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David S. Kershaw

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A New Method for Numerical Solution of the Transport Equation*

David S. Kershaw

University of California, Lawrence Livermore Laboratory
Livermore, California 94550

One of the basic equations of physics is the transport equation which has the general form

$$\left(\frac{\partial}{\partial t} + \vec{v} \cdot \frac{\partial}{\partial \vec{x}} + \vec{F} \cdot \frac{\partial}{\partial \vec{p}} \right) \rho(\vec{x}, \vec{p}, t) = J(\rho), \quad (1)$$

where ρ is the probability density for finding a particle at position $\vec{x}$ with momentum $\vec{p}$ at time t , $\vec{v}$ is the velocity, $\vec{F}$ is the external force field, and

$$J(\rho) = \int d^3\vec{p}' K(\vec{p}, \vec{p}') \rho(\vec{x}, \vec{p}', t) + S(\vec{p})$$

is the collision term, where S and K give the probability for emission, absorption and scattering off the background matter.

A standard technique for numerical solution of this equation is the method of spherical harmonics⁽¹⁾. In this method the angular dependence of $\rho(\vec{x}, \vec{p}, t)$ is represented by an expansion in spherical harmonics (Legendre polynomials in one dimensional problems) with coefficients depending on $\vec{x}$, E (energy of particle) and t . Thus,

$$\rho(\vec{x}, \vec{p}, t) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} Y_{\ell m}(\hat{p}) f_{\ell m}(\vec{x}, E, t),$$

where $\hat{p}$ is the unit vector in the $\vec{p}$ direction. Multiplying equation (1) by the various $Y_{\ell m}^*(\hat{p})$ and integrating over all directions one obtains

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an infinite set of coupled equations for the quantities $f_{\ell m}$. Setting $f_{\ell m} = 0$ for $\ell > L$, gives a finite set of coupled equations which approximates the transport equation. If, as is usually true, $K(\vec{p}, \vec{p}')$ tends to isotropize ρ over all directions, then the great virtue of the spherical harmonic method is that in very opaque materials (K very large) ρ is very well approximated by just a few ℓ . In particular if we keep just $\ell = 0, 1$ and set $f_{\ell m} = 0$ for $\ell \geq 2$ we get the diffusion approximation. The most serious drawback of this method has been that in very thin materials (K very small) higher ℓ components are not small and setting $f_{\ell m} = 0$ for large ℓ is a poor approximation. In particular in the diffusion approximation (for a physically typical $K(\vec{p}, \vec{p}')$ and $S(\vec{p})$) one has:

$$f^0 = \int d\Omega \rho,$$

$$\vec{f}^1 = \int d\Omega \rho \vec{v} = v \int d\Omega \rho \hat{p},$$

$$\frac{\partial f^0}{\partial t} + \vec{\nabla} \cdot \vec{f}^1 = \alpha(g - f^0) \quad (2a)$$

$$\vec{f}^1 = -\beta \vec{\nabla} f^0, \quad (2b)$$

where the $\ell = 1$ equation has relaxed to steady state. If the matter gets very thin (β very large) then $|\vec{f}^1|$ can get $\gg v f^0$ which is clearly wrong. This is the most common example of the errors introduced by setting $f_{\ell m} = 0$ for $\ell > L$ in thin materials, and at this point people have either switched to a different scheme such as S_n , gone to higher L , or tried to patch up diffusion theory with some sort of ad hoc scheme for forcing

$$|\vec{f}^1| \leq v f^0$$

to remain true. This last option is usually called flux limiting (2) and typically equation (2b) is modified to read

$$\vec{f}^1 = \frac{-\beta \vec{\nabla} f^0}{1 + \left(\frac{\beta}{v}\right) \left| \frac{\vec{\nabla} f^0}{f^0} \right|} \quad (3a)$$

or

$$f^1 = \begin{cases} -\beta \vec{\nabla} f^0, & \text{if } \beta |\vec{\nabla} f^0| \leq v f^0 \\ -v f^0 \left(\frac{\vec{\nabla} f^0}{|\vec{\nabla} f^0|} \right), & \text{if } \beta |\vec{\nabla} f^0| > v f^0 \end{cases} \quad (3b)$$

From a mathematical point of view the flux limit condition

$$|\vec{f}^1| \leq v f^0$$

is a simple consequence of the fact that f^0 and $\vec{f}^1$ are the zeroth and first moments of a probability distribution, i.e.

$$\rho(\vec{x}, \vec{p}, t) \geq 0$$

which implies for all unit vectors $\hat{u}$,

$$\int d\Omega (1 - \hat{u} \cdot \hat{p}) \rho(\vec{x}, \vec{p}, t) \geq 0,$$

and so for all $\hat{u}$

$$f^0 - \left(\frac{\hat{u} \cdot \vec{f}^1}{v} \right) \geq 0,$$

and therefore, $v f^0 \geq |\vec{f}^1|$.

Realizing this, one immediately suspects that there are also inequalities that the higher moments must satisfy simply by virtue of the fact that they are moments of some probability distribution on the unit sphere. In fact there is an extensive literature on this subject which is called

the "Theory of Moments"⁽³⁾. The basic problem of the theory of moments (for probability measures on the unit sphere) may be stated:

Given a set of numbers (moments)

$$f_{\ell m} \quad \begin{pmatrix} m = -\ell, -\ell + 1, \dots, +\ell \\ \ell = 0, 1, 2, \dots \end{pmatrix}$$

find a necessary and sufficient set of inequalities on the $f_{\ell m}$ in order that there exists a probability measure $\rho(\hat{p}) \geq 0$ with

$$f_{\ell m} = \int d\Omega Y_{\ell m}^*(\hat{p}) \rho(\hat{p})$$

for all ℓ and m .

In what follows various solutions to this problem will be discussed and it will be shown that:

- 1) The flux limit condition is just the first of a series of inequalities which set definite limits to the value of each of the higher moments.
- 2) The usual procedure of setting $f_{\ell m} = 0$, for $\ell > L$, violates these inequalities badly except in very diffusive problems. Therefore in the usual spherical harmonic method apriori knowledge about the moments is actually being thrown away. If instead of setting $f_{\ell m} = 0$ for $\ell > L$, we give $f_{\ell m}$ for $\ell = L + 1$ a value compatible with the inequalities derived from the theory of moments we should certainly improve agreement with the exact solution.
- 3) By choosing $f_{(L+1),m}$ in this way the equations become automatically flux limiting. Even for $L = 1$, (the diffusion approximation) $v f^0 > |\vec{f}^1|$ is a rigorous consequence of the equations obtained.
- 4) This choice of $f_{(L+1),m}$ insures that $f^0 \geq 0$ remains true.

- 5) This choice of $f_{(L+1),m}$ gives for $L = 1$ a hyperbolic system of equations whose characteristic velocities vary from $-v$ to $+v$ and take on all possible values in between. This is exactly the range of characteristic velocities for the transport equation.
- 6) This choice of $f_{(L+1),m}$ gives a set of equations which has the same free streaming solution as the exact transport equation, i.e.

$$f^0(\vec{x}, t) = g(\vec{x} - \vec{v}t)$$

$$f^1(\vec{x}, t) = \vec{v} g(\vec{x} - \vec{v}t)$$

for an arbitrary function g is an exact solution of the truncated set of equations as well as the exact transport equation.

Note that the usual choice $f_{(L+1),m} = 0$ gives a set of equations which has none of the properties 3) through 6).

Thus by simply choosing $f_{(L+1),m}$ consistent with our apriori knowledge about the moments of a probability distribution on the unit sphere we can greatly improve the accuracy of our truncated set of equations.

In part (I) various solutions to the problem of moments on the unit sphere are discussed.

In part (II) these inequalities are applied to the spherical harmonic method for solution of the transport equation and various properties of the resultant truncated set of equations are obtained.

I.

The problem of moments can be stated as follows: Given a set of numbers

$$f_{\ell m}, \quad 0 \leq \ell \leq (L+1), \quad -\ell \leq m \leq +\ell$$

find a necessary and sufficient condition on the $f_{\ell m}$ for there to exist a probability distribution $\rho(p)$ such that

$$f_{\ell m} = \int d\Omega Y_{\ell m}^* (\hat{p}) \rho(\hat{p})$$

$$0 \leq \ell \leq (L+1), -\ell \leq m \leq +\ell.$$

A set of moments which satisfies these conditions will be called a good set.

First consider one dimensional problems (slab or spherical symmetry). For that case $\rho(\hat{p}) = \rho(\cos\theta)$ and we can use for our basis functions $\cos^\ell\theta$. Then the moments are

$$g_\ell = \int_{-1}^{+1} d(\cos\theta) (\cos\theta)^\ell \rho(\cos\theta)$$

It is well known ⁽⁴⁾ that a necessary and sufficient condition on the g_ℓ is that if $(L+1) = 2M$ the two matrices

$$E_{ij}^{(M)} = g_{(i+j)}, \quad 0 \leq i, j \leq M \quad (4a)$$

$$\text{and } F_{ij}^{(M-1)} = g_{(i+j)} - g_{(i+j+2)}, \quad 0 \leq i, j \leq M-1 \quad (4b)$$

must be non negative ⁽⁵⁾, and if $(L+1) = 2M-1$ the two matrices

$$G_{i,j}^{(M-1)} = g_{(i+j)} + g_{(i+j+1)}, \quad 0 \leq i, j \leq M-1 \quad (5a)$$

$$H_{i,j}^{(M-1)} = g_{(i+j)} - g_{(i+j+1)}, \quad 0 \leq i, j \leq M-1 \quad (5b)$$

must be non negative (the superscript refers to the dimension of the matrix).

It is also well known that a matrix O^N of dimension N is non negative if and only if each leading principal submatrix of dimension $R \leq N$

$$O_{ij}^R = O_{ij}^N, \quad 1 \leq i, j \leq R$$

satisfies

$$\det (O_{ij}^R) \geq 0.$$

For our application, given a good set of moments, g_ℓ for $\ell = 0, \dots, L$ we wish to find the upper and lower bounds for $g_{(L+1)}$.

CASE I) $L + 1 = 2M$

From (5a) it is necessary and sufficient that

$$\det (E^M) \geq 0$$

$$\det (F^{(M-1)}) \geq 0,$$

but,

$$\det (E^M) = g_{(L+1)} \det (E^{(M-1)}) + \det (\bar{E}^M) \geq 0$$

where $\bar{E}^M$ is identical to E^M except that $\bar{E}_{M,M}^M = 0$. Now $E^{(M-1)}$ and $\bar{E}^M$ depend only on g_ℓ for $\ell = 0, 1, \dots, L$ and since by assumption the g_ℓ for $\ell = 0, 1, \dots, L$ are a good set of moments

$$\det (E^{(M-1)}) \geq 0.$$

Therefore assuming $\det (E^{(M-1)}) > 0$, we have

$$g_L + 1 \geq \frac{-\det(\bar{E}^M)}{\det(E^{(M-1)})} \quad (6a)$$

for a greatest lower bound. Similarly one obtains

$$(g_{(L-1)} - g_{(L+1)}) \det(F^{(M-2)}) + \det(\bar{F}^{(M-1)}) \geq 0,$$

where $\bar{F}^{(M-1)}$ is identical to $F^{(M-1)}$ except that $\bar{F}_{(M-1)(M-1)}^{(M-1)} = 0$. Therefore

$$g_{(L-1)} + \frac{\det(\bar{F}^{(M-1)})}{\det(F^{(M-2)})} \geq g_{(L+1)} \quad (6b)$$

CASE II) $L + 1 = 2M - 1$

Similar arguments show that

$$\begin{aligned} g_L + \frac{\det(\bar{H}^{(M-1)})}{\det(H^{(M-2)})} &\geq g_L + 1 \\ &\geq -g_L - \frac{\det(\bar{G}^{(M-1)})}{\det(G^{(M-2)})} \end{aligned} \quad (7a)$$

Now let us look in detail at the first few g_ℓ . Since ρ is a probability distribution,

$$\int_{-1}^{+1} d(\cos\theta) \rho(\cos\theta) = g_0 = 1,$$

The explicit upper and lower bounds for $\ell = 1, 2, 3$ and 4 are:

$$-1 \leq g_1 \leq +1, \quad (8a)$$

$$g_1^2 \leq g_2 \leq 1, \quad (8b)$$

$$-g_2 + \frac{(g_1 + g_2)^2}{(1 + g_1)} \leq g_3 \leq g_2 - \frac{(g_1 - g_2)^2}{(1 - g_1)} \quad (8c)$$

$$\frac{(g_2^3 - g_3^2 + 2 g_1 g_2 g_3)}{(g_2 - g_1^2)} \leq g_4 \leq g_2 - \frac{(g_1 - g_3)^2}{(1 - g_2)} \quad (8d)$$

If for any $\ell < (L + 1)$, the ℓ th moment g_ℓ is equal to one of its two boundary values, then $\rho(\cos\theta)$ is uniquely determined and all $g_{\ell'}$, for $\ell' > \ell$ are uniquely determined.⁽⁶⁾ To determine these higher $g_{\ell'}$, we cannot use the above expressions for the upper and lower bounds since (except for $g_{(\ell + 1)}$) they will be indeterminate (they have the form 0/0). Instead one must solve for $\rho(\cos\theta)$, which will be zero except at a finite set of points.

Then ρ can be used to find $g_{\ell'}$, for $\ell' > \ell$. Explicitly for $\ell = 1, 2, 3$ and 4:

$$\begin{aligned} \text{If } \ell = 1, g_1 &= \pm 1, \\ \text{then } \rho(\cos\theta) &= \delta(1 \pm \cos\theta), \end{aligned} \quad (9a)$$

($\delta(x)$ is the Dirac delta function)

$$\text{and } g_{\ell'} = (\pm 1)^{\ell'} \text{ for all } \ell' > \ell.$$

$$\begin{aligned} \text{If } \ell = 2, g_2 &= 1, \\ \text{then } \rho &= \frac{(1 + g_1)}{2} \delta(1 - \cos\theta) + \frac{(1 - g_1)}{2} \delta(1 + \cos\theta), \end{aligned} \quad (9b)$$

$$\text{and } g_{\ell'} = \begin{cases} 1 & \text{if } \ell' \text{ even,} \\ g_1 & \text{if } \ell' \text{ odd.} \end{cases}$$

$$\begin{aligned} \text{If } \ell = 2, g_2 &= g_1^2, \\ \text{then } \rho &= \delta(g_1 - \cos\theta), \\ \text{and } g_{\ell'} &= (g_1)^{\ell'} \end{aligned}$$

$$\text{If } \ell = 3, g_3 = \pm g_2 \mp \frac{(g_1 \mp g_2)^2}{(1 \mp g_1)},$$

$$\text{then } \rho = \rho_a \delta(1 \mp \cos\theta) + \rho_b \delta(x_b - \cos\theta), \quad (9c)$$

where

$$\rho_a = (g_2 - g_1^2) / (1 \mp 2g_1 + g_2),$$

$$\rho_b = (1 \mp g_1)^2 / (1 \mp 2g_1 + g_2),$$

$$x_b = (g_1 \mp g_2) / (1 \mp g_1),$$

and

$$g_{\ell'} = \rho_a + \rho_b (x_b)^{\ell'}.$$

$$\text{If } \ell = 4, g_4 = g_2 - \frac{(g_1 - g_3)^2}{(1 - g_2)},$$

$$\text{then } \rho = \rho_a \delta(1 + \cos\theta) + \rho_b \delta(x_b - \cos\theta) + \rho_c \delta(1 - \cos\theta),$$

where

$$\rho_a = \frac{(g_1 - g_3)(1 - g_1) - (1 - g_2)(g_1 - g_2)}{2(g_1 - g_3) + (g_1 - g_2)},$$

$$\rho_c = \frac{(g_1 - g_3)(1 + g_1) - (1 - g_2)(g_1 + g_2)}{2(g_1 - g_3) - (1 - g_2)}, \quad (9d)$$

$$\rho_b = \frac{(1 - g_2)^3}{(1 - g_2)^2 - (g_1 - g_3)^2},$$

$$x_b = \frac{(g_1 - g_3)}{(1 - g_2)},$$

and

$$g_{\ell'} = \rho_a (-1)^{\ell'} + \rho_b (x_b)^{\ell'} + \rho_c$$

If

$$\ell = 4, g_4 = \frac{(g_2^3 - g_3^2 + 2 g_1 g_2 g_3)}{(g_2 - g_1^2)}$$

then

$$\rho = \rho_a \delta (x_a - \cos \theta) + \rho_b \delta (x_b - \cos \theta)$$

where x_a and x_b are the two roots of the polynomial

$$\begin{aligned} & x^2 (g_2 - g_1^2) - x (g_3 - g_1 g_2) + (g_1 g_3 - g_2^2) \\ & = (g_2 - g_1^2) (x - x_a) (x - x_b) \end{aligned}$$

and

$$\rho_a = \frac{(g_1 - x_b)}{(x_a - x_b)} \quad , \quad (9e)$$

$$\rho_b = \frac{(g_1 - x_a)}{(x_b - x_a)}$$

and

$$g_{\ell'} = \rho_a (x_a)^{\ell'} + \rho_b (x_b)^{\ell'}$$

Now let us consider three dimensional problems. For the three dimensional case there is no general theory so we consider $\ell = 1$ and 2 first.

For $\ell = 1$

$$\text{let } f^0 = \int d\Omega \rho(\hat{p}) = 1 ,$$

$$\vec{f}^1 = \int d\Omega \rho(\hat{p}) \hat{p} .$$

Then

$$\int d\Omega \rho(\hat{p}) (1 - \hat{u} \cdot \hat{p}) = 1 - \hat{u} \cdot \vec{f}^1 \geq 0 ,$$

where $\hat{u}$ is an arbitrary unit vector,

$$\text{implies } |\vec{f}^1| \leq f^0 .$$

Conversly, given $f^0 = 1$, $\vec{f}^1$ with $|\vec{f}^1| \leq f^0$ let $\hat{f}^1$ be the unit vector in $\vec{f}^1$ direction

$$\text{and } \rho(\hat{p}) = \frac{(1 + |\vec{f}^1|)}{2} \delta^2(\hat{p} - \hat{f}^1) + \frac{(1 - |\vec{f}^1|)}{2} \delta^2(\hat{p} + \hat{f}^1) ,$$

$$\text{then clearly } \int \rho d\Omega = 1$$

$$\int \rho \hat{p} d\Omega = \vec{f}^1 ,$$

so $f^0 = 1$ and $|\vec{f}^1| \leq f^0$ is both necessary and sufficient for there to exist a probability distribution $\rho(\hat{p})$ with moments f^0 and $\vec{f}^1$. Note that if $\vec{f}^1$ attains its boundary value, i.e. $|\vec{f}^1| = 1$, then the probability distribution and all higher moments are uniquely determined.

$$\text{Proof: if } |\vec{f}^1| = 1, \text{ then } \int d\Omega \rho(\hat{p}) (1 - \vec{f}_1 \cdot \hat{p}) = 0, \text{ but this}$$

can only be true if $\rho(\hat{p})$ is zero everywhere except at $\hat{p} = \vec{f}_1$, implies

$$\rho(\hat{p}) = \delta^2(\hat{p} - \vec{f}_1) .$$

Therefore the higher moments are

$$f_{i_1, i_2, \dots, i_\ell}^\ell = \int d\Omega \rho \hat{p}_{i_1} \hat{p}_{i_2} \dots \hat{p}_{i_\ell}$$

$$= f_{i_1}^1, f_{i_2}^1, \dots, f_{i_\ell}^1$$

For $\ell = 2$

$$\text{let } f_{ij}^2 = \int d\Omega \rho(\hat{p}) \hat{p}_i \hat{p}_j$$

$$\text{then } \text{Tr} f^2 = \sum_i f_{ii}^2 = 1$$

$$\text{and } \int d\Omega \rho(\hat{p}) (\hat{p}_i - f_i^1) (\hat{p}_j - f_j^1) = f_{ij}^2 - f_i^1 f_j^1$$

is clearly a non negative quadratic form,

$$\left(f_{ij}^2 - f_i^1 f_j^1 \right) \geq 0 \text{ (note the resemblance to equation (8b)).}$$

Conversely if $f^0 = 1$, $|\vec{f}^1| \leq 1$, $\text{Tr} f^2 = 1$

and $f_{ij}^2 - f_i^1 f_j^1$ is non negative,

then rotate to a basis in which

$$\left(f_{ij}^2 - f_i^1 f_j^1 \right) \text{ is diagonal. In this basis,}$$

$$\left(f_{ij}^2 - f_i^1 f_j^1 \right) = \lambda_i \delta_{ij},$$

$$\lambda_i \geq 0 \text{ and } \sum \lambda_i = 1 - |\vec{f}^1|^2 = n.$$

Let $\alpha_i = \lambda_i/n$, implies $\sum \alpha_i = 1, \alpha_i \geq 0$.

$$\text{Let } \hat{p}(1, \pm) = \left(\pm \sqrt{n + (f_1^1)^2}, f_2^1, f_3^1 \right),$$

$$\hat{p}(2, \pm) = \left(f_1^1, \pm \sqrt{n + (f_2^1)^2}, f_3^1 \right),$$

$$\hat{p}(3, \pm) = \left(f_1^1, f_2^1, \pm \sqrt{n + (f_3^1)^2} \right),$$

and
$$\rho(i, \pm) = \frac{\alpha_i}{2} \left(1 \pm \frac{f_i^1}{\sqrt{n + (f_i^1)^2}} \right) \geq 0.$$

Then
$$\sum_{\pm} \sum_{i=1}^3 \rho(i, \pm) = 1$$

$$\sum_{\pm} \sum_{i=1}^3 \rho(i, \pm) \hat{p}(i, \pm) = \vec{f}^1,$$

$$\sum_{\pm} \sum_{i=1}^3 \rho(i, \pm) (\hat{p}_k(i, \pm) - f_k^1) (\hat{p}_j(i, \pm) - f_j^1) = \lambda_j \delta_{kj}$$

Therefore $f^0 = 1$, $|\vec{f}^1| \leq 1$, $\text{Tr} f^2 = 1$, $f_{ij}^2 - f_i^1 f_j^1 \geq 0$, (10)

is a necessary and sufficient set of conditions for there to exist a probability distribution with moments f^0 , f^1 , and f_{ij}^2 . If f_{ij}^2 attains one of its boundary values, then at least one of λ_1 , λ_2 , or $\lambda_3 = 0$. W.l.g. assume $\lambda_3 = 0$, then in the basis which diagonalizes f^2 ,

$$\int d\Omega \rho(\hat{p}) (\hat{p}_3 - f_3^1)^2 = 0,$$

implies $\rho(\hat{p}) = 0$ everywhere except on the line of latitude $\hat{p}_3 = f_3^1$, and all higher moments are constrained by the theory of moments for probability measures on the unit circle⁽⁷⁾.

For $\ell > 2$ although it is possible to write down necessary conditions on $f_{i_1 i_2 \dots i_\ell}^\ell$ which are analogous to equations (6), (7) and (8), I have been unable to prove that these are also sufficient. Furthermore, these equations for $\ell > 2$ have a complicated form which is hard to work with.

A more promising approach for $L > 2$ is to drop the sufficiency requirement and look for a set of conditions on the moments up to order $(L + 1)$ which

- 1) is a necessary set of conditions
- 2) is numerically tractable
- 3) becomes a sufficient set of conditions in the limit as $L \rightarrow \infty$.

One nice way to obtain a set of conditions satisfying 1), 2) and 3) is with the Bernstein polynomials⁽⁸⁾.

Consider the polynomials

$$P_{j_1 j_2 j_3}^{i_1 i_2 i_3}(\hat{p}) = \prod_{k=1}^3 \left[(1 + \hat{p}_k)^{i_k} (1 - \hat{p}_k)^{j_k} \right]$$

Clearly $P \geq 0$ everywhere on the unit sphere so if we consider all polynomials for which

$$\sum_{k=1}^3 (i_k + j_k) \leq L + 1,$$

then

$$\int d\Omega \rho(\hat{p}) P_{j_1 j_2 j_3}^{i_1 i_2 i_3}(\hat{p}) = E \left[P_{j_1 j_2 j_3}^{i_1 i_2 i_3} \right] \geq 0$$

$(E[f(\hat{p})])$ is the expectation value of $f(\hat{p})$ gives a necessary set of conditions on the moments up to order $(L + 1)$.

To prove sufficiency in the limit $L \rightarrow \infty$, consider the Bernstein polynomial

$$P_{j_1 j_2 j_3}^{i_1 i_2 i_3}(\hat{p}) = N_n B_n(\hat{u}, \hat{p})$$

where $\hat{u}$ is an arbitrary unit vector,

$$i_k = \left[\frac{(1+\hat{u}_k)}{2} \right], \quad k = 1, 2, 3.$$

$$j_k = n i_k \text{ and } N_n = \int d\Omega \rho_{j_1 j_2 j_3}^{i_1 i_2 i_3}(\hat{p}), \text{ is a normalization coefficient.}$$

It is shown in Reference (8) that

$$\lim_{n \rightarrow \infty} B_n(\hat{u}, \hat{p}) = \delta^2(\hat{u} - \hat{p})$$

the two dimensional Dirac data function on the unit sphere.

In the limit $L \rightarrow \infty$ our necessary set of conditions becomes the requirement that any Bernstein polynomial have expectation value ≥ 0 . Therefore if we let

$$\rho(\hat{u}) = \lim_{n \rightarrow \infty} E(B_n(\hat{u}, \hat{p})) \geq 0$$

then ρ is a probability distribution with the required moments, and our set of conditions is sufficient in the limit $L \rightarrow \infty$.

This for example, given f^0, f_i^1, f_{ij}^2 satisfying equations (10) we have as our conditions on f_{ijk}^3 ,

$$E((1 \pm \hat{p}_i)(1 \pm \hat{p}_j)(1 \pm \hat{p}_k)) \geq 0$$

$$\begin{aligned} \text{which implies, } & \left[1 \mp \left(\pm f_i^1 + f_j^1 + f_k^1 \right) + \left(f_{jk}^2 + f_{ij}^2 + f_{ik}^2 \right) \right] \geq f_{ijk}^3 \\ & \geq \left[-1 \mp \left(\pm f_i^1 + f_j^1 + f_k^1 \right) - \left(f_{jk}^2 + f_{ij}^2 + f_{ik}^2 \right) \right] \end{aligned} \quad (11)$$

Here the $\pm$ signs within a [] are linked.

Note that since these constraints for a finite order ℓ are necessary but not sufficient, when we go to a higher order $\ell' > \ell$ the consistency of the higher order inequalities imply additional constraints on the lower order moments.

II.

We will now consider a spherical harmonic expansion of the transport equation keeping only the zeroth and first moments of the equation.

Let
$$n(E, \vec{x}, t) = \int d\Omega \rho(\vec{x}, \vec{p}, t),$$

$$n \vec{f}_i^1 v = \vec{F}_i(E, \vec{x}, t) = \int d\Omega \rho(\vec{x}, \vec{p}, t) \vec{v}$$

(v is the velocity of particle with energy E).

Then the 1st two moments of the transport equation are

$$\frac{\partial n}{\partial t} + \vec{v} \cdot \vec{F} = \alpha(g - n), \quad (12)$$

$\frac{\partial F_i}{\partial t} + \nabla_j (n v^2 f_{ij}^2) = -\alpha F_i$, where g is a given emission spectrum of the background matter ($g \geq 0$). f_{ij}^2 is to be chosen in accordance with the constraints (10).

Substituting $n f_i^1 v$ for F_i in (12) and after a little algebra (12) can be rewritten as

$$\left(\frac{\partial}{\partial t} + v \vec{f}_i^1 \cdot \vec{\nabla} \right) n + n v \vec{v} \cdot \vec{f}_i^1 = \alpha(g - n) \quad (13a)$$

$$\left(\frac{\partial}{\partial t} + v \vec{f}_i^1 \cdot \vec{\nabla} \right) f_i^1 + \nabla_j \left[n v (f_{ij}^2 - f_i^1 f_j^1) \right] = -\alpha g f_i^1. \quad (13b)$$

The constraints (10) imply that if $|\vec{f}_1| = 1$, then $f_{ij}^2 = f_i^1 f_j^1$, for if $|\vec{f}_1| = 1$ then $\text{Tr} (f_{ij}^2 - f_i^1 f_j^1) = 1 - 1 = 0$ and a non negative matrix has zero trace i.f.f. $f_{ij}^2 - f_i^1 f_j^1 = 0$. We may think of equation (13b) like a hydrodynamic force equation

$$n \left(\frac{\partial}{\partial t} + v \vec{f}_1 \cdot \vec{\nabla} \right) f_i^1 = -\nabla_j \left[n v (f_{ij}^2 - f_i^1 f_j^1) \right] - \alpha g f_i^1 v,$$

where $n v (f_{ij}^2 - f_i^1 f_j^1)$ is analogous to the (velocity dependent) pressure tensor and $-\alpha g f_i^1 v$ is a viscous drag force.

Then we see immediately that if initially $|\vec{f}_1| \leq 1$ everywhere it can never become >1 because the viscous drag term will always try to decrease $|\vec{f}_1|$ in magnitude and the pressure tensor (the only force that can increase $|\vec{f}_1|$) will (because of the constraints (10)) always vanish as $1 - |\vec{f}_1|^2$ as $|\vec{f}_1| \rightarrow 1$. Thus our equations (13) are automatically flux limiting.

Looking at (13a), we see that it has just the form of the hydrodynamics equation of continuity (with a source term which is always positive when $n < g$) and therefore since the velocity $\vec{f}_1$ is always bounded, it must keep n always positive.

If in equations (13) the matter is very thin, then $\alpha = 0$. At $t=0$, let n be arbitrary and $\vec{f}_1 = \vec{u}$ everywhere. Then since $f_{ij}^2 - f_i^1 f_j^1 = 0$, $\vec{f}_1(\vec{x}, t) = \vec{u}$ and $n(\vec{x}, t) = n(\vec{x} - \vec{u}t, 0)$ is an exact solution of (13) with the given initial conditions. That is, equations (13) have the same free streaming solution as the exact transport equation in the limit of very thin background matter.

In general, one will want to choose f_{ij}^2 within the range allowed by eqs. (10) in accordance with one's physical intuition as to what the actual distribution $\rho(\hat{p})$ looks like in a given region.

However, if a general expression is desired, the simplest way to choose f_{ij}^2 in accordance with the constraints (10) is by observing that in the diffusion limit

$$f_{ij}^2 = \frac{1}{3} \delta_{ij} ,$$

and in the free streaming limit

$$f_{ij}^2 = f_i^1 f_j^1 ,$$

so interpolating between these two extremes one obtains

$$f_{ij}^2 = f_i^1 f_j^1 + \frac{1}{3} \delta_{ij} (1 - |\vec{f}^1|^2) . \quad (14)$$

Note that with this choice,

$$\text{Tr} f_{ij}^2 = 1$$

and $f_{ij}^2 - f_i^1 f_j^1 = \frac{1}{3} \delta_{ij} (1 - |\vec{f}^1|^2) \geq 0$, so the constraints (10) are indeed satisfied. Substituting (14) into (13) our equations become

$$\frac{\partial n}{\partial t} + v \vec{\nabla} \cdot (\vec{f}^1) = \alpha(g-n) \quad (15a)$$

$$\begin{aligned} n \frac{\partial \vec{f}^1}{\partial t} + n v (\vec{f}_1 \cdot \vec{\nabla}) \vec{f}^1 + \frac{v}{3} \vec{\nabla} \left[n (1 - |\vec{f}^1|^2) \right] \\ = - \alpha g \vec{f}^1 \end{aligned} \quad (15b)$$

It is interesting to note that if we solve equations (15) for a one dimensional steady state problem, and if in some regions of the problem (e.g. between two parallel plates of differing temperature) the flux $F_i = n f_i^1$ is constant ($\frac{\partial F}{\partial x} = 0$), then equations (15) with

$$f_{ij}^2 = f_i^1 f_j^1 + \frac{1}{3} \delta_{ij} (1 - |\vec{f}^1|^2)$$

give

$$-\left(\frac{v}{3\alpha}\right) \left(\frac{\partial n}{\partial x}\right) = \frac{f^1}{1 - 2(f^1)^2} \quad (16)$$

or

$$f^1 = \frac{-2Z}{\sqrt{1 + 1 + 8Z^2}}$$

where

$$Z = \left(\frac{v}{3\alpha}\right) \left(\frac{\partial n}{\partial x} / n\right)$$

Note the resemblance to the usual flux limiter (eq. (3a)) in this special case. In the diffusion limit, $Z \ll 1$

$$\text{and} \quad f^1 = -\left(\frac{v}{3\alpha}\right) \left(\frac{\partial n}{\partial x} / n\right) + O(Z^2)$$

In the free streaming limit, $Z \gg 1$

$$\text{and} \quad f^1 = \frac{1}{\sqrt{2}} + O\left(\frac{1}{Z}\right) \quad \text{or} \quad ,$$

$$F = \frac{v}{\sqrt{2}} + O\left(\frac{1}{Z}\right) .$$

Now let us look at the characteristic velocity associated with equation (15). The characteristic velocities in the direction $\hat{u}$ are given by the eigenvalues of the 4 x 4 matrix:

$$A = \begin{bmatrix} v (\hat{u} \cdot \vec{f}^1) & v n u_x & v n u_y & v n u_z \\ u_x (\frac{v}{3})(1-|\vec{f}^1|^2)/n & & & \\ u_y (\frac{v}{3})(1-|\vec{f}^1|^2)/n & & (v(u \cdot \vec{f}^1) \delta_{ij} - \frac{2v}{3} u_i f_j^1) & \\ u_z (\frac{v}{3})(1-|\vec{f}^1|^2)/n & & & \end{bmatrix}$$

If we rotate so that $\hat{u}_x = 1$ and $\hat{u}_y = \hat{u}_z = 0$, then

$$A = \begin{bmatrix} v f_x^1 & n v & 0 & 0 \\ (\frac{v}{3})(1-|\vec{f}^1|^2)/n & \frac{v}{3} f_x^1 & -\frac{2v}{3} f_y^1 & -\frac{2v}{3} f_z^1 \\ 0 & 0 & v f_x^1 & 0 \\ 0 & 0 & 0 & v f_x^1 \end{bmatrix}$$

So

$$\det (\lambda I - A) = (\lambda - v (\hat{u} \cdot \vec{f}^1))^2 \left(\lambda^2 - \frac{4}{3} v \lambda (\hat{u} \cdot \vec{f}^1) - \frac{v^2}{3} (1-|\vec{f}^1|^2) - (\hat{u} \cdot \vec{f}^1)^2 \right)$$

and the characteristic velocities are

$$\lambda_t = v (\hat{u} \cdot \vec{f}^1) \text{ for transverse waves,}$$

and

$$\lambda_\ell = \frac{2v}{3} (\hat{u} \cdot \vec{f}^1) \pm \frac{v}{3} \sqrt{3(1-|\vec{f}^1|^2) + (\hat{u} \cdot \vec{f}^1)^2}$$

for longitudinal waves.

(17)

For $|\vec{f}^1| \leq 1$ and $-|\vec{f}^1| \leq (\hat{u} \cdot \vec{f}^1) \leq |\vec{f}^1|$,

it is easy to show that

$$-1 \leq \lambda_t, \lambda_\ell \leq +1$$

and λ_t, λ_ℓ take on all values within this range. Therefore, the range of characteristic velocities for our $L = 1$ approximate equation is exactly that of the transport equation.

Clearly all these results also apply to the one dimensional case.

Conclusion

The transport equation may be solved by expanding it in spherical harmonics, Y_{lm} , and truncating the resultant infinite set of equations at some finite order L . This procedure leaves the $(L + 1)$ th order moments which appear in the L th order equation undetermined and the standard procedure for obtaining a closed set of equations has been to set all the $(L + 1)$ th order moments to zero.

It has been shown above that this procedure actually violates our apriori knowledge that we are solving for the moments of a probability measure on the unit sphere. Using the theory of moments as discussed above, the $(L + 1)$ th order moments can be chosen in accordance with our apriori knowledge. The resultant truncated set of equations has properties much truer to the original transport equation than the usual set obtained by setting the $(L + 1)$ th order moments to zero. In particular our truncated set of equations gets the solution of the transport equation exactly right in both the diffusion limit and the free streaming limit. Furthermore, this has been achieved by merely truncating our set of equations properly and not by any ad hoc changes in our basic equations as is the case in the approaches that use flux limiters.

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3. J. A. Sohat and J. D. Tamarkin, "The Problem of Moments", American Mathematical Society, Mathematical Surveys #1, N. Y. (1943). N. I. Aheizer and M. Krein, "Theory of Moments", American Mathematical Society Translations of Mathematical Monographs, Vol. 2, Providence (1962).
4. IBID, Aheizer and Krein, p. 35.
5. A real matrix M_{ij} is non negative if and only if for all real vectors X_i .
$$\sum_{ij} M_{ij} X_i X_j \geq 0.$$
6. IBID, Aheizer and Krein, p. 38. The method for finding ρ is given on pps. 39, 40.
7. IBID, Aheizer and Krein, p. 12.
8. IBID, Sohat and Tamarkin, p. 8.

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