$$\int_{-1}^{+1} \frac{u}{g(u)} \phi(\pm\nu_j, u) \phi(\pm\nu_i, u)\, du = I(\pm\nu_j)\, \delta_{ji} \qquad (58a)$$

$$I(\pm\nu_j) = \frac{c^2}{4} \nu_j^2 \int_{-1}^{+1} \frac{u g(u)}{(\nu_j \pm u)^2}\, du \qquad (58b)$$

If ν belongs to the continuum, then

$$\int_{-1}^{+1} \frac{u}{g(u)} \phi(\nu, u) \phi(\nu', u)\, du = \frac{\nu \Lambda^2(\nu)}{g(\nu)} \delta(\nu - \nu') \qquad (59)$$

It was found that the set of normal modes $\{\phi(\nu, u)\}$ is orthogonal, with weight function $u/g(u)$, on the interval $u \epsilon (-1, +1)$. For the remainder of this section assume that the normal modes are also complete in the space of functions which satisfy a Holder condition on the interval $u \epsilon (-1, +1)$. Appendix B, in measure, substantiates this hypothesis by demonstrating the existence of the modal expansion coefficients. In so doing, the interval of completeness is generalized to include all physically relevant cases.

Assuming that the normal modes form a complete set on the interval $u \epsilon (-1, +1)$, the general solution of Eq. (41) is in the form

$$F(x, u) = \sum_{\nu} a(\nu) \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) \qquad (60)$$

where the summation indicates integration over continuous spectra when applicable. In many problems there are boundary conditions which can be formulated as

$$F(0, u) = \phi(u) = \sum_{\nu} a(\nu) \phi(\nu, u) \text{ for } u \epsilon (-1, +1) \qquad (61)$$

and the orthogonality relations can be used to determine the expansion coefficients, $a(\nu)$. In detail, Eq. (61) is rewritten as

$$\phi(u) = \sum_j a(+\nu_j) \phi(+\nu_j, u) + \sum_j a(-\nu_j) \phi(-\nu_j, u) + \int_{-1}^{+1} a(\nu) \phi(\nu, u)\, d\nu \text{ for } u \epsilon (-1, +1) \qquad (62)$$

Direct application of the discrete index orthogonality relation, Eq. (58), yields the discrete indexed expansion coefficients,

$$a(\pm\nu_j) = \frac{1}{I(\pm\nu_j)} \int_{-1}^{+1} \frac{u}{g(u)} \phi(u) \phi(\pm\nu_j, u)\, du \qquad (63)$$

Using Eq. (57) in Eq. (62) gives the result

$$\int_{-1}^{+1} \frac{u}{g(u)} \phi(u) \phi(\nu, u)\, du = \int_{-1}^{+1} du \frac{u}{g(u)} \phi(\nu, u) \times \int_{-1}^{+1} a(\nu') \phi(\nu', u)\, d\nu' \qquad (64)$$

There appears a doubly singular Cauchy integral and thus the order of integration in Eq. (64) may not be reversed without due caution. The doubly singular term appears as

$$\frac{c^2}{4} \nu \int_{-1}^{+1} du \frac{u g(u)}{\nu - u} \int_{-1}^{+1} \frac{\nu' a(\nu')}{\nu' - u} d\nu'$$

Assume that $a(\nu)$ satisfies a Holder condition for $\nu \epsilon (-1, +1)$ and follow the dictates of the Poincaré-Bertrand formula for inverting the integration order (Ref. 5, p. 57). Then

$$\frac{C^2}{4} \nu \int_{-1}^{+1} du \frac{u g(u)}{\nu - u} \int_{-1}^{+1} \frac{\nu' a(\nu')}{\nu' - u} d\nu' = \pi^2 \frac{c^2}{4} \nu^2 g(\nu) a(\nu) + \frac{c^2}{4} \nu \int_{-1}^{+1} d\nu' \frac{\nu' a(\nu')}{\nu' - u} \int_{-1}^{+1} \frac{u g(u)}{\nu - u} du \qquad (65)$$

Using Eqs. (59) and (65) results in the more useful "orthogonality relation,"

$$\int_{-1}^{+1} du \frac{u}{g(u)} \phi(\nu, u) \int_{-1}^{+1} a(\nu') \phi(\nu', u)\, d\nu' = I(\nu) a(\nu) \text{ for } \nu \epsilon (-1, +1) \qquad (66a)$$

$$I(\nu) = \nu g(\nu) \left[\left(\frac{\Lambda(\nu)}{g(\nu)}\right)^2 + \left(\frac{\pi c \nu}{2}\right)^2\right] \qquad (66b)$$

Now, applying Eq. (66) to the problem of finding the continuum expansion coefficients in Eq. (62),

$$a(\nu) = \frac{1}{I(\nu)} \int_{-1}^{+1} \frac{u}{g(u)} \phi(u)\, \phi(\nu, u)\, du \qquad (67)$$

for $\nu \epsilon (-1, +1)$

G. The Green's Function for the Case of Isotropic Scattering

As a specific example of the use of the relations just developed, consider the problem of finding the infinite medium Green's function for isotropic, plane sources. In this case, the source density, $S(x, u)$, of Eq. (41) represents a unit, plane, isotropic emission of neutrons at a position which is designated $x = 0$, i.e., $S(x, u) = g(u)\,\delta(x)/2$. Integration of Eq. (41) over a vanishing interval about $x = 0$ yields the boundary condition

$$u\,[F(0^+, u) - F(0^-, u)] = \frac{g(u)}{2} \text{ for } u \epsilon (-1, +1) \qquad (68)$$

The additional condition that as $|x| \to \infty$, $F(x, u) \to 0$ is imposed and the solution is expressed in the form

$$F(x, u) = \sum_j a(+\nu_j)\, \phi(+\nu_j, u) \exp\left(\frac{-x}{\nu_j}\right) + \int_0^{+1} a(\nu)\, \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x > 0 \qquad (69a)$$

$$F(x, u) = -\sum_j a(-\nu_j)\, \phi(-\nu_j, u) \exp\left(\frac{x}{\nu_j}\right) - \int_{-1}^{0} a(\nu)\, \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x < 0 \qquad (69b)$$

The source condition, Eq. (68), then takes the form of the general boundary condition, Eq. (62). Specifically

$$\frac{u}{g(u)} \sum_j a(+\nu_j)\, \phi(+\nu_j, u) + \frac{u}{g(u)} \sum_j a(-\nu_j)\, \phi(-\nu_j, u) + \frac{u}{g(u)} \int_{-1}^{+1} a(\nu)\, \phi(\nu, u)\, d\nu = \frac{1}{2} \qquad (70)$$

Whence, employing the normalization expressed by Eq. (49),

$$a(\pm\nu_j) = \frac{1}{2I(\pm\nu_j)} \qquad (71a)$$

$$a(\nu) = \frac{1}{2I(\nu)} \text{ for } \nu \epsilon (-1, +) \qquad (71b)$$

and the solution of the Green's function has been completed.

Some aspects of the Green's function will be examined. For simplicity, assume that there is only one pair of zeroes of $\Lambda(\nu)$, $\pm\nu_0$. A sufficient condition for this property is developed in Appendix A. The Green's function is then given by

$$F(x, u) = \frac{\phi(+\nu_0, u)}{2I(+\nu_0)} \exp\left(\frac{-x}{\nu_0}\right) + \int_0^{+1} \frac{\phi(\nu, u)}{2I(\nu)} \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x > 0 \qquad (72a)$$

$$F(x, u) = -\frac{\phi(-\nu_0, u)}{2I(-\nu_0)} \exp\left(\frac{x}{\nu_0}\right) - \int_{-1}^{0} \frac{\phi(\nu, u)}{2I(\nu)} \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x < 0 \qquad (72b)$$

With the definition

$$\phi_n(\nu) = \int_{-1}^{+1} \phi(\nu, u)\, P_n(u)\, du \qquad (73)$$

and the easily derived symmetry properties,

$$I(-\nu_0) = -I(+\nu_0) \text{ and } I(-\nu) = -I(\nu),$$

the collision density moments for the neutron distribution from a unit, plane, isotropic source, are

$$F_n^j = \frac{j!}{2} [\phi_n(+\nu_0) + (-1)^j \phi_n(-\nu_0)] \frac{\nu_0^{j+1}}{I(+\nu_0)} + \frac{j!}{2} \int_0^{+1} [\phi_n(\nu) + (-1)^j \phi_n(-\nu)] \frac{\nu^{j+1}}{I(\nu)} d\nu \qquad (74)$$

Using Eqs. (9), (43c), (48), and (49), a recurrence relation is obtained for the set $\{\phi_n(\nu)\}$,

$$(2n+1)\,\nu\,\phi_n(\nu) = n\phi_{n-1}(\nu) + (n+1)\,\phi_{n+1}(\nu) + c\nu g_n \tag{75}$$

and the normalization $\phi_0(\nu) = 1$. Note that Eq. (75) implies that $\phi_n(\nu)$ is an even, or odd, polynomial in ν of degree n. Therefore, $\phi_n(-\nu) = (-1)^n\phi_n(+\nu)$, and Eq. (74) reduces to

$$F_n^j = j!\left[\frac{\nu_0^{j+1}}{I(+\nu_0)}\phi_n(+\nu_0) + \int_0^{+1}\frac{\nu^{j+1}}{I(\nu)}\,\phi_n(\nu)\,d\nu\right] \qquad \text{if } j+n \text{ is even} \tag{76a}$$

$$F_n^j = 0 \qquad \text{if } j+n \text{ is odd} \tag{76b}$$

Already considered is the moments set $\{F_n^j\}$. For this particular case the $\{F_n^j\}$ is determined from Eq. (45) and the source condition $S_n^j = \delta_{n0}\delta_{j0}$. In passing, note that the consistency of Eq. (45) and (76) is easily demonstrated via the recurrence relation Eq. (75). Moreover, equating the F_0^0 and F_0^2 moments as derived by the two relations gives

$$\frac{\nu_0}{I(+\nu_0)} + \int_0^{+1}\frac{\nu}{I(\nu)}\,d\nu = \frac{1}{1-cg_0} \tag{77a}$$

$$\frac{\nu_0^3}{I(+\nu_0)} + \int_0^{+1}\frac{\nu^3}{I(\nu)}\,d\nu = \frac{1}{3}\,\frac{1+\dfrac{2cg_2}{5}}{(1-cg_0)^2} \tag{77b}$$

From Eqs. (77a and b) an explicit expression for the discrete index ν_0 is obtained:

$$\nu_0^2 = \frac{\dfrac{1}{3}\,\dfrac{\left(1+\dfrac{2cg_2}{5}\right)}{(1-cg_0)^2} - \displaystyle\int_0^{+1}\frac{\nu^3}{I(\nu)}\,d\nu}{\dfrac{1}{1-cg_0} - \displaystyle\int_0^{+1}\frac{\nu}{I(\nu)}\,d\nu} \tag{78}$$

For $c < 1$, ν_0 is real and is interpreted as the exact asymptotic diffusion length [here, measured in units of $\lambda(1)$]. It should be noted that the integral terms in Eq. (78) depend on c and $\{g_n\}$ via the dependence of $I(\nu)$ on these parameters [cf., Eq. (66b)].

III. REMARKS REGARDING APPLICATION OF THE THEORY

A limited number of considerations relevant to the application of the theory presented in Section II will be developed as a brief illustration of possible methods of application of the present theory to physical problems. Many interesting calculations are possible, and with the accomplishment of experimental measurements of neutron distributions in the types of media under discussion, many comparisons of theoretical and experimental results would be profitable.

Methods of determining the proper variation of mean free path are certainly required if these mathematical formulations are to be applied to physical problems. In this section the general types of heterogeneity, toward which the current theory applies, will be discussed. A simple method will be detailed, using known diffusion lengths, to specify the angular dependence of the mean free path for a particular type of heterogeneity.

A. Types of Heterogeneity

The motivation of the present effort, as mentioned earlier, is the establishment of a method of homogenization of regular arrays of vacuum channels for the purpose of neutron diffusion calculations. Also imposed was the necessary restriction that, in general, the type of heterogeneity considered should yield two characteristic orthogonal directions. As an example of the caution which must be exercised in application of the theory, consider a type of heterogeneity which, at first approach, appears to satisfy the necessary requirements, but which actually is unsuitable for these methods. Specifically, examine the case of a periodic slab array of scatterer and vacuum. This heterogeneity exhibits two characteristic orthogonal directions; perpendicular to slab, and the directions in the plane of the slab. Moreover, the direction perpendicular to the slabs (transverse to slab "channels") yields considerations which are algebraically easily accomplished.

If $\lambda(\mu, x)$ represents the mean distance traveled to a collision by a neutron located at a position x to the left of the right-hand-face of a slab of scatterer, traveling with direction cosine μ relative to the slab perpendicular direction, gives

$$\lambda(\mu, x) = \lambda_s + \frac{\frac{T_v}{\mu}\exp\left(\frac{-x}{\lambda_s \mu}\right)}{1 - \exp\left(\frac{-T_s}{\lambda_s \mu}\right)} \quad \text{for } x \leqq T_s, \mu > 0 \tag{79}$$

In Eq. (79), λ_s is the mean free path in the scatterer material which has slab thickness T_s, and T_v is the vacuum slab thickness. For the homogenized medium we require a function $\lambda(\mu)$ which, it would seem, should be a "suitable" average of $\lambda(\mu, x)$. For the case of isotropic scattering, the average

$$\lambda(\mu) = \frac{\int_0^{T_s} \lambda(\mu, x)\, \psi_0(x)\, dx}{\int_0^{T_s} \psi_0(x)\, dx} \tag{80}$$

is clearly indicated. In Eq. (80), $\psi_0(x)$ represents the actual angular integrated neutron flux. Note that, in the present case, $\psi_0(x)$ can be found. Far from neutron sources there is $\psi_0(x) \to \exp(x/L_s)$ where L_s is the "asymptotic" diffusion length in the scatterer material. A note in passing: if $T_s/L_s << 1$, then $\psi_0(x)$ is approximately constant and Eq. (80) gives the result

$$\lambda(\mu) = \lambda_s\left(1 + \frac{T_v}{T_s}\right) \tag{81}$$

which is the "simply homogenized" parameter. Of course, the condition $T_s/L_s << 1$ should yield the homogeneous limit.

If x now represents the direction perpendicular to the slabs we have the asymptotic result $\psi_0(x) \to \exp(-x/L_s)$ when the position x falls in a scatterer slab and $\psi_0(x)$ is a constant when x falls in a vacuum slab. The "best fit" to this flux, for the homogenized medium is $\psi_0(x) \to \exp(-x/L)$ where L is the simply homogenized diffusion length, i.e., $L = L_s(1 + T_v/T_s)$. This result would be obtained if Eq. (81) were used. In this particular case, the situation is that a calculation based on an angular-dependent mean free path yields results less representative than the simply homogenized calculation. It is expected that, in the orthogonal characteristic direction (i.e., in the plane of the slab), use of an angular-dependent mean free path is indicated.

The case of a calculation in the slab perpendicular direction for a periodic slab array is certainly excluded from the present considerations. Moreover, no motivation should be felt toward developing a theory for that case since it is easily treated by a standard method, i.e., change of position variable to "optical thickness." Consider now the details of a macroscopic-parameter-based calculation for a heterogeneity for which the present methods were clearly intended, i.e., a regular array of cylindrical vacuum channels.

B. Cylindrical Channels in a Regular Array

Consider a regular array of vacuum channels of cylindrical cross section. With every vacuum channel of cross sectional area A_v a cross sectional area of scatterer material A_s is associated such that $V = A_v/A_s$ is the ratio of vacuum volume to scatterer volume characteristic of the medium. Label the axial, or longitudinal, direction with x and direction cosine μ, and the radial, or transverse direction with y and direction cosine η. Due to streaming along channels, different diffusion properties in the x- and y-directions are expected with both of these cases being different than the simply homogenized diffusion. The simply homogenized mean free path is given by

$$\lambda_h = \lambda_s(1 + V) \tag{82}$$

Before presenting a specific method for obtaining a representative $\lambda(\mu)$, some general comments will be made regarding the features of such a calculation. It is clear that only two representative directions are being considered: axial, or x-direction; and transverse, or y direction. It is also clear that in the present lattice the actual description of a straight line path in the transverse direction starting from a point in the scattering material depends upon both the azimuthal angle about the x-direction and the particular position in the scattering material relative to, say, the center of a vacuum channel. A "suitable" averaging technique must be employed. Furthermore, the same difficulty is encountered when considering a description of an axially-oriented path. Let $\lambda_x(\mu)$ and $\lambda_y(\eta)$ represent the angular-dependent mean free paths with respect to x-direction diffusion and y-direction diffusion.

The following constraints on the "suitable" averaging technique seem intuitively reasonable:

1. The average mean free path based on axial and transverse directions should be equal, i.e.,

$$\int_{-1}^{+1} \lambda_x(\mu)\, d\mu = \int_{-1}^{+1} \lambda_y(\eta)\, d\eta \tag{83}$$

2. The axial mean free path in the transverse direction (i.e., at $\mu = 0$) should be equal to the transverse mean free path in the transverse direction (i.e., at $\eta = \pm 1$), i.e.,

$$\lambda_x(0) = \lambda_y(\pm 1) \tag{84}$$

3. Both axial and transverse mean free paths should be symmetric, i.e.,

$$\lambda_x(\mu) = \lambda_x(-\mu) \tag{85a}$$

$$\lambda_y(\eta) = \lambda_\eta(-\eta) \tag{85b}$$

A possible method of obtaining $\lambda(\mu)$ is to find, as a function of starting position in the scatterer, the mean free path length traveled in all directions. Then, upon "suitably" weighting this quantity, according to whether $\lambda_x(\mu)$ or $\lambda_y(\eta)$ is desired, an average yields the angular-dependent mean free path. In even the simplest lattice this is a geometric task of considerable magnitude. Here, for the sake of brevity, an alternate, albeit certainly less self-contained, route will be taken. Assume certain macroscopic diffusion parameters, such as diffusion length, are given and use the general constraints of Eqs. (83–85) to obtain a representation of the mean free path which yields the given parameters. To be specific, assume that $\lambda_x(\mu)$ and $\lambda_y(\eta)$ are even quadratics of the respective variables. Thus, in terms of the Legendre polynomial expansion

$$\lambda_x(\mu) = \lambda_{x0} + \lambda_{x2} P_2(\mu) \tag{86a}$$

$$\lambda_y(\eta) = \lambda_{y0} + \lambda_{y2} P_2(\mu) \tag{86b}$$

From Eq. (83) $\lambda_{x0} = \lambda_{y0}$, and this result used in Eq. (84) yields $\lambda_{y2} = -\lambda_{x2}/2$. Therefore, in terms of the two unknowns, λ_0 and λ_2, Eq. (86) may be reformulated as

$$\lambda_x(\mu) = \lambda_0 + \lambda_2 P_2(\mu) \tag{87a}$$

$$\lambda_y(\eta) = \lambda_0 - \frac{1}{2}\lambda_2 P_2(\eta) \tag{87b}$$

The arguments used here with respect to the mean free path also apply to the determination of the total cross section. Thus, the general constraints are expected:

1. $\int_{-1}^{+1} \sigma_x(\mu)\, d\mu = \int_{-1}^{+1} \sigma_y(\eta)\, d\eta$
2. $\sigma_x(0) = \sigma_y(\pm 1)$
3. $\sigma_x(\mu) = \sigma_x(-\mu)$

and

$$\sigma_y(\eta) = \sigma_y(-\eta)$$

If the total cross section is assumed to be an even quadratic, then in terms of the two unknowns, σ_0 and σ_2,

$$\sigma_x(\mu) = \sigma_0 + \sigma_2 P_2(\mu)$$

$$\sigma_y(\eta) = \sigma_0 - \frac{1}{2}\sigma_2 P_2(\eta)$$

For the remainder of this discussion assume that the neutron collision density is used as dependent variable and thus the mean free path is the relevant parameter. These considerations can be equally well applied to the neutron flux and total cross section.

From Eqs. (28) and (87) results are

$$L_x^2 = \frac{\left(\lambda_0 + \frac{2\lambda_2}{5}\right)^2}{3(1-c)(1-cf_1)} \tag{88a}$$

$$L_y^2 = \frac{\left(\lambda_0 - \frac{\lambda_2}{5}\right)^2}{3(1-c)(1-cf_1)} \tag{88b}$$

Also,

$$L_s^2 = \frac{\lambda_s^2}{3(1-c)(1-cf_1)} \tag{89}$$

From Eqs. (88 and 89)

$$\frac{\lambda_0}{\lambda_s} = \frac{\langle L \rangle}{L_s} \tag{90a}$$

$$\langle L \rangle = \frac{L_x}{3} + \frac{2L_y}{3} \tag{90b}$$

$$\frac{\lambda_2}{\lambda_s} = \frac{5}{3}\left[\frac{L_x}{L_s} - \frac{L_y}{L_s}\right] \tag{90c}$$

Measured values of L_x and L_y, or other theoretical treatments, can be used to find L_x and L_y in order to determine

λ_0/λ_s and λ_2/λ_s. For example, if Behren's theoretical formulation (Ref. 1) is used,

$$\left(\frac{L_x}{L_s}\right)^2 = 1 + 2V + \frac{2RV}{\exp\left(\frac{2R}{V}\right) - 1} + 2RV \tag{91a}$$

$$\left(\frac{L_y}{L_s}\right)^2 = 1 + 2V + \frac{2RV}{\exp\left(\frac{2R}{V}\right) - 1} + RV \tag{91b}$$

where R is the ratio of the vacuum channel radius to λ_s. In Fig. 2 L_x/L_s and L_y/L_s are presented as a function of R, $R \in (0, 5)$, for the cases $V = 0.5$, 1.0 and 2.0 as determined by Eq. (91). Then in Fig. 3 for the same values of R and V, the results for λ_0/λ_s and λ_2/λ_s are based on the curves in Fig. 2.

It should be noted that what is referred to as L_x^2 and L_y^2 is Eq. (91) are actually calculated by Behrens (Ref. 1) as $\langle x^2\rangle/2$ and $\langle y^2\rangle/2$ and, via Eq. (38),

$$\langle x^2\rangle = 2L_x^2 + \frac{18}{175}\frac{\lambda_2^2}{(1-c)(1-cf_3)} \tag{92a}$$

$$\langle y^2\rangle = 2L_y^2 + \frac{18}{175}\frac{\frac{\lambda_2^2}{4}}{(1-c)(1-cf_3)} \tag{92b}$$

If $\lambda_2^2 > 1$ the validity of Fig. 3 as a relevant representation for $\lambda(\mu)$ is questionable. However, truncation of $\lambda(\mu)$ at a quadratic would, in that case, also be of questionable usefulness.

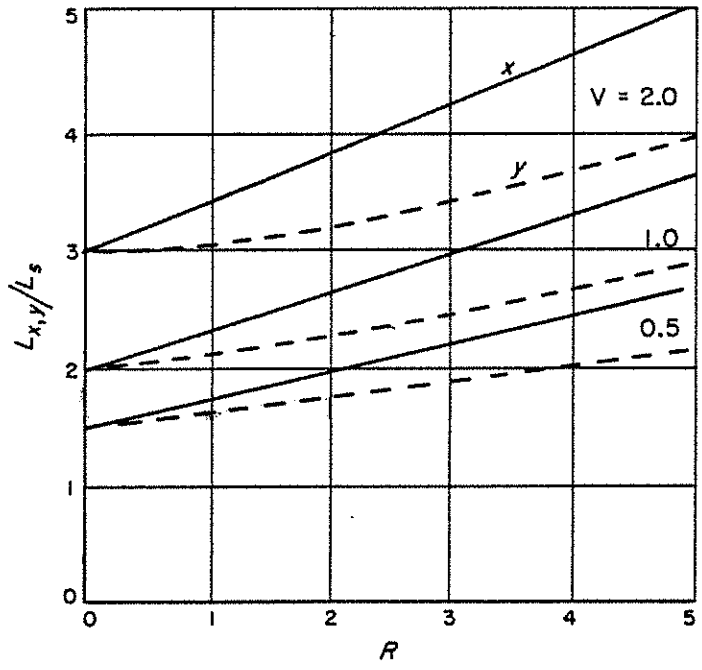


Fig. 2. Neutron diffusion lengths as found by Behren's theoretical formulation

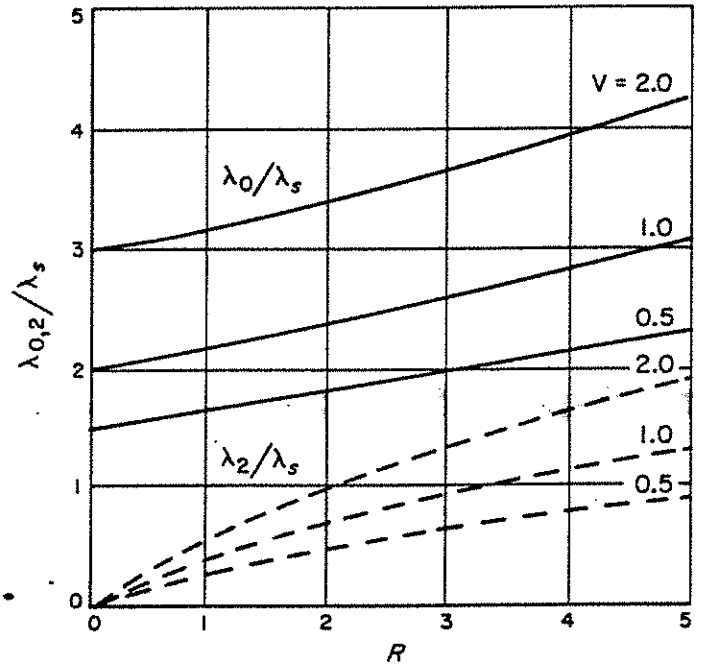


Fig. 3. Expansion coefficients for an even quadratic representation of the mean free path angular dependence

IV. SUMMARY

The mathematical formulation has been developed of a new approach to the homogenization of certain types of heterogeneous media (such as a regular array of vacuum channels) for the purpose of neutron diffusion calculations.

The new method is based on the inclusion of an angular-dependent mean free path in the theory of neutron transport. In the present effort, calculations are restricted to media with plane symmetry and monoenergetic neutron theory is employed. Extension to energy-dependent theory and to other symmetries would probably follow the general lines for the familiar, angular-independent case without significant additional complication. However, it seems clear that the requirement of the existence of two orthogonal characteristic directions in the development of the angular dependence of the mean free path must be imposed.

It was found in this Report that a neutron flux based theory and a collision density based theory can lead to significantly different results when low-order approximations, such as diffusion theory, are employed in the solution of the transport equation. For the case of isotropic scattering, the normal mode technique is applicable, and exact, closed-form solutions can be determined.

Evaluating the results implied by the present theory with respect to measurements is impossible. There is a current lack of pertinent experimental results for neutron distribution description in the relevant type of media.

APPENDIX A

The Function $\Lambda(\nu)$

It has been found previously that the zeroes of $\Lambda(\nu)$ for $\nu \notin (-1, +1)$ are the discrete set of normal mode indices and that they appear in pairs, $\pm\nu_j$. The number of these allowed discrete indices will be discussed. To this end, and for relationships which are useful in Section II G, there follows a brief study of the general properties of the function $\Lambda(\nu)$ as defined by Eqs. (51) and (53), i.e.,

$$\Lambda(\nu) = 1 + i\pi c\nu G(\nu)$$

$$G(\nu) = \frac{1}{2\pi i}\int_{-1}^{+1} \frac{g(u)}{u-\nu}\,du$$

In terms of the set $\{g_n\}$, as defined in Eq. (43c), $\Lambda(\nu)$ may be rewritten

$$\Lambda(\nu) = 1 - c\nu \sum_n g_n Q_n(\nu) \qquad \text{(A-1)}$$

where $Q_n(\nu)$ is a Legendre function of the second kind defined for the entire ν-plane by an extension of the Neumann formula (Ref. 2, p. 51) to include $\nu \notin (-1, +1)$, i.e.,

$$Q_n(\nu) = \frac{1}{2}\int_{-1}^{+1} \frac{P_n(u)}{\nu-u}\,du \qquad \text{(A-2)}$$

with singular integrals evaluated as the Cauchy principal value. For large ν, $\nu Q_n(\nu)$ varies as ν^{-n}. Thus, $\Lambda(\nu)$ is bounded for large ν. Furthermore, the $Q_n(\nu)$ are analytic in the ν-plane excluding $\nu \in (-1, +1)$ and, therefore, $\Lambda(\nu)$ is analytic in this same region. The contour illustrated in Fig. A-1 and the argument theorem (Ref. 6, p. 116) establishes the number of zeroes of $\Lambda(\nu)$ in the region $\nu \notin (-1, +1)$. Since the zeroes of $\Lambda(\nu)$ appear in pairs, the number of zeroes are denoted by $2J$. The argument theorem applied here yields

$$4\pi J = \text{change in arg } \Lambda^+(u) \text{ on } C_+ + \text{change in arg } \Lambda^-(u) \text{ on } C_- \qquad \text{(A-3)}$$

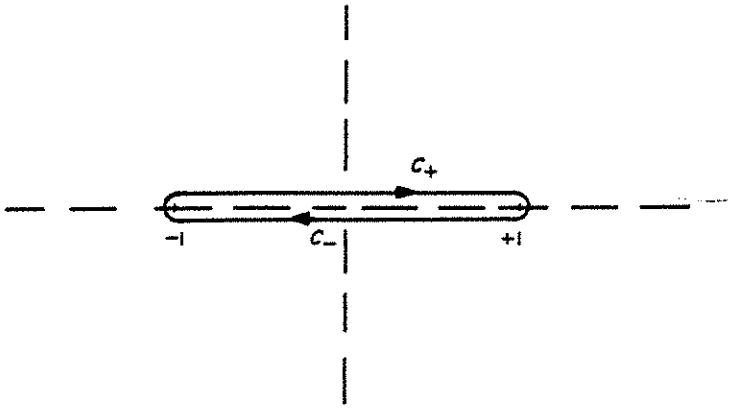


Fig. A-1. Contour in ν-plane used in determination of the number of zeroes of the function $\Lambda(\nu)$

It was assumed that $g(u)$ satisfies a Holder condition on $u \epsilon (-1, +1)$ and therefore $G(\nu)$ is a Cauchy integral. The Plemelj formulae (Ref. 5, p. 43) are applied to find the limit values $G^{\pm}(u)$. It is found that

$$G^{\pm}(u) = G(u) \pm \frac{1}{2} g(u) \tag{A-4}$$

where $G^{+}(u)$ and $G^{-}(u)$ refer to the limit values of $G(\nu)$ as ν approaches u from above and below the real line respectively. From Eq. (A-4) the limit values

$$\Lambda^{\pm}(u) = \Lambda(u) \pm \frac{i\pi}{2} cug(u) \tag{A-5}$$

Now, $\Lambda(u)$ with $u \epsilon (-1, +1)$ is a real function (with singularities at $u = \pm 1$), so that $\Lambda(0) = 1$ and $g(u)$ is a symmetric function. Whence, the relations

$$\arg \Lambda^{+}(u) = -\arg \Lambda^{-}(u) \tag{A-6a}$$

$$\arg \Lambda^{+}(0) = \arg \Lambda^{-}(0) = 0 \tag{A-6b}$$

$$\Lambda^{+}(u) = \Lambda^{-}(-u) \tag{A-6c}$$

These results used in Eq. (A-3) yield the number of pairs of zeroes J in terms of the single angle $\arg \Lambda^{+}(+1)$, i.e.,

$$J = \frac{1}{\pi} \arg \Lambda^{+}(+1) \tag{A-7}$$

It should be noted that Eq. (A-3) contains the implicit requirement that $\Lambda^{+}(u) \neq 0$ for $u \epsilon (-1, +1)$. This assumption is not completely necessary; however, it probably applies to most cases of physical interest and its application greatly simplifies these considerations.

A sufficient condition for $J = 1$ will be developed in the case that $g(u)$ is an N-degree polynomial in u, i.e.,

$$g(u) = \sum_{n=0}^{N} g_n P_n(u) \tag{A-8}$$

Note that the Legendre functions, $Q_n(\nu)$, can be expressed as

$$Q_n(\nu) = P_n(\nu) Q_0(\nu) - W_{n-1}(\nu) \tag{A-9a}$$

$$Q_0(\nu) = \operatorname{arc\,tanh} \nu, \nu \epsilon (-1, +1)$$

$$= \operatorname{arc\,tanh} \frac{1}{\nu}, \nu \notin (-1, +1) \tag{A-9b}$$

where $W_{n-1}(\nu)$ is an even, or odd, polynomial in ν of degree $n-1$ (Ref. 2, p. 51). In these terms $\Lambda(\nu)$ is rewritten as

$$\Lambda(\nu) = 1 - c\nu Q_0(\nu) \sum_{n=0}^{N} g_n P_n(\nu) + \sum_{n=0}^{N} g_n W_{n-1}(\nu) \tag{A-10}$$

Also, as $u \to +1$, $Q_0(u) \to +\infty$ and $P_n(+1) = 1$. Clearly, $W_n(+1)$ is bounded, and thus, if

$$\sum_{n=0}^{N} g_n > 0 \tag{A-11}$$

then as $u \to +1$, $\Lambda(\nu) \to -\infty$. From Eq. (A-5), in the present case,

$$\Lambda^{+}(u) = \Lambda(u) + \frac{i\pi}{2} cu \sum_{n=0}^{N} g_n P_n(u) \tag{A-12}$$

Therefore, the following may be concluded: if Eq. (A-11) holds and, in the range $u \epsilon (0, +1)$,

$$\sum_{n=0}^{N} g_n P_n(u) > 0 \tag{A-13}$$

then $\arg \Lambda^{+}(+1) = \pi$ and we have the desired result, $J = 1$. It should be stressed that Eqs. (A-11) and (A-13) give a sufficient, not necessary, condition for the number of pairs of discrete indexed normal modes to be unity.

APPENDIX B

A Relevant Hilbert Problem

In Section II F the existence of the modal expansion coefficients $\{a(\pm\nu_j),\ j=1,2,\cdots,J, a(\nu),\ \nu\in(-1,+1)\}$ was assumed. Moreover, the orthogonality relations are based on the whole angle range $u\in(-1,+1)$ and thus only provide a means of determining expansion coefficients for the case of a boundary condition given over all angles. It is found, by reducing the problem of finding expansion coefficients to the solution of an inhomogeneous Hilbert problem, that the existence of expansion coefficients can be demonstrated, and a method prescribed for determining the value of the coefficients for problems involving all physically relevant boundary conditions. The techniques elegantly described by Muskhelishvili (Ref. 5), are followed closely.

I. REDUCTION OF TRANSPORT PROBLEM TO AN INHOMOGENEOUS HILBERT PROBLEM

Transport problem boundary conditions will be encountered, in general, of the form

$$\phi(u)=\sum_{j=1}^{J} a(+\nu_j)\,\phi(+\nu_j,u)+\sum_{j=1}^{J} a(-\nu_j,u)\,\phi(-\nu_j,u)+\int_{\alpha}^{\beta} a(\nu)\,\phi(\nu,u)\,d\nu \text{ for } u\in(\alpha,\beta) \tag{B-1}$$

where $-1\leqq\alpha<\beta\leqq+1$. If it were possible by some method to determine the set of discrete indexed coefficients $\{a(\pm\nu_j),\ j=1,2,\cdots,J\}$, and define

$$\phi'(u)=\phi(u)-\sum_{j=1}^{J} a(+\nu_j)\,\phi(+\nu_j,u)-\sum_{j=1}^{J} a(-\nu_j)\,\phi(-\nu_j,u) \tag{B-2}$$

then there would be an integral equation for $a(\nu)$, $\nu\in(\alpha,\beta)$, i.e.,

$$\int_{\alpha}^{\beta} a(\nu)\,\phi(\nu,u)\,d\nu=\phi'(u) \text{ for } u\in(\alpha,\beta) \tag{B-3}$$

Using the derived form of $\phi(\nu,u)$ Eq. (50)

$$\Lambda(u)\,a(u)+\frac{c}{2}\,g(u)\int_{\alpha}^{\beta}\frac{\nu a(\nu)}{\nu-u}\,d\nu=\phi'(u) \text{ for } u\in(\alpha,\beta) \tag{B-4}$$

From Eq. (A-5)

$$\frac{c}{2}\,ug(u)=\frac{1}{2\pi i}\left[\Lambda^{+}(u)-\Lambda^{-}(u)\right] \tag{B-5a}$$

$$\Lambda(u)=\frac{1}{2}\left[\Lambda^{+}(u)+\Lambda^{-}(u)\right] \tag{B-5b}$$

and therefore Eq. (B-4) may be rewritten as

$$\frac{1}{2}\left[\Lambda^{+}(u)+\Lambda^{-}(u)\right]ua(u)+\left[\Lambda^{+}(u)-\Lambda^{-}(u)\right]A(u)=u\,\phi'(u) \tag{B-6a}$$

$$A(u)=\frac{1}{2\pi i}\int_{\alpha}^{\beta}\frac{\nu a(\nu)}{\nu-u}\,d\nu \text{ for } u\in(\alpha,\beta) \tag{B-6b}$$

There is assurance that $A(u)$, as defined in Eq. (B-6b), exists if $a(u)$ satisfies a Holder condition on $u\in(\alpha,\beta)$. For the moment, assume that this condition is fulfilled and define the Cauchy integral, $A(\nu)$, over the entire ν-plane,

$$A(\nu)=\frac{1}{2\pi i}\int_{\alpha}^{\beta}\frac{ua(u)}{u-\nu}\,du \tag{B-7}$$

The Plemelj formulae yield the limit relations on the line $u\in(\alpha,\beta)$,

$$A^{+}(u)-A^{-}(u)=ua(u) \tag{B-8a}$$

$$A^{+}(u)+A^{-}(u)=2A(u) \tag{B-8b}$$

The results of Eqs. (B-5) and (B-8) applied to Eq. (B-6) give the alternate form

$$\Lambda^+(u)\,A^+(u) - \Lambda^-(u)\,A^-(u) = u\,\phi'(u) \text{ for } u \in (\alpha, \beta) \tag{B-9}$$

It was assumed that $\Lambda^{\pm}(u) \neq 0$ for $u \in (\alpha, \beta)$. With this restriction Eq. (B-9) can be easily transformed to the form of a boundary condition for an inhomogeneous Hilbert problem on an arc (Ref. 5, chapter 10). The problem of determining $a(u)$ restated in these terms is: Find the sectionally analytic function, $A(\nu)$, vanishing at infinity, with boundary condition on the line $u \in (\alpha, \beta)$,

$$A^+(u) = \frac{\Lambda^-(u)}{\Lambda^+(u)} A^-(u) + \frac{u\phi'(u)}{\Lambda^+(u)} \tag{B-10}$$

Note that the assumptions on $g(u)$ and $\Lambda^{\pm}(u)$ imply that $\Lambda^-(u)/\Lambda^+(u)$ is a function satisfying a Holder condition and not vanishing on $u \in (\alpha, \beta)$, and, if it is assumed that the angle boundary condition, $\phi(u)$, satisfies a Holder condition and $a(\pm\nu_i)$ exist, then $u\phi'(u)/\Lambda^+(u)$ satisfies a Holder condition on $u \in (\alpha, \beta)$.

Summarizing will help clarify the procedure. If it is assumed (what is to be proved) that $a(u)$ satisfies a Holder condition on $u \in (\alpha, \beta)$, then the integral $A(\nu)$, defined by Eq. (B-7), is of the Cauchy type. Now, Cauchy integrals are sectionally analytic functions with boundary the line of integration. Specifically, if (α, β) is the line of integration:

1. $A(\nu)$ is analytic in ν-plane excluding (α, β).
2. $A(\nu)$ approaches well-defined limits as $u \in (\alpha, \beta)$ is approached from either side of (α, β) with possible exception of the end points, α and/or β.
3. Near the end points, $A(\nu)$ satisfies the conditions

$$|A(\nu)| \leq \frac{A}{|\nu - \alpha|^a} \text{ as } \nu \to \alpha$$

$$|A(\nu)| \leq \frac{B}{|\nu - \beta|^b} \text{ as } \nu \to \beta$$

where a, b, A and B are real constants, and $a < 1$ and $b < 1$.

Moreover, $A(\nu)$ vanishes as $|\nu| \to \infty$. The integral equation for $a(u)$ has been transformed into the boundary condition Eq. (B-10) which is the form of an inhomogeneous Hilbert problem boundary condition. Thus, the original transport problem has been reduced to an inhomogeneous Hilbert problem. If a solution $A(\nu)$ which introduces no physical ambiguity can be found, then the assumption of the existence of $a(u)$, $u \in (\alpha, \beta)$, will be substantiated.

II. SOLUTION OF THE HILBERT PROBLEM

In terms of

$$\theta(u) = \arg \Lambda^+(u),\ \Lambda^-(u)/\Lambda^+(u) = \exp[-2i\theta(u)]$$

the Hilbert problem boundary condition [cf., Eq. (B-10)] becomes

$$A^+(u) = \exp[-2i\,\theta(u)]\,A^-(u) + \frac{u\phi'(u)}{\Lambda^+(u)} \text{ for } u \in (\alpha, \beta) \tag{B-11}$$

Since $A(\nu)$ must also vanish $|\nu| \to \infty$, the solution (Ref. 5) is

$$A(\nu) = \frac{H(\nu)}{2\pi i} \int_\alpha^\beta \frac{u\phi'(u)}{(u-\nu)\,\Lambda^+(u)\,H^+(u)}\,du \tag{B-12}$$

where $H(\nu)$ is the fundamental solution of the associated homogeneous Hilbert problem and is given by

$$H(\nu) = (\alpha - \nu)^{-\Theta(\alpha)/\pi}\,(\beta - \nu)^{\Theta(\beta)/\pi}\,e^{\Theta(\nu)} \tag{B-13}$$

The Cauchy integral $\Theta(\nu)$ is defined by

$$\Theta(\nu) = -\frac{1}{\pi} \int_\alpha^\beta \frac{\theta(u)}{u - \nu}\,du \tag{B-14}$$

Providing $\kappa = \theta(\beta)/\pi - \theta(\alpha)/\pi$ is a positive integer, there are the κ additional requirements

$$\int_\alpha^\beta \frac{u^{n+1}\phi'(u)}{\Lambda^+(u)\,H^+(u)}\,du = 0 \qquad \text{for } n = 0, 1, \cdots, \kappa - 1 \tag{B-15}$$

These additional requirements are a necessary feature of the solution. It should be recalled that the function $\phi'(u)$, $u \in (\alpha, \beta)$, is not completely specified, i.e., the discrete indexed expansion coefficients, $a(\pm\nu_j)$, in Eq. (B-2) are, as yet, unknown. For the general problems considered later, it will be demonstrated that, in each case, the κ requirements are necessary and sufficient for the complete specification of all discrete and continuum expansion coefficients.

III. APPLICATION OF THE HILBERT PROBLEM SOLUTION

Plane symmetry transport problems fall into two general categories:

1. Infinite media problems with full-angle-range boundary conditions (such as the Green's function solved in Section II G).
2. Half-space media problems with half-angle-range boundary conditions (such as albedo or Milne type problems).

Combinations of the solutions of these type problems lead to the solution of cases with finite media (slabs). For full-range boundary conditions, the orthogonality of the normal modes provides a direct method for determining expansion coefficients. The solution of the Hilbert problem in these cases demonstrates the existence of the coefficients and thus partially supports the completeness hypothesis. For half-range boundary problems, there are no apparent orthogonality properties of the normal modes. In these cases, the solution of the Hilbert problem not only provides proof of existence, but also gives a well-defined prescription for the determination of expansion coefficients. The application of the Hilbert problem solution will now be outlined to the categories of full-range and half-range boundary conditions.

In the case of an infinite medium, full-range boundary condition problem, a source condition is usually given at some position, which is chosen to be designated $x = 0$. For $c < 1$, it follows that $F(x, u)$ should vanish as $|x| \to \infty$. Thus, the general form of solution is that given in Eq. (69). The source condition can be formulated as

$$\phi(u) = \sum_{j=1}^{J} a(+\nu_j)\,\phi(+\nu_j, u) + \sum_{j=1}^{J} a(-\nu_j)\,\phi(-\nu_j, u) + \int_{-1}^{+1} a(\nu)\,\phi(\nu, u)\,d\nu \qquad \text{for } u \in (-1, +1) \tag{B-16}$$

Instead of using the obviously indicated orthogonality properties, consider the coefficient evaluation by the route prescribed in the Hilbert problem solution. Note that $\alpha = -1$ and $\beta = +1$. From Eqs. (A-6) and (A-7), the results are $\theta(-1) = -J\pi$ and $\theta(+1) = J\pi$. Therefore, in this case, $\kappa = 2J$ and there are $2J$ requirements of the form of Eq. (B-15). Specifically,

$$\int_{-1}^{+1} \frac{u^{n+1}\phi'(u)}{\Lambda^+(u)\,H^+(u)}\,du = 0 \qquad \text{for } n = 0, 1, \cdots, 2J-1 \tag{B-17}$$

Equation (B-17) provides a sufficient number of equations to find the discrete indexed expansion coefficients, $a(\pm\nu_j)$, $j = 1, 2, \cdots, J$. The fundamental solution $H(\nu)$, [cf., Eq. (B-13)], is given by

$$H(\nu) = (-1-\nu)^J\,(1-\nu)^J e^{\Theta(\nu)} \tag{B-18a}$$

$$\Theta(\nu) = -\frac{1}{\pi}\int_{-1}^{+1} \frac{\theta(u)}{u-\nu}\,du \tag{B-18b}$$

Thus, $A(\nu)$ is determined [by Eq. (B-12)] and $a(u)$ for $u \in (-1, +1)$ can be found from the limit relation [cf., Eq. (B-8a)]

$$ua(u) = A^+(u) - A^-(u) \qquad \text{for } u \in (-1, +1) \tag{B-19}$$

Since the problem has been completely and unambiguously solved, it is clear that the supposition that $a(u)$ satisfies a Holder condition is substantiated and the existence of the expansion coefficients has been demonstrated.

For half-space media, consider two types of problems. An "albedo problem" is described by a boundary con-

dition at the medium surface ($x = 0$ with medium occupying $x > 0$) specified for $u \epsilon (0, +1)$ and the condition that $F(x, u)$ vanish as $x \to \infty$. A "Milne problem" is described by a similar boundary condition at $x = 0$, but with $F(x, u) \to \phi(-\nu, u) \exp(x/\nu)$ with $\nu = \nu_j$, $j = 1, 2, \cdots, J$, or $\nu \epsilon (0, +1)$, as $x \to \infty$. These problems have been specified as boundary conditions on the half-range $u \epsilon (0, +1)$. With obvious modifications, the procedure is easily applied to half-space media occupying $x < 0$ and boundary conditions on $u \epsilon (-1, 0)$. With the half-space occupying $x > 0$, the general solution of an albedo problem is

$$F(x, u) = \sum_{j=1}^{J} a(+\nu_j)\, \phi(+\nu_j, u) \exp\left(\frac{-x}{\nu_j}\right) + \int_0^{+1} a(\nu)\, \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x > 0 \tag{B-20}$$

and for a Milne problem,

$$F(x, u) = A\phi(-\nu, u) \exp\left(\frac{x}{\nu}\right) + \sum_{j=1}^{J} a(+\nu_j)\, \phi(+\nu_j, u) \exp\left(\frac{-x}{\nu_j}\right) + \int_0^{+1} a(\nu)\, \phi(\nu, u) \exp\left(\frac{-x}{\nu}\right) d\nu \text{ for } x > 0 \tag{B-21}$$

In both cases, the boundary condition at $x = 0$ can be expressed in the form of Eq. (B-1), i.e.,

$$\phi(u) = \sum_{j=1}^{J} a(+\nu_j)\, \phi(+\nu_j, u) + \int_0^{+1} a(\nu)\, \phi(\nu, u)\, d\nu \quad \text{for } u \epsilon (0, +1) \tag{B-22}$$

Now, $\alpha = 0$ and $\beta = +1$ and, from Eqs. (A-6) and (A-7), $\theta(0) = 0$ and $\theta(+1) = J\pi$. Thus, $\kappa = J$ and we have the J requirements

$$\int_0^{+1} \frac{u^{n+1} \phi'(u)}{\Lambda^+(u)\, H^+(u)}\, du = 0 \qquad \text{for } n = 0, 1, \cdots, J-1 \tag{B-23}$$

These are sufficient to determine the discrete indexed coefficients, $a(+\nu_j)$, $j = 1, 2, \cdots, J$. The fundamental solution takes the form

$$H(\nu) = (1 - \nu)^J \exp(\Theta(\nu)) \tag{B-24a}$$

$$\Theta(\nu) = -\frac{1}{\pi} \int_0^{+1} \frac{\theta(u)}{u - \nu}\, du \tag{B-24b}$$

The Hilbert problem solution, $A(\nu)$, $\nu \epsilon (0, +1)$, and the continuum expansion coefficients, $a(u)$, $u \epsilon (0, +1)$, are found as in the case of a full-range boundary problem. Again, substantiation is found for the supposition of the existence of the relevant members of $\{a(\nu)\}$. Moreover, a prescription is found for calculating the expansion coefficients when the use of orthogonality conditions is impossible.

NOMENCLATURE

- a modal expansion coefficients of F
- A Cauchy integral with density a
- A_s cross-sectional area of scatterer material per lattice cell
- A_v cross-sectional area of vacuum per lattice cell
- A_{lmn} triple Legendre polynomial integral
- c neutron scattering probability
- D diffusion coefficient
- f neutron scattering distribution
- f_n Legendre polynomial expansion coefficients of f
- F neutron collision density
- F_n Legendre polynomial expansion coefficients of F
- F_n^j angle-space-moments of F
- g Jacobian of angle-variable change, i.e. $g(u) = |d\mu/du|$
- g_n Legendre polynomial expansion coefficients of g

NOMENCLATURE (Cont'd)

G Cauchy integral with density g

H fundamental solution of Hilbert problem

I orthogonality integral value

J half of the number of discrete indexed eigenmodes

L_F neutron diffusion length based on an F-expansion

L_ψ neutron diffusion length based on a ψ-expansion

L_s asymptotic diffusion length in scatterer material

L_x diffusion length with respect to x-direction

L_y diffusion length with respect to y-direction

P_n Legendre polynomial

Q_n Legendre functions of the second kind

R ratio of vacuum channel radius to λ_s

S neutron source distribution

S_n Legendre polynomial expansion coefficients of S

S_n^j angle-space-moments of S

t time variable

T_s slab thickness of scatterer material

T_v slab thickness of vacuum material

u angle variable defined by $u = \mu\lambda(\mu)/\lambda(1)$

v neutron speed

V ratio of vacuum volume to scatterer volume, i.e. $V = A_v/A_s$

W_n regular part of Legendre functions of the second kind

x position variable

$\langle x^2 \rangle$ mean value of x^2

y position variable perpendicular to x-direction

δ Dirac δ-distribution

δ_{mn} Kronecker δ-distribution

ϵ included in the interval

η direction cosine of neutron travel relative to y-direction

θ argument of the function Λ

Θ Cauchy integral with density θ

κ index of the Hilbert problem

λ neutron mean free path

λ_h simply homogenized medium mean free path

λ_n Legendre polynomial expansion coefficients of λ

λ_x mean free path with respect to x-direction

λ_y mean free path with respect to y-direction

Λ coefficient of δ-distribution in angle eigenmode

μ direction cosine of neutron travel relative to x-direction

ν angular flux eigenvalues

ν_j discrete indexed angular flux eigenvalues

σ total cross section

σ' absorption cross section

σ_n Legendre polynomial expansion coefficients of σ

σ_x total cross section with respect to x-direction

σ_y total cross section with respect to y-direction

ϕ angular flux eigenmodes (and angular boundary conditions)

ϕ_n Legendre polynomial expansion coefficients of ϕ

ψ neutron flux distribution

ψ_n Legendre polynomial expansion coefficients of ψ

ψ_n^j angle-space-moments of ψ

Ω unit vector in direction of neutron travel

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