On the Number of Moments in Radiative Transfer Problems

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In a recent paper (Struchtrup, Annals of Physics, **257**, 1997) we set up an extended moment method for radiative transfer problems, which involves matrices of mean absorption and scattering coefficients. In the present paper, we examine the resulting moment equations for one-dimensional radiative transfer problems. In particular we are interested in the number of moments which one has to choose in order to have satisfactory agreement between solutions of the moment equations and solutions of the radiative transfer equation. We show that the moment theory will describe a one-dimensional beam properly, if moments with a tensorial rank of about 30 are taken into account. © 1998 Academic Press

1. INTRODUCTION

In a previous paper [10], we presented a system of moment equations for radiative transfer problems. In that paper we investigated the covariant form of the equations as well as the non-relativistic limit. We also tested the equations for two important cases: local radiative equilibrium and homogeneous processes.

The present paper treats one-dimensional non-equilibrium processes, in particular radiation beams travelling through gases. For simplicity, we restrict our attention to the case of homogeneous matter at rest, i.e., the density and the temperature of matter are constant in space and time and the velocity equals zero.

The moment equations for this case were derived in [10] from the covariant radiative transfer equation by means of the entropy maximum principle. Nevertheless, we review their derivation in Appendix A, where we consider the equations in the rest frame of the matter.

The moments on which the theory is based are defined as

$$u_{\langle i_{1}i_{2}\cdots i_{n}\rangle}^{r} = \left(\frac{\hbar}{c}\right)^{r+3} \int \omega^{r+2} n_{\langle i_{1}}\cdots n_{i_{n}\rangle} f \, d\omega \, d\Omega, \qquad r = 1, ..., R; \quad n = 0, ..., N,$$
(1)

where ω is the photon frequency, n_i denotes the photon direction vector and f is the phase density of photons; \hbar is Planck's constant and c is the speed of light. The indices in angular brackets denote a symmetric traceless tensor. The densities of

radiative energy e and momentum p_i and the radiative pressure tensor N_{ij} are related to the moments by the relations

$$e = cu^{1}, \quad p_{i} = u_{i}^{1}, \quad N_{ij} = \frac{1}{3}e\delta_{ij} + cu_{\langle ij \rangle}^{1};$$
 (2)

the other moments have no obvious intuitive physical meaning.

Thus, the total number of moments in the theory is given by the product of the two numbers R and N. To begin with, the theory is developed for an arbitrary number of moments and the question arises of how to choose the number of moments in order to obtain reasonable results from the moment equations. In particular, the moment equations must predict the same space-time behavior for a process as the radiative transfer equation. As in [10], we will consider some simple processes for which both moment equations and the radiative transfer equation are solved. The comparison of the results will provide information about the number of moments needed.

Our set of moment equations differs from those of other authors, e.g., [4, 7, 9, 11], mostly in the production terms and in the occurrence of the number R. Those of our results which concern the number N for R = 1 are valid for these theories, too.

The plan of the paper is as follows: In Section 2 we briefly review the moment equations. These are solved in Section 3 for the propagation of a one-dimensional beam. We shall determine the necessary number of moments N by the consideration of two distinctive limits, the damped wave limit (absorption dominates) and the diffusion limit (scattering dominates). Whereas in the latter case N = 1 will be sufficient, we show that in the first case one must choose $N \simeq 30$ in order to describe the radiation in accordance with nature.

In order to obtain the necessary number R, we solve the radiative transfer equation in Section 4 for a beam that penetrates into an atmosphere in the damped wave limit. The solutions of the radiative transfer equation and of the moment equations are compared, and we show that they agree, if $R \simeq 6$ holds in the case of absorption by bremsstrahlung.

2. THE MOMENT EQUATIONS

The moment equations read (see Appendix A for derivation)

$$\frac{\partial u^{r}}{\partial t} + c \frac{\partial u^{r}_{k}}{\partial x_{k}} = -\sum_{q=1}^{R} \Theta_{rq}(u^{q} - u^{q}_{|E})$$

$$\frac{\partial u^{r}_{\langle i_{1}i_{2}\cdots i_{n}\rangle}}{\partial t} + \frac{n}{2n+1} c \frac{\partial u^{r}_{\langle i_{1}i_{2}\cdots i_{n-1}\rangle}}{\partial x_{i_{n}\rangle}} + c \frac{\partial u^{r}_{\langle i_{1}i_{2}\cdots i_{n}k\rangle}}{\partial x_{k}} = -\sum_{q=1}^{R} \hat{\Theta}_{rq} u^{q}_{\langle i_{1}i_{2}\cdots i_{n}\rangle} \quad (3)$$

$$\frac{\partial u^{r}_{\langle i_{1}i_{2}\cdots i_{N}\rangle}}{\partial t} + \frac{N}{2N+1} c \frac{\partial u^{r}_{\langle i_{1}i_{2}\cdots i_{N-1}\rangle}}{\partial x_{i_{N}\rangle}} = -\sum_{q=1}^{R} \hat{\Theta}_{rq} u^{q}_{\langle i_{1}i_{2}\cdots i_{N}\rangle},$$

r = 1, ..., R; n = 0, ..., N. The matrix of mean absorption coefficients Θ_{rs} and the matrix of mean absorption and scattering coefficients $\hat{\Theta}_{rs}$ are given by

$$\Theta_{rs} = \left(\frac{k_B T}{c}\right)^{r-s} \sum_{t=1}^{R} \mathscr{C}_{ts}^{-1} \int \kappa(\Xi) \frac{e^{\Xi}}{(e^{\Xi} - 1)^2} \Xi^{t+r+2} d\Xi$$
(4)

and

$$\hat{\Theta}_{rs} = \Theta_{rs} + \left(\frac{k_B T}{c}\right)^{r-s} \sum_{t=1}^{R} \mathscr{C}_{ts}^{-1} \int \varsigma(\Xi) \frac{e^{\Xi}}{(e^{\Xi} - 1)^2} \Xi^{t+r+2} d\Xi$$
(5)

with $\mathscr{C}_{rs} = \Gamma(s+r+3) \zeta(s+r+2)$; $u_{|E}^{r}(T)$ denotes the equilibrium value of the moments,

$$u_{|E}^{r}(T) = 4\pi y \left(\frac{k_{B}T}{c}\right)^{r+3} \Gamma(r+3) \zeta(r+3), \qquad u_{\langle i_{1}i_{2}\cdots i_{n}\rangle|E}^{r}(T) = 0$$
(6)

and T is the temperature of matter; k_B denotes Boltzmann's constant.

 $\kappa(\Xi)$ and $\varsigma(\Xi)$ are the spectral absorption and scattering coefficients, respectively, written as functions of the dimensionless parameter $\Xi = \hbar \omega / k_B T$. As in [10], we consider only Thomson scattering on electrons and the absorption of bremsstrahlung with [1, 11]

$$\varsigma_T = const.$$
 $\kappa_{ff}(\Xi) = D_{ff} \frac{1 - \exp(-\Xi)}{\Xi^3}.$ (7)

The constant D_{ff} depends on atomic constants of the matter. For the matrices, we obtain

$$\Theta_{rs} = D_{ff} \left(\frac{k_B T}{c}\right)^{r-s} \sum_{t} \Gamma(t+r) \zeta(t+r) \mathscr{C}_{ts}^{-1}$$
(8)

and

$$\hat{\Theta}_{rs} = \Theta_{rs} + \zeta_T \delta_{rs}. \tag{9}$$

With (3) we have R hierarchies of moment equations, each one consisting of tensor equations up to rank N. The main problem is the determination of R and N appropriate to the phenomenon under consideration.

3. PENETRATION OF A BEAM OF RADIATION INTO MATTER

3.1. One-Dimensional Field Equations

We consider the propagation of a one-dimensional beam of radiation into matter. A typical example occurs when a sun beam penetrates the earth's atmosphere which here we suppose to have the uniform and constant temperature T.

The appropriate system of equations is (3) except that now we specialize the system to one dimension, the direction of the 1-axis or x-axis. We obtain

$$\frac{\partial u_{\langle 0 \rangle}}{\partial t} + c \frac{\partial u_{\langle 1 \rangle}}{\partial x} = -\sum_{q} \Theta_{rq} (u_{\langle 0 \rangle}^{q} - u_{\langle 0 \rangle | E}^{q})$$

$$\frac{\partial u_{\langle n \rangle}}{\partial t} + \frac{n^{2}}{4n^{2} - 1} c \frac{\partial u_{\langle n-1 \rangle}}{\partial x} + c \frac{\partial u_{\langle n+1 \rangle}}{\partial x} = -\sum_{q} \hat{\Theta}_{rq} u_{\langle n \rangle}^{q}$$

$$\frac{\partial u_{\langle N \rangle}}{\partial t} + \frac{N^{2}}{4N^{2} - 1} c \frac{\partial u_{\langle N-1 \rangle}}{\partial x} = -\sum_{q} \hat{\Theta}_{rq} u_{\langle n \rangle}^{q}.$$
(10)

Here we have introduced the abbreviation

$$u_{\langle n \rangle}^{r} = u_{\langle 11 \cdots 1 \rangle}^{r}.$$
(11)

Also in what follows we shall abbreviate $n^2/(4n^2-1)$ as α_n .

3.2. Characteristic Speeds and Amplitudes of a Propagating Beam

Since free-flying photons travel with the speed of light c, we know that a beam propagates with c. The fastest propagation speed implied by the system (10) of moments, however, is equal to the largest characteristic speed of the system. This knowledge provides a criterion for the break-off of the system: The number N of moments $u_{\langle n \rangle}^{r}$ —needed for the representation of a beam—is such that the largest characteristic speed equals c.

The characteristic speeds of the system (10) are the eigenvalues of the matrix¹

$$\mathcal{A}_{AB} = c \begin{bmatrix} 0 & 1 & & & \\ \alpha_1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \alpha_N & 0 \end{bmatrix},$$
(12)

which are easy to determine numerically. The value of the largest eigenvalue—and thus the largest characteristic speed—is plotted in Fig. 1 for different values of N. Inspection shows that the value c is rapidly approached as N grows. For $N \ge 30$ we may say that the largest characteristic speed is equal to c.

Thus for a proper description of a beam of radiation we need as many as 30 moments, at least according to the speed criterion.

¹ Note that the matrix is the same for all of the R systems.



FIG. 1. The largest characteristic speed of the moment equations approaches the speed of light rapidly as N increases.

A beam in vacuum is described by (10) with $\Theta_{rq} = \hat{\Theta}_{rq} = 0$. The solution is obtained by transformation to the principal axes of (12) and reads

$$u_{\langle n\rangle}^{r} = \sum_{\gamma} R_{n}^{\gamma} f^{\gamma}(x - V^{\gamma}t), \qquad (13)$$

where R_n^{γ} is the eigenvector corresponding to the eigenvalue V^{γ}/c and $f^{\gamma}(x)$ is the amplitude; V^{γ} are the characteristic speeds.

For the calculation of the eigenvectors, it is useful to know that the determinant

$$D_{n+1}^{\gamma} = \begin{vmatrix} -V^{\gamma}/c & 1 \\ \alpha_1 & -V^{\gamma}/c & 1 \\ \alpha_2 & -V^{\gamma}/c & 1 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n-1} & -V^{\gamma}/c & 1 \\ \alpha_n & -V^{\gamma}/c \end{vmatrix}, \quad n \ge 2 \quad (14)$$

obeys the recurrence relation

$$D_{n+1}^{\gamma} = -V^{\gamma}/c \ D_n^{\gamma} - \alpha_n D_{n-1}^{\gamma}, \quad \text{with} \quad D_0^{\gamma} = 11, \quad D_1^{\gamma} = -V^{\gamma}/c.$$
(15)

The eigenvalues are the solutions of $D_{N+1}^{\gamma} = 0$. It is easy to show that the eigenvectors are given by the relation

$$R_n^{\gamma} = (-1)^n \, D_n^{\gamma},\tag{16}$$

where we have set R_n^{γ} equal to 1. The eigenvectors form an orthogonal set with $\sum_n R_n^{\gamma} R_n^{\varepsilon} = \sum_n R_n^{\gamma} R_n^{\gamma} \delta_{\gamma \varepsilon}$.

Since we know that the beam propagates with just one speed, $V_{\text{max}} \simeq c$, we have to stipulate that other characteristic speeds of the system should not appear in the mathematical description of a beam. This requires that the initial or boundary data for the beam be chosen properly. Let us consider:

For a beam in x-direction the phase density is a delta function of angle, so that the moments

$$u_{i_{1}i_{2}\cdots i_{n}}^{r} = \left(\frac{\hbar}{c}\right)^{r+3} \int \omega^{r+2} n_{i_{1}}\cdots n_{i_{n}} f \, d\omega \, d\Omega, \qquad r = 1, ..., R; \quad n = 0, ..., N, \quad (17)$$

have vanishing components unless $i_1 = i_2 = \cdots = i_n = 1$ holds. We have

$$u_{1,1,\dots,1}^r = u^r$$
, $r = 1, \dots, R; n = 0, \dots, N$

independent of n and find, by means of equation (3.27) of [10],

$$u_{\langle n \rangle}^{r} = u_{\langle 1 \cdots 1 \rangle}^{r} = \overline{D}_{n} u^{r}$$
(18)

with

$$\overline{D}_{n} = \sum_{k=0}^{\|n/2\|} \frac{(-1)^{k}}{\prod_{j=0}^{k-1} (2n-2j-1)} \frac{n!}{(n-2k)! \, 2^{k} \, k!}, \qquad \|n/2\| = \begin{cases} n/2 & n \text{ even} \\ (n-1)/2 & n \text{ uneven.} \end{cases}$$
(19)

The coefficients \overline{D}_n obey the recurrence relation

$$\bar{D}_{n+1} = \bar{D}_n - \alpha_n \bar{D}_{n-1}$$
 with $\bar{D}_0 = 1$, $\bar{D}_1 = 1$. (20)

We consider (15) with the maximum characteristic speed $V^{\gamma} = V_{\text{max}}$. If we have a large number N of moments so that—according to Fig. 1— $V_{\text{max}}/c \simeq 1$ holds, we find by comparison of (15) and (16)

$$(-1)^n D_n^{\max} \simeq \overline{D}_n,\tag{21}$$

where D_n^{max} is the determinant (14) with $V^{\gamma} = V_{\text{max}}$. Thus by (16) and (21) we may write, instead of (18), for the moments in a beam

$$u_{\langle n \rangle}^r \simeq R_n^{\max} u^r, \qquad r = 1, ..., R; \quad n = 0, ..., N,$$
 (22)

where R_n^{max} is the eigenvector corresponding to V_{max} . Note that we have $u_{\langle n \rangle}^r = 0$ for n > N in this approximation which corresponds to the very small values of \overline{D}_n for large n.

If the boundary and initial data obey (22) the general solution of (13) reduces to

$$u_{\langle n\rangle}^{r} = R_{n}^{\max} f(x - V_{\max} t).$$
⁽²³⁾

Thus the beam travels with the maximum characteristic speed. It should be emphasized that this result follows from the special form (22) of the initial and boundary data which was constructed by physical arguments. Due to (22) the initial values of the moments are not independent. From a mathematical point of view the initial values of the moments may be chosen independent of each other. In this case one would find all characteristic speeds in the solution (13). We think that it is impossible to create initial data of this kind.² If this assumption is correct, the other characteristic speeds have no physical meaning.

If the beam propagates into an equilibrium state so that $u_{\langle n \rangle}^r = 0$ $(n \ge 1)$ holds in front of the beam, we have for $n \ge 1$

$$u_{\langle n \rangle}^{r} = R_{n}^{\max}(u_{\langle 0 \rangle}^{r} - u_{\langle 0 \rangle | E}^{r}).$$

$$(24)$$

3.3. Plane Harmonic Waves and Dispersion Relation (General)

The hierarchies (10) are coupled through the right hand sides. But they may easily be decoupled by a linear transformation of the form

$$u_{\langle n \rangle}^{r} - u_{\langle n \rangle | E}^{r} = \sum_{s} M_{rs} w_{\langle n \rangle}^{s}$$
⁽²⁵⁾

such that the matrix M_{rs} is the matrix of right eigenvectors of the matrix Θ_{rq} . We have

$$\sum_{r,q} M_{sr}^{-1} \Theta_{rq} M_{qp} = \mu_s \delta_{sp} ,$$

where μ_s are the eigenvalues of Θ_{rq} . The decoupling is possible, because Θ_{rq} and $\hat{\Theta}_{rq}$ differ only by a unit matrix, see (9). It follows that we may rewrite the *R* coupled systems (10) as *R* uncoupled systems for $w_{\langle n \rangle}^s$,

$$\frac{\partial w_{\langle 0\rangle}^{s}}{\partial t} + c \frac{\partial w_{\langle 1\rangle}^{s}}{\partial x} = -\mu_{s} w_{\langle 0\rangle}^{s}$$

$$\frac{\partial w_{\langle n\rangle}^{s}}{\partial t} + \alpha_{n} c \frac{\partial w_{\langle n-1\rangle}^{s}}{\partial x} + c \frac{\partial w_{\langle n+1\rangle}^{s}}{\partial x} = -\hat{\mu}_{s} w_{\langle n\rangle}^{s}$$

$$\frac{\partial w_{\langle N\rangle}^{s}}{\partial t} + \alpha_{N} c \frac{\partial w_{\langle N-1\rangle}^{s}}{\partial x} = -\hat{\mu}_{s} w_{\langle N\rangle}^{s};$$
(26)

 $\hat{\mu}_s$ equals $\mu_s + \varsigma_T$.

We investigate plane harmonic waves of the form

$$\tilde{w}_{\langle n \rangle}^{s,\Omega} \exp i(\Omega t - q_s x) \tag{27}$$

 2 A similar problem would be to prescribe temperature and heat flux independent of each other at a wall.

as solutions of the s-system (26). $\tilde{w}_{\langle n \rangle}^{s,\Omega}$ are complex amplitudes and Ω and q_s are frequency and wave numbers, respectively. The phase speeds and attenuation coefficients are given by

$$v_{Ph} = \frac{\Omega}{\operatorname{Re}(q)}, \qquad \alpha_s = -\operatorname{Im}(q).$$
 (28)

Insertion of (27) into (26) provides homogenous algebraic systems of the form

where

$$\beta_s = \frac{\hat{\mu}_s + i\Omega}{icq_s}, \qquad \gamma_s = \frac{\mu_s + i\Omega}{\hat{\mu}_s + i\Omega}.$$
(30)

These systems have non-trivial solutions, if the determinant vanishes, a condition which requires the dispersion relation

$$\begin{vmatrix} -\gamma\beta & 1 & & \\ \alpha_{1} & -\beta & 1 & & \\ & \alpha_{2} & -\beta & 1 & & \\ & & \alpha_{3} & -\beta & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha_{N-1} & -\beta & 1 \\ & & & & \alpha_{N} & -\beta \end{vmatrix} = 0.$$
(31)

3.4. Intense Absorption: The Damped Wave Limit

If there is much more absorption and emission than scattering, we may neglect ς . Hence the difference between $\hat{\mu}_s$ and μ_s vanishes, so that $\gamma_s = 1$ holds.

In that case β_s are the eigenvalues of the matrix \mathscr{A} in (12)—independent of *s* or, in other words, the characteristic speeds of the system (10). If the initial and boundary data are chosen according to (22) the eigenvectors—here $\tilde{w}_{\langle n \rangle}^{s,\Omega}$ by (29)—vanish for all but the largest β_s . That largest value is equal to V_{\max}/c or, if N is large enough, it is equal to 1. Thus, by (30), we obtain

$$q_s = \frac{\Omega - i\mu_s}{c} \tag{32}$$

so that there is no dispersion and the damping is independent of Ω . We have

$$v_{Ph} = c$$
 and $\alpha = \mu_s/c.$ (33)

The amplitudes are related according to (24)

$$\tilde{w}^{s,\Omega}_{\langle n\rangle} = (-1)^n D_n \tilde{w}^{s,\Omega}_{\langle 0\rangle}.$$
(34)

The $w_{\langle n \rangle}^s$ -part of the beam can be represented by a superposition of harmonic waves—Fourier harmonics with different frequencies Ω —so that we may write

$$w^{s}_{\langle n \rangle} = \int_{-\infty}^{\infty} \tilde{w}^{s,\Omega}_{\langle n \rangle} e^{i(\Omega t - q_{s} x)} d\Omega,$$

or by (32)

$$w_{\langle n \rangle}^{s} = \int_{-\infty}^{\infty} \tilde{w}_{\langle n \rangle}^{s, \,\Omega} e^{i\Omega(t - x/c)} \, d\Omega \, e^{-\mu_{s} x/c}.$$
(35)

If we return to the moments $u_{\langle n \rangle}^r$, we thus obtain

$$u_{\langle n \rangle}^{r} - u_{\langle n \rangle | E}^{r} = \sum_{s} M_{rs} \int_{-\infty}^{\infty} \tilde{w}_{\langle n \rangle}^{s, \Omega} e^{i\Omega(t - x/c)} d\Omega e^{-\mu_{s} x/c}.$$
 (36)

Therefore, the beam penetrates the matter as a damped wave propagating with velocity c. Let the wave be created by a boundary stimulus at x = 0 given by the functions

$$(\overset{0}{u_{\langle 0\rangle}} - \overset{0}{u_{\langle 0\rangle | E}})(t) = \sum_{s} M_{rs} \int_{-\infty}^{\infty} \tilde{w}_{\langle 0\rangle}^{s,\Omega} e^{i\Omega t} d\Omega,$$
 (37)

$${}^{0}_{u_{\langle n \rangle}}^{r} = (-1)^{n} D_{n}(u_{\langle 0 \rangle}^{r} - u_{\langle 0 \rangle \mid E}^{r}).$$
(38)

The propagating damped wave may then be written in the form³

$$(u_{\langle n \rangle}^{r} - u_{\langle n \rangle \mid E}^{r})(x, t) = (-1)^{n} D_{n} \sum_{t} \left(\sum_{s} M_{rs} e^{-\mu_{s} x/c} M_{st}^{-1} \right) (u_{\langle 0 \rangle}^{t} - u_{\langle 0 \rangle \mid E}^{0}) \left(t - \frac{x}{c} \right).$$
(39)

Note that, starting from (32), the formulae are valid, if $N \ge 30$ holds, because otherwise V_{max} is not equal to c.

³ Recall that all $u'_{\langle n \rangle | E} = 0$ for $n \ge 1$, since we let the beam propagate into an equilibrium state.

3.5. Intense Scattering: The Diffusion Limit

If scattering is more important than absorption and emission, we may set $\mu_s = 0$ and $\hat{\mu}_s = \varsigma_T = \varsigma$. This gives the system (29) the form

$$\begin{bmatrix} -\frac{\Omega}{cq_s} & 1 & & \\ \alpha_1 & -\frac{\zeta + i\Omega}{icq_s} & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{N-1} & -\frac{\zeta + i\Omega}{icq_s} & 1 \\ & & & \alpha_N & -\frac{\zeta + i\Omega}{icq_s} \end{bmatrix} \begin{bmatrix} \tilde{w}_{\langle 0 \rangle} \\ & \tilde{w}_{\langle 1 \rangle} \\ & & & \\ &$$

We proceed to solve this system for the special case of small frequencies, i.e., $\Omega \ll \varsigma$ and $(cq_s/\varsigma)^2 \ll 1$. In that case the system (40) may be reduced to two recurrence equations, viz.

$$-\frac{\Omega}{cq}\tilde{w}^{s,\Omega}_{\langle 0\rangle} + \tilde{w}^{s,\Omega}_{\langle 1\rangle} = 0, \qquad \frac{icq}{\zeta}\alpha_n\tilde{w}^{s,\Omega}_{\langle n-1\rangle} - \tilde{w}^{s,\Omega}_{\langle n\rangle} = 0 \qquad (n \ge 1).$$
(41)

Hence it follows that all amplitudes vanish unless we have

$$q_s = \pm \sqrt{-i(3\varsigma \Omega/c^2)},\tag{42}$$

independent of s.

Just as the eigenvalue problem (39) belongs to the differential system (26), the new—approximate—eigenvalue problem (41) belongs to the differential system

$$\frac{\partial w_{\langle 0\rangle}^{s}}{\partial t} + c \frac{\partial w_{\langle 1\rangle}^{s}}{\partial x} = 0$$

$$\alpha_{n} c \frac{\partial w_{\langle n-1\rangle}^{s}}{\partial x} = -\varsigma w_{\langle n\rangle}^{s} \qquad (n = 1, ..., N).$$
(43)

Therefore we conclude that the approximations employed here have reduced the system to two equations, one for n = 0 and n = 1. These two equations combine to give the diffusion equation

$$\frac{\partial w_{\langle 0\rangle}^s}{\partial t} - \frac{c^2}{3\varsigma} \frac{\partial^2 w_{\langle 0\rangle}^s}{\partial x^2} = 0.$$
(44)

All moments $w_{\langle n \rangle}^s$ with $n \ge 1$ may be obtained from the solution of (44) by differentiation, cf. (43)₂. We conclude that the predominance of scattering over absorption and emission makes radiation propagate into matter diffusively. Only $w_{\langle 0 \rangle}^s$ —hence $u_{\langle 0 \rangle}^s$ —is important now and, if we consider it as a superposition of harmonic waves, we may write

$$w^{s}_{\langle 0 \rangle} = \int_{-\infty}^{\infty} \tilde{w}^{s, \Omega}_{\langle 0 \rangle} e^{i(\Omega t - q_{s} x)} d\Omega.$$

To calculate the corresponding fields $(u_{\langle 0 \rangle}^r - u_{\langle 0 \rangle | E}^r)(x, t)$ is both easier and more difficult than in the case of intense absorption: easier, because q_s is independent of s now, and more difficult, since q is not a linear function of Ω . We obtain

$$(u_{\langle 0\rangle}^{r} - u_{\langle 0\rangle|E}^{r})(x, t) = \int_{-\infty}^{\infty} (u_{\langle 0\rangle}^{t} - u_{\langle 0\rangle|E}^{t})(\tau) \left[\int_{0}^{\infty} e^{-\sqrt{(3\varsigma \Omega/2c^{2})}x} \cos\left(\Omega(t-\tau) - \sqrt{\frac{3\varsigma \Omega}{2c^{2}}}x\right) d\Omega \right] d\tau,$$

$$(45)$$

where

$$(\overset{0}{u_{\langle 0\rangle}^{t}}-\overset{0}{u_{\langle 0\rangle|E}^{t}})(t)$$

are the boundary values as functions of time.

3.6. The General Case and a Simple Example

In general, we shall have both absorption and emission, as well as scattering. The beam created by a boundary stimulus is then quite difficult to calculate and it would not be very instructive to describe the method that must be followed. But the result is bound to be given—at least qualitatively—as shown in Fig. 2 which refers to a short-pulse-stimulus: The damped pulse arrives first and it drags a wake of scattered radiation behind it.

The curve of Fig. 2 has been calculated for the case R = 1 and N = 4 and for κ and ς independent of k. The duration of the pulse Δt was chosen to make t, x, κ and ς dimensionless

$$\bar{t} = t/\Delta t, \qquad \bar{x} = x/c\Delta t, \qquad \bar{\kappa} = \kappa \Delta t, \qquad \bar{\zeta} = \zeta \Delta t.$$

The total energy supply $e = hc(u^1 - u_{|E}^1) \Delta t$ (i.e., the area below the curve) was equal to e_0 when the pulse was created and at $\bar{x} = 20$ —in Fig. 2—it has already dropped to less than $0.00081e_0$. The peak is due to photons that have passed the matter without any interaction and the long wake behind the peak stems from scattered photons. Note that the peak does not propagate with the speed of light, since we have chosen N equal to 4.



FIG. 2. Propagation of a damped pulse followed by a wake of scattered radiation.

4. A BEAM IN AN ABSORBING ATMOSPHERE

4.1. Phase Density in Distance r from a Star

We consider a star of radius R_{\odot} which emits black body radiation of temperature T_{\odot} . An observer outside the star sees only radiation with direction vectors pointing from the sun to the observer. In this direction, the frequency distribution is given by the equilibrium phase density

$$f_{|E}(T_{\odot}) = \frac{1}{4\pi^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1},$$
(46)

while it is equal to zero in all other directions. If we define angles such that the photon direction vector is given by $n_i = \{\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta\}_i$, we find for the distribution function in distance r

$$f_r = \begin{cases} f_{|E}(T_{\odot}), & \vartheta \in \left(0, \arcsin\frac{R_{\odot}}{r}\right), \quad \varphi \in (0, 2\pi) \\ 0, & \vartheta \in \left(\arcsin\frac{R_{\odot}}{r}, \pi/2\right), \quad \varphi \in (0, 2\pi). \end{cases}$$
(47)

4.2. Moments in Distance r

We calculate the moments from (1) with the phase density (46) far away from the star, i.e. when $R_{\odot}/r \ll 1$ holds. In this limit, the only non-vanishing part of the moments is

$$u_{3\dots3}^{r} = \left(\frac{\hbar}{c}\right)^{r+3} \int \omega^{r+2} n_{3} \cdots n_{3} f \, d\omega \, d\Omega$$
$$= \left(\frac{\hbar}{c}\right)^{r+3} \int_{0}^{\infty} \omega^{r+2} f_{|E}(T_{\odot}) \, d\omega \int_{0}^{\arcsin(R_{\odot}/r)} \cos^{n} \vartheta f \sin \vartheta \, d\vartheta \int_{0}^{2\pi} d\varphi$$
$$\simeq \frac{u_{|E}^{r}(T_{\odot})}{4} \left(\frac{R_{\odot}}{r}\right)^{2}.$$

We are only interested in the traceless part of $u_{3...3}^r$ and obtain, with equation (34) in [10],

$$u_{\langle n \rangle}^{r} = u_{\underbrace{\langle 3 \cdots 3 \rangle}_{n-\text{times}}}^{r} = \overline{D}_{n}u^{r} \qquad \text{with} \quad u^{r} = \frac{u_{|E}^{r}(T_{\odot})}{4} \left(\frac{R_{\odot}}{r}\right)^{2}; \tag{48}$$

 \overline{D}_n is given by (19). Equation (48) agrees with our result from the moment equations (22) if we set $V_{\text{max}}/c = 1$ in (15).

4.3. A Beam (Boundary Value Problem)

Now we consider the penetration of a short plane radiation pulse into an isothermal absorbing atmosphere of constant density. We consider this to be a one-dimensional problem and write the one-dimensional radiative transfer equation as [4, 7]

$$\frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = -\kappa (f - f_{|E}(T)). \tag{49}$$

 κ is the absorption coefficient and T denotes the temperature of the atmosphere. We consider the following initial and boundary values

$$f(t, x=0) = f_{|E}(T) + f_r(T_{\odot}) F(t),$$
(50)

$$f(t=0, x) = f_{|E}(T),$$
(51)

where $f_r(T_{\odot})$ is given by $(47)^4$ and F(t) is a window function, viz.

$$F(t) = \begin{cases} 1, & t \in (0, \Delta t) \\ 0, & \text{else.} \end{cases}$$
(52)

In terms of moments, the initial and boundary data read

$$u_{\langle n \rangle}^{r}(t, x=0) = u_{\langle n \rangle | E}^{r}(T) + \bar{D}_{n} \frac{u_{|E}^{r}(T_{\odot})}{4} \left(\frac{R_{\odot}}{r}\right)^{2} F(t)$$
(53)

⁴ We neglect the expansion of the beam, i.e. we consider only distances which are much smaller than the distance from the star.

and

$$u_{\langle n \rangle}^{r}(t=0,x) = u_{\langle n \rangle | E}^{r}(T).$$
 (54)

4.4. Solution of Radiative Transfer Equation

The solution of (49)-(52) is given by

$$f(t, x) = f_{|E}(T) + f_r(T_{\odot}) F\left(t - \frac{x}{c}\right) \exp -\kappa \frac{x}{c}.$$
(55)

Now we are able to compute the moments as functions of space and time. We introduce dimensionless measures for the scalar moments, viz.

$$v^{r} = 4 \frac{u^{r} - u^{r}_{|E}(T)}{u^{r}_{|E}(T_{\odot})(R_{\odot}/r)^{2}}$$
(56)

and obtain for their space-time dependence⁵

$$v^{r}(t,x) = \frac{F(t - (x/c))}{\Gamma(r+3)\,\zeta(r+3)} \int \frac{\Xi_{\odot}^{r+2}}{e^{\Xi_{\odot}} - 1} \, e^{-\kappa((T_{\odot}/T)\,\Xi_{\odot})(x/c)} \, d\Xi_{\odot}$$
(57)

and

$$v_{\langle n \rangle}^{r}(t,x) = \overline{D}_{n}v^{r}(t,x), \qquad (58)$$

where Ξ_{\odot} stands for $\hbar\omega/k_B T_{\odot}$. The integral in (57) must be evaluated numerically. The interpretation of (57) is simple: The boundary stimulus moves with the speed of light *c* into the atmosphere, and its amplitude is damped due to absorption processes. We will compare this solution with the solution of the moment equations in the next section.

4.5. Solution of Moment Equations

From (39), we obtain with (53), (54), (56)

$$v^{r}(t,x) = F\left(t - \frac{x}{c}\right) \sum_{t} \sum_{s} M_{rs} M_{st}^{-1} \frac{(k_{B}T_{\odot}/c)^{t} \Gamma(t+3) \zeta(t+3)}{(k_{B}T_{\odot}/c)^{r} \Gamma(r+3) \zeta(r+3)} e^{-\mu_{s} x/c}$$
(59)

and

$$v_{\langle n \rangle}^{r}(t,x) = D_{n}v^{r}(t,x), \tag{60}$$

⁵ We consider the absorption coefficient given as function of the dimensionless parameter $\Xi = \hbar\omega/k_B T$, where T is the temperature of the atmosphere. We have $\Xi = (T_{\odot}/T) \Xi_{\odot}$.

where μ_s are the eigenvalues of the matrix of mean absorption coefficients, given by (4)

$$\Theta_{rs} = \left(\frac{k_B T}{c}\right)^{r-s} \sum_{t=1}^{R} \mathscr{C}_{ts}^{-1} \int \kappa(\Xi) \frac{e^{\Xi}}{(e^{\Xi} - 1)^2} \Xi^{t+r+2} d\Xi.$$
(61)

We rewrite (59) as

$$v^{r}(t,x) = F\left(t - \frac{x}{c}\right) \sum_{t} \sum_{s} \tilde{M}_{rs} \tilde{M}_{st}^{-1} e^{-\mu_{s} x/c}$$
(62)

where \tilde{M}_{rs} is the matrix of right eigenvectors of

$$\widetilde{\Theta}_{rs} = \frac{(k_B T_{\odot}/c)^s \Gamma(s+3) \zeta(s+3)}{(k_B T_{\odot}/c)^r \Gamma(r+3) \zeta(r+3)} \Theta_{rs}$$
$$= \left(\frac{T}{T_{\odot}}\right)^{r-s} \frac{\Gamma(s+3) \zeta(s+3)}{\Gamma(r+3) \zeta(r+3)} \sum_{t=1}^R \mathscr{C}_{ts}^{-1} \int \kappa(\Xi) \frac{e^{\Xi}}{(e^{\Xi}-1)^2} \Xi^{t+r+2} d\Xi, \quad (63)$$

which has the same eigenvalues μ_s as Θ_{rq} . Here only the ratio T_{\odot}/T occurs and we conclude that the absolute values of the temperatures play no role in the calculation of the dimensionless variables v^r .

4.6. Comparison of Solutions

We need to compare only the damping parts of (57) and (59), i.e., the quantities without the factor F(t - (x/c)). We consider bremsstrahlung absorption with κ given by (7), introduce the dimensionless space variable

$$\tilde{x} = \frac{D_{ff}}{c} \left(\frac{T}{T_{\odot}}\right)^3 x \tag{64}$$

and obtain for these parts

$$\hat{v}^{r}(t,x) = \frac{1}{\Gamma(r+3)\,\zeta(r+3)} \int \frac{\Xi_{\odot}^{r+2}}{e^{\Xi_{\odot}} - 1} \, e^{-\left[1 - \exp(-(T_{\odot}/T)\,\Xi_{\odot})/\Xi_{\odot}^{3}\right]\,\tilde{x}} \, d\Xi_{\odot} \tag{65}$$

and

$$\check{v}^{r}(t,x) = \sum_{t} \sum_{s} \tilde{M}_{rs} \tilde{M}_{st}^{-1} e^{-\tilde{\mu}_{s}\tilde{x}},$$
(66)

where \hat{v}^r refers to the solution of the radiative transfer equation and \check{v}^r to the solution of the moment equations. $\tilde{\mu}_s$ in (66) are the eigenvalues of

$$\tilde{\tilde{\Theta}}_{rs} = \frac{1}{D_{ff}} \left(\frac{T_{\odot}}{T}\right)^3 \tilde{\Theta}_{rs}$$
(67)

$$= \left(\frac{T_{\odot}}{T}\right)^{s-r+3} \frac{\Gamma(s+3)\,\zeta(s+3)}{\Gamma(r+3)\,\zeta(r+3)} \sum_{t=1}^{R} \mathscr{C}_{ts}^{-1} \Gamma(r+t)\,\zeta(r+t).$$
(68)

The moment equations were derived from the radiative transfer equation in order to replace the latter by a finite number of moment equations. Therefore, we consider solutions of the moment equations as satisfactory, if they agree with the solution of the radiative transfer equation. In the following, we will compare only \hat{v}^1 and \check{v}^1 , which are measures for the energy density of the beam.

While the solution of the radiative transfer equation (65) depends on the single parameter T_{\odot}/T , the moment solution (66) depends on T_{\odot}/T and on the number R of moments. We will compare both solutions for several values T_{\odot}/T and different values of R. In all figures to follow, the solution of the radiative transfer equation is drawn as a dashed line, while solid lines refer to solutions of the moment equations.

We start with the case $T_{\odot}/T = 1$. Figure 3 shows that the moment theory with R = 1 gives only qualitative agreement with the radiative transfer equation, while the moment theory with R = 6 agrees almost perfectly with that solution. The same is true for moment theories with $R \ge 6$.

In summary we conclude that we have to choose a moment theory with moment numbers $N \simeq 30$ and R = 6 in order to describe the beam in the absorbing atmosphere in accordance with the radiative transfer equation. In [10], we found the same value R = 6 when we considered the homogeneous compression of radiation. Note that the value R = 6 holds for the special case of bremsstrahlung absorption;



FIG. 3. $v^1(\tilde{x})$ according to the radiative transfer equation (dashed line) and according to moment theories with R = 1 and R = 6 (solid line). $T_{\bigcirc}/T = 1$.

other values will result for R when different absorption and emission mechanisms dominate.

Now we ask whether R = 6 gives reasonable results for other values of the temperature ratio T_{\odot}/T , i.e., if the temperature of the star and the absorbing atmosphere are different. The result is as follows: In the range $0.5 \le T_{\odot}/T \le 1.8$, there is no visible change in the figure. But if T_{\odot}/T lies outside this domain, the picture changes considerably. As an example, Fig. 4 shows the result for $T_{\odot}/T = 0.25$. It is clearly seen from the figure that we have to increase the number R to a value of R = 14 in order to have agreement with the solution of the radiative transfer equation.

Most probably the number R must be further increased for lower values of T_{\odot}/T but here we have had problems with the numerical accuracy in solving the eigenvalue problem in (66).

In the case $T_{\odot}/T \ge 1.8$, the situation is worse: The solutions of the moment theories become non-monotone with high, even negative, peaks, and an increase of R gives even worse results. Since this may be due to numerical inaccuracies, we do not present the curves for this case.⁶

4.7. A Better Approximation

We conclude that the moment theory in its present form gives very good results in the case that T_{\odot}/T lies in the vicinity of one. But typically T_{\odot}/T has values which differ considerably from one; for a sun-beam and the earth's atmosphere we find $T_{\odot}/T \simeq 20$.

In order to understand why the moment equations give good results for $T_{\odot}/T \simeq 1$ and why the number of moments must be increased—at the cost of considerable numerical difficulties—when T_{\odot}/T exceeds the value 1.8, we comment on the derivation of the matrix of mean absorption coefficients (4) which may be found in Appendix A.

This derivation includes a series expansion of the phase density obtained from the entropy maximum principle about the local equilibrium phase density, which is determined by the local temperature T. An expansion is needed because it is impossible to calculate integrals over the original phase density. It is only on account of this expansion that the temperature occurs in the matrices of mean absorption and scattering coefficients.

Now, if the phase density differs considerably from the local equilibrium phase density, e.g., for the sun-beam, we need a lot of expansion coefficients in order to have a good approximation of the phase density. Since the number of moments equals the number of expansion coefficients, we need many moments as well.

After these remarks it is understandable that an expansion about a non-local equilibrium phase density may give better results. Appendix B discusses the procedure in detail. It is shown that the only change in the moment equation occurs in

⁶ The numerical inaccuracy results mainly from the inversion of the matrix $\mathscr{C}_{rs} = \Gamma(s+r+3) \times \zeta(s+r+2)$. The elements of this matrix differ in magnitude by several orders.



FIG. 4. $v^1(\tilde{x})$ according to the radiative transfer equation (dashed line) and according to moment theories with R = 1, R = 6 and R = 14 (solid line). $T_{\bigcirc}/T = 0.25$.

the definition of the matrices Θ_{rs} and $\hat{\Theta}_{rs}$. If θ is the temperature of the non-local equilibrium, we find for instance that Θ_{rs} must be replaced by (A.34)

$$\Theta_{rs}^{\theta} = \left(\frac{k_B\theta}{c}\right)^{r-s} \sum_{t} \mathscr{C}_{ts}^{-1} \int \kappa \left(\Xi_{\theta} \frac{\theta}{T}\right) \frac{e^{\Xi_{\theta}}}{(e^{\Xi_{\theta}} - 1)^2} \Xi_{\theta}^{t+r+2} d\Xi_{\theta}, \tag{69}$$

where $\Xi_{\theta} = \hbar \omega / k_B \theta$. Specificially for the beam problem, we need the eigenvalues and eigenvectors of the matrix (see (63), (68))

$$\widetilde{\Theta}_{rs} = \frac{1}{D_{ff}} \left(\frac{T_{\odot}}{T}\right)^3 \frac{(k_B T_{\odot}/c)^s \, \Gamma(s+3) \, \zeta(s+3)}{(k_B T_{\odot}/c)^r \, \Gamma(r+3) \, \zeta(r+3)} \, \Theta_{rs},\tag{70}$$

and we find with Θ_{rs} replaced by (69)

$$\tilde{\tilde{\Theta}}_{rs} = \left(\frac{T_{\odot}}{\theta}\right)^{s-r+3} \frac{\Gamma(s+3)\,\zeta(s+3)}{\Gamma(r+3)\,\zeta(r+3)} \sum_{t=1}^{R} \mathscr{C}_{ts}^{-1} \int \frac{(1 - \exp(-\Xi_{\theta}(\theta/T)))\,e^{\Xi_{\theta}}}{(e^{\Xi_{\theta}} - 1)^{2}} \Xi_{\theta}^{t+r+1}\,d\Xi_{\theta}.$$
(71)

 $\tilde{\Theta}_{rs}$ must be calculated numerically. With θ , we have an additional parameter in the system of moment equations. In the problem under consideration it is suggestive to take θ equal to the temperature of the beam, $\theta = T_{\odot}$. Figure 5 shows results from the moment equations with this choice for large differences between beam and atmospheric temperature. It is clearly seen that the choice R = 6 gives an excellent agreement between the solutions of moment equations and radiative transfer equation for all values of the ratio T_{\odot}/T .



FIG. 5. $v^1(\tilde{x})$ according to the radiative transfer equation (dashed line) and according to moment theories with R = 1 and R = 6 (solid line) for $T_{\odot}/T = 0.01$ and $T_{\odot}/T = 40$.

4.8. A Comment on Absorption Coefficients

The matrices Θ_{rq} , $\hat{\Theta}_{rq}$ (4), (5) depend strongly on the absorption and scattering coefficients under consideration. In particular it follows that the number of moments R which was discussed in the previous sections of this paper depends on the choice of the absorption coefficient κ . While for the proper description of gray matter ($\kappa = const.$) a value of R = 1 gives excellent results, one needs very large values of R for more complex absorption coefficients.

As an example we considered a simple model absorption coefficient for bremsstrahlung absorption and single-line photo-absorption, viz.

$$\kappa = \begin{cases} D_{ff} \frac{1 - \exp(-\Xi)}{\Xi^3} & 0 < \Xi < \Xi_0 \\ D_{ff} (1+a) \left(\frac{1 - \exp(-\Xi)}{\Xi^3}\right) & \Xi > \Xi_0. \end{cases}$$
(72)

Numerical tests show that the necessary number R depends on the values Ξ_0 and the "step" a. A moment number R = 12 gives excellent results for $\Xi_0 = 0.5$, a < 8.6; $\Xi_0 = 1$, a < 3.8 and $\Xi_0 = 2$, a < 1.5. Thus the moments method works for discontinuous absorption coefficients if the step is not to big.

It was not possible to obtain accurate results for higher values of the step *a*. Most probably this is due to numerical inaccuracies which occur in the inversion of the matrices and the calculation of the eigenvalues. In theses cases the moment method should not be used.

5. CONCLUSION

We have shown in this paper that the extended moment theory with matrices of mean absorption and scattering coefficients, originally presented in [10], is a good tool for the calculation of non-homogeneous non-equilibrium processes. In particular, we have shown that the number of moments in the theory may be adjusted so that, at least for the simple case of a beam penetrating an isothermal atmosphere, the moment theory gives the same results as the radiative transfer equation.

We strongly believe that the extended moment theory will give excellent results in more complex cases too, and we suggest that the simple beam process of the present paper may serve as an indicator for the number of moments which are needed.

APPENDIX A. THE EQUATIONS OF RADIATION THERMODYNAMICS

A.1. Distribution Function and Radiative Transfer Equation

We describe radiation in the photon picture. Photons are characterized by their momentum p_i^{Ph} or, alternatively, by their frequency ω and their direction vector n_i with $p_i^{Ph} = \hbar \omega/c$; the photon energy is $E = \hbar \omega$. \hbar denotes Planck's constant divided by 2π and c is the speed of light. The photon distribution function

$$f(x_i, t, p_i) d\mathbf{p} = \left(\frac{\hbar}{c}\right)^3 f(x_i, t, \omega, n_i) \omega^2 d\omega d\Omega$$
(A.1)

gives the number density of photons with momenta in the vicinity of **p** or with frequencies in $(\omega, \omega + d\omega)$ and directions within the solid angle $d\Omega = \sin \vartheta \, d\vartheta \, d\varphi$. The

photon distribution function f satisfies the radiative transfer equation which reads in the rest frame of matter [2, 4, 7]

$$\frac{\partial f}{\partial t} + cn_k \frac{\partial f}{\partial x_k} = \mathscr{S} = -\kappa (f - f_{|E}) - \varsigma \left[f(\omega, n_i) - \frac{1}{4\pi} \int f(\omega, n'_i) \, d\Omega' \right].$$
(A.2)

Here the right hand side accounts for the creation and annihilation of photons due to interaction with matter. The first term describes absorption and emission. $\kappa(\omega)$ is the effective absorption coefficient and

$$f_{|E} = \frac{1}{4\pi^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$
(A.3)

denotes the equilibrium distribution. k_B is Boltzmann's constant and T is the temperature of matter. Scattering processes are described by the second term; here we restrict the attention to the case of isotropic scattering. $\varsigma(\omega)$ is the scattering coefficient. The functions $\varsigma(\omega)$, $\kappa(\omega)$ depend on the mechanisms of interaction.

A.2. Moments and Moment Equations

The moments of the phase density are defined as

$$u_{\langle i_1 i_2 \cdots i_n \rangle}^r = \left(\frac{\hbar}{c}\right)^{r+3} \int \omega^{r+2} n_{\langle i_1} \cdots n_{i_n \rangle} f \, d\omega \, d\Omega. \tag{A.4}$$

 $n_{\langle i_1} \cdots n_{i_n \rangle}$ are spherical harmonics which form an orthogonal set of functions [12]. The moment equations follow by multiplication of the radiative transfer equation with $\omega^r n_{\langle i_1} \cdots n_{i_n \rangle}$ and integration. They read

$$\frac{\partial u_{\langle i_1 i_2 \cdots i_n \rangle}}{\partial t} + \frac{n}{2n+1} c \frac{\partial u_{\langle i_1 i_2 \cdots i_{n-1} \rangle}}{\partial x_{i_n \rangle}} + c \frac{\partial u_{\langle i_1 i_2 \cdots i_n k \rangle}}{\partial x_k} = P_{\langle i_1 i_2 \cdots i_n \rangle}.$$
 (A.5)

The quantities

$$P^{r}_{\langle i_{1}i_{2}\cdots i_{n}\rangle} = \left(\frac{h}{c}\right)^{r+3} \int \omega^{r+2} n_{\langle i_{1}}\cdots n_{i_{n}\rangle} \mathscr{S} \, d\omega \, d\Omega \tag{A.6}$$

are called the productions of the moments $u_{\langle i_1 i_2 \cdots i_n \rangle}^r$.

A.3. Closure Problem

Equations (A.5) form an infinite set of coupled PDEs. Since we need a finite number of equations, we assume that the knowledge of the moments

$$u_{\langle i_1 i_2 \cdots i_n \rangle}^r$$
, $r = 1, ..., R; n = 0, 1, ..., N$ (A.7)

with $R, N \ge 1$ describes the process with sufficient accuracy⁷. Equations (A.5) with r = 1, ..., R; n = 0, ..., N do not form a closed set of equations. Therefore, we need equations of state which relate the moments

$$u_{\langle i_1 i_2 \cdots i_{N+1} \rangle}^r, \quad r = 1, ..., R,$$
 (A.8)

and the productions

$$P^{r}_{\langle i_{1}i_{2},...i_{n}\rangle}, \quad r=1,...,R; \quad n=0,\,1,...,N.$$
 (A.9)

to the moments (A.7). We find the equations of state by means of the entropy maximum principle [3] in the next section. The entropy maximum principle is equivalent to the entropy principle of extended thermodynamics [5].

A.4. The Entropy Maximum Principle

Since the quantities (A.8), (A.9) follow from the distribution function by (A.4), (A.6), we may find the required equations of state if we have the distribution function as function of the moments (A.7), $f = f(u_{\langle i_1 i_2 \cdots i_n \rangle}^r(x_i, t), \omega, n_i)$. Such a distribution function follows from the entropy maximum principle which states that f has to be the function that maximizes the entropy of radiation [6, 8]

$$h = -k_B \int \left[f \ln \frac{f}{y} - (y+f) \ln \left(1 + \frac{f}{y}\right) \right] d\mathbf{p}, \quad \text{with} \quad y = 2/(2\pi\hbar)^3 \quad (A.10)$$

under the constraint of given values of the $u_{\langle i_1 i_2 \cdots i_n \rangle}^r$. By a common procedure, we obtain

$$f = \frac{y}{\exp \Xi - 1} \qquad \text{with} \quad \Xi = \frac{1}{k_B} \sum_{r, n} \Lambda^r_{\langle i_1 i_2 \cdots i_n \rangle} \left(\frac{h\omega}{c}\right)^r n_{\langle i_1} \cdots n_{i_n \rangle}, \quad (A.11)$$

where the $\Lambda^r_{\langle i_1 i_2 \cdots i_n \rangle}$ are Lagrange multipliers. The $\Lambda^r_{\langle i_1 i_2 \cdots i_n \rangle}$ must be determined from the constraints

$$u_{\langle i_1 i_2 \cdots i_n \rangle}^r = \left(\frac{h}{c}\right)^{r+3} \int \omega^{r+2} n_{\langle i_1} \cdots n_{i_n \rangle} f \, d\omega \, d\Omega, \qquad r = 1, ..., R; \quad n = 0, ..., N.$$
(A.12)

A.5. Expansion about Local Equilibrium

Unfortunately it is not possible to calculate integrals over the function (A.11). For this reason, we expand (A.11) about equilibrium. Comparison with the

⁷ It is necessary to start with r = 1 instead of r = 0, see [10].

equilibrium distribution (A.3) shows that almost all Lagrange multipliers vanish in equilibrium,

$$\Lambda^{r}_{\langle i_{1}i_{2}\cdots i_{n}\rangle \mid E} = \begin{cases} \frac{c}{T}, & r = 1, \quad n = 0\\ 0, & \text{else.} \end{cases}$$
(A.13)

We therefore write

$$\frac{1}{k_B} \Lambda^r_{\langle i_1 i_2 \cdots i_n \rangle} = \frac{c}{k_B T} \,\delta^{r_1} \delta_{n_0} + \lambda^r_{\langle i_1 i_2 \cdots i_n \rangle} \tag{A.14}$$

and assume that the $\lambda_{\langle i_1 i_2 \cdots i_n \rangle}^r$ are small. A Taylor expansion gives

$$f \approx f_{|E}(k, T) + \frac{df_{|E}}{d\Xi_{|E}} \sum_{r, n} \lambda_{\langle i_1 i_2 \cdots i_n \rangle}^r \left(\frac{\hbar\omega}{c}\right)^r n_{\langle i_1} \cdots n_{i_n \rangle}.$$
 (A.15)

Thus, f is an expansion in ω^r and $n_{\langle i_1} \cdots n_{i_n \rangle}$. From (A.12), (A.15), we obtain the $\lambda^r_{\langle i_1, i_2, \cdots, i_n \rangle}$ as

$$\lambda_{\langle i_1 i_2 \cdots i_n \rangle}^t = -\frac{\prod_{j=0}^n (2j+1)}{n!} \sum_r \mathscr{C}_{tr}^{-1} \frac{u_{\langle i_1 i_2 \cdots i_n \rangle}^r - u_{\langle i_1 i_2 \cdots i_n \rangle | E}^r}{4\pi y (k_B T/c)^{r+t+3}}$$
(A.16)

with the abbreviations

$$u_{|E}^{r}(T) = 4\pi y \left(\frac{k_{B}T}{c}\right)^{r+3} \Gamma(r+3) \zeta(r+3), \qquad u_{\langle i_{1}i_{2}\cdots i_{n}\rangle|E}^{r}(T) = 0 \quad (A.17)$$

and

$$\mathscr{C}_{rs} = \Gamma(s+r+3)\,\zeta(s+r+2), \qquad r, s = 1, ..., R.$$
(A.18)

 $\Gamma(x)$ denotes the Gamma function and $\zeta(x)$ is Riemann's Zeta function.

A.6. Equations of State

With (A.15), (A.16), we are able to calculate the equations of state (A8), (A.9). We obtain

$$u_{\langle i_1 i_2 \cdots i_{N+1} \rangle}^r = 0, \qquad r = 1, ..., R$$
 (A.19)

for the highest moments while the productions are given by

$$P^{r} = -\sum_{s} \Theta_{rs}(u^{s} - u^{s}_{|E}(T))$$
(A.20)

and

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$$P^{r}_{\langle i_{1}i_{2}\cdots i_{n}\rangle} = -\sum_{s} \hat{\Theta}_{rs} u^{s}_{\langle i_{1}i_{2}\cdots i_{n}\rangle}.$$
(A.21)

Here, Θ_{rs} is the matrix of mean absorption coefficients (4), and $\hat{\Theta}_{rs}$ is the matrix of mean absorption and scattering coefficients (5).

APPENDIX B. EXPANSION ABOUT NON-LOCAL EQUILIBRIUM

B.1. Phase Density

The expansion of (A.11) about the local equilibrium phase density is not suitable for all processes. In particular, it is not if a sun beam enters into an atmosphere. This is due to the fact that the spectrum of the beam is determined by the temperature of the sun. Therefore an expansion about the local equilibrium phase density, which is determined by the local temperature, is not suitable. Here, we have the possibility to expand about a non-local equilibrium phase density with temperature θ . Instead of (A.14), we write

$$\frac{1}{k_B} \Lambda^r_{\langle i_1 i_2 \cdots i_n \rangle} = \frac{c}{k_B \theta} \,\delta^{r_1} \delta_{n0} + \hat{\lambda}^r_{\langle i_1 i_2 \cdots i_n \rangle},\tag{A.22}$$

and, by the assumption that the $\hat{\lambda}^{r}_{\langle i_{1},i_{2},...,i_{n}\rangle}$ are small, we obtain instead of (A.15)

$$f \approx f_{\theta}(k, \theta) + \frac{df_{\theta}}{d\Xi_{\theta}} \sum_{r, n} \hat{\lambda}_{\langle i_1 i_2 \cdots i_n \rangle}^r \left(\frac{h\omega}{c}\right)^r n_{\langle i_1} \cdots n_{i_n \rangle}, \qquad (A.23)$$

where we have introduced the abbreviations

$$f_{\theta} = \frac{y}{\exp \Xi_{\theta} - 1}, \qquad \Xi_{\theta} = \frac{\hbar\omega}{k_B \theta}.$$
 (A.24)

For the Lagrange multipliers we obtain in this case

$$\hat{\lambda}_{\langle i_1 i_2 \cdots i_n \rangle}^r = -\frac{\prod_{j=0}^n (2j+1)}{n!} \sum_t \mathscr{C}_{rt}^{-1} \frac{u_{\langle i_1 i_2 \cdots i_n \rangle}^t - u_{\langle i_1 i_2 \cdots i_n \rangle \mid \theta}^t}{4\pi y (k_B \theta / c)^{r+t+3}}, \qquad (A.25)$$

where

$$u_{|\theta}^{r} = 4\pi y \left(\frac{k_{B}\theta}{c}\right)^{r+3} \Gamma(r+3) \,\zeta(r+3), \qquad u_{\langle i_{1}i_{2}\cdots i_{n} \rangle |\theta}^{r} = 0. \tag{A.26}$$

But now we have a problem with the local equilibrium phase density: If we introduce the local equilibrium values (A.17) of the moments into (A.23), (A.25), we should obtain—at least approximately—the local equilibrium phase density. If we do so, we obtain

$$f_{|E} \approx f_{\theta} - \frac{df_{\theta}}{d\Xi_{\theta}} \sum_{r} \hat{\lambda}_{|E}^{r}(T,\theta) \left(\frac{\hbar\omega}{c}\right)^{r}$$
(A.27)

with

$$\hat{\lambda}_{|E}^{r}(T,\theta) = \sum_{t} \mathscr{C}_{rt}^{-1} \frac{u_{|E}^{t}(T) - u_{|\theta}^{t}(\theta)}{4\pi y (k_{B}\theta/c)^{r+t+3}}.$$
(A.28)

Only if we expand both the actual phase density f and the local equilibrium phase density according to (A.23), (A.27) will the photon production density \mathscr{S} vanish in equilibrium. We may eliminate f_{θ} between (A.23) and (A.27) and find for the phase density

$$f \approx f_{|E} + \frac{df_{\theta}}{d\Xi_{\theta}} \sum_{r,n} \tilde{\lambda}_{\langle i_1 i_2 \cdots i_n \rangle}^r \left(\frac{h\omega}{c}\right)^r n_{\langle i_1} \cdots n_{i_n \rangle}$$
(A.29)

with

$$\tilde{\lambda}_{\langle i_1 i_2 \cdots i_n \rangle}^r = \frac{\prod_{j=0}^n (2j+1)}{n!} \sum_t \mathscr{C}_{rt}^{-1} \frac{u_{\langle i_1 i_2 \cdots i_n \rangle}^t - u_{\langle i_1 i_2 \cdots i_n \rangle \mid E}^t(T)}{4\pi y (k_B \theta / c)^{r+t+3}}.$$
 (A.30)

We will use the phase density (A.29) for the calculation of the equations of state.

Note: The procedure of this section seems to be artificial, but it may be justified by the results which it gives. While we have taken θ as an external and constant input, one could think also of θ as a variable which goes to T when the radiation reaches equilibrium. But that would require an equation for θ —which should then replace one of the moment equations, of course—and it is not clear how to obtain that equation. Also one must bear in mind that no temperature would occur in the phase density f, if we were able to calculate the integrals (A.11).

B.2. Equations of State

With (A.29), (A.30) we are able to calculate the equations of state (A.8), (A.9). Again we obtain

$$u_{\langle i_1 i_2 \cdots i_{N+1} \rangle}^r = 0, \qquad r = 1, ..., R$$
 (A.31)

for the highest moments, while the productions turn out to be

$$P^{r} = -\sum_{s} \Theta_{rs}^{\theta} (u^{s} - u_{|E}^{s}(T))$$
(A.32)

and

$$P^{r}_{\langle i_{1}i_{2}\cdots i_{n}\rangle} = -\sum_{s} \hat{\Theta}^{\theta}_{rs} u^{s}_{\langle i_{1}i_{2}\cdots i_{n}\rangle}.$$
(A.33)

Now, Θ_{rs}^{θ} and $\hat{\Theta}_{rs}^{\theta}$ are given by

$$\Theta_{rs}^{\theta} = \left(\frac{k_B \theta}{c}\right)^{r-s} \sum_{t} \mathscr{C}_{ts}^{-1} \int \kappa \left(\Xi_{\theta} \frac{\theta}{T}\right) \frac{e^{\Xi_{\theta}}}{(e^{\Xi_{\theta}} - 1)^2} \Xi_{\theta}^{t+r+2} d\Xi_{\theta}$$
(A.34)

and

$$\hat{\Theta}^{\theta}_{rs} = \Theta^{\theta}_{rs} + \left(\frac{k_{B}\theta}{c}\right)^{r-s} \sum_{t} \mathscr{C}^{-1}_{ts} \int \varsigma \left(\Xi_{\theta} \frac{\theta}{T}\right) \frac{e^{\Xi_{\theta}}}{\left(e^{\Xi_{\theta}} - 1\right)^{2}} \Xi^{t+r+2}_{\theta} d\Xi_{\theta}.$$
(A.35)

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