IDEALISED MODELS FOR CLOSED SYSTEM RELAXATION

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ABSTRACT

A class of model non-linear systems which describe the energy exchange of molecules with internal degrees of freedom is examined. The models,which arise purely from a consideration of the combinatorics of energy exchange,may also be formulated as models of 'collective games' and 'economic systems'. Their transport properties are determined by a Boltzmann-like equation which is first studied in a more general formalism giving useful insight into this type of problem. The equation's properties and it's approximations (viz. the linearised equation and a non-linear Fokker-Planck equation) are derived from first principles and studied in detail.

Four particular inter-related models are then considered with both discrete and continuous state variables. Two of these (one discrete and one continuous) fall under the heading of 'molecules with diffuse scattering', and have a definite analogy with the case of Maxwell molecules in the classical Boltzmann equation, whilst the other two may be termed 'persistent scattering molecules' and in allowing persistence of state can be said to be more realistic. For each of these models an exact similarity solution of the non-linear Boltzmann equation is found in closed form, and in the case of diffuse scattering molecules this is compared with the solution of the corresponding linearised equation. These similarity solutions are only valid for a particular class of initial distributions, which although apparently close to equilibrium still differ appreciably from the linearised solution.

An exact solution of these models for an arbitrary initial distribution can only be found in terms of the moments which can be calculated sequentially, and this is discussed for each model. This is the first known case of a soluble Boltzmann equation with persistent rather than diffuse scattering, moreover only in the former case is a Fokker-Planck approximation conceivable.

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CHAPTER ONE : INTRODUCTION

1.1 Non-Equilibrium Physics

The problem of describing the state of a gas in thermal equilibrium can be solved in a straightforward manner, and is the subject matter of a large number of textbooks on statistical mechanics. In contrast, however, the non-equilibrium properties of a gas present many more problems, generally concerning the irreversibility paradox (see e.g. Tolman (1938)) or the connection of the reversible laws of motion to the irreversible nature of the system as a whole. The researches of a number of early physicists into the kinetic theory of gases culminated in the famous H-Theorem and equation of Boltzmann (1872).

1.2 The Boltzmann Equation

The Boltzmann equation is a non-linear integro-differential equation first established in 1872 (Boltzmann (1872)) to describe the time evolution of the one particle distribution in a dilute gas governed by binary collisions. In standard notation the equation reads,

$$\frac{\partial f}{\partial t} + \underline{v}\cdot\frac{\partial f}{\partial \underline{r}} + \frac{\underline{F}}{m}\cdot\frac{\partial f}{\partial \underline{v}} = \int d\underline{v}_1 \int d\hat{n}\, g\, I(g,\chi)\,(f'f_1' - f f_1) \qquad (1.1a)$$

$$= \iiint d\underline{v}_1\, d\underline{v}'\, d\underline{v}_1'\; W(\underline{v}_1', \underline{v}' \,|\, \underline{v}, \underline{v}_1)\,(f'f_1' - f f_1) \qquad (1.1b)$$

where $f_1' = f(\underline{v}_1', \underline{r}, t)$ etc. and $f(\underline{v}, \underline{r}, t)$ is the average number of particles between $\underline{v}$ and $\underline{v}+\underline{dv}$ at a point in space between $\underline{r}$ and $\underline{r}+\underline{dr}$. For the spatially homogeneous case all terms on the left hand side apart from the first are zero and $f_1' = f(v_1',t)$ etc. only. Primes denote the values after collision, and g is the relative speed before collision, $g = |\underline{v}-\underline{v}_1|$. The differential scattering cross- section is I and $\hat{n}$ is a unit vector parallel to g. In (1.1b) the Boltzmann equation is expressed in terms of the transition probability $W(\underline{v}',\underline{v}_1' \mid \underline{v},\underline{v}_1)$ per unit time of particles with velocities $(\underline{v},\underline{v}_1)$ scattering into $(\underline{v}',\underline{v}_1')$. There are several inherent properties of (1.1a,b), namely conservation of the number of particles, energy and momentum ;the H-Theorem states that the function

$$H(t) = \int f \ln f \, \underline{dv} \tag{1.2}$$

is non-increasing; and the stationary solution is the Maxwellian (Maxwell (1879)).

The derivation of the Boltzmann equation, and discussions of the underlying assumptions have been given in many textbooks (e.g. Balescu (1975)) and it is appropriate that they should be mentioned here since they are implicit in all of the future work. They are,

1) The duration of a collision (τ_c) is very much less than the time between collisions (τ_r)

$$\tau_c \ll \Delta t \ll \tau_r \tag{1.3}$$

This is staisfied for the case of a dilute gas.

2) That the distribution function $f(\underline{v},\underline{r},t)$ does not change appreciably in space during a time Δt.

3) The 'Stosszahlansatz' or molecular chaos assumption that there are no correlations between the particles, or more particularly that the two body distribution function $f_2(\underline{v},\underline{r};\underline{v}_1,\underline{r};t)$ is the product of two one particle distribution functions,

$$f_2(\underline{v},\underline{r};\underline{v}_1,\underline{r};t) = f(\underline{v},\underline{r};t)\, f(\underline{v}_1,\underline{r};t) \tag{1.4}$$

It is this last assumption that has been at the heart of much criticism of the Boltzmann equation and for further discussion and justification one is refered to a standard text (Balescu (1975)).

The properties of the classical Boltzmann equation have also received some attention (see e.g. Resibois & de Leener (1977)) but will be discussed and proved with particular reference to scalar systems in Chapter 2.

1.3 Solutions

In the case of a linear equation (e.g. a Master equation) it is sufficient to find the solution for a delta function initial distribution so that the solution for an arbitrary initial distribution can be constructed by using the principle of superposition. However in the case of a non-linear equation like the Boltzmann equation there is no such principle and a general solution must contain all of the information about the initial distribution.

We thus draw the distinction between the general solution which holds for an arbitrary initial distribution and an exact one which will hold for some particular class of initial conditions. In addition the exact form of the solution (whether it is in closed form or in terms of an infinite series) may well determine the usefulness of it.

At the present no general solutions of the full Boltzmann equation (1.1) are known for the spatially uniform or non-uniform case and it is because of this that certain simplifications are made either to the model (e.g. Maxwell molecules) or to the equation (e.g. the linearised equation).

Dealing with the latter of these first, it is obvious that the main stumbling block in finding solutions of (1.1) is due to the complicated nature of the collision integral on the right hand side. This can be considerably simplified by assuming that the effect of a collision is always to restore a local equilibrium desribed by the distribution function $f^{(0)}(\underline{v},\underline{r},t)$. Furthermore if we assume that, if the molecular distribution is disturbed from the local equilibrium so that the actual distribution $f(\underline{v},\underline{r},t)$ is different from $f^{(0)}(\underline{v},\underline{r},t)$ then the effect of the collision is simply to restore f to $f^{(0)}$ exponentially with a relaxation time τ_r which is of the order of the time between collisions then (1.1) reduces to

$$\frac{\partial f}{\partial t} + \underline{v}\cdot\frac{\partial f}{\partial \underline{r}} + \frac{\underline{F}}{m}\cdot\frac{\partial f}{\partial v} = -\frac{(f - f^{(0)})}{\tau_r} \tag{1.5}$$

This is a linear partial differential equation for f and is the Boltzmann equation with the relaxation time assumption. Such theories as this have attained wide usage through the work of Bhatnagar, Gross & Krook (1954).

An alternative approximation for systems close to equilibrium is to assume that the distribution function can be expanded about the equilibrium distribution function and hence derive a linear equation for the deviation from from equilibrium. The derivation of such an equation is standard bookwork (see e.g. Cercignani (1975)) and in this particular reference a discussion as to the validity of such an equation is well presented. It is worthy of note that recently Ernst & Hendriks (1979) have shown for a particular model system that the linearised equation does not describe the relaxation of that system when it is near to equilibrium, especially in the high energy tail.

A third, alternative simplification is the Fokker-Planck equation, which arises from the case of Brownian particles where the change in velocity at each collision is small. It is often derived from the linearised equation when the result is a linear partial differential equation in f. The more general case of the derivation from the full non-linear equation is dealt with in the next chapter when a non-linear partial differential equation is the result.

Apart from a few rare cases however it has been impossible to determine exactly how well these approximate forms of the Boltzmann equation describe the exact solution of the non-linear equation. For this reason simple models are investigated, for which exact solutions are availiable, to give valuable information of the features of the solutions of the non-linear Boltzmann equation. Many of these models have recently centred around the use of Maxwell molecules, altough work on more idealised models without particular reference to kinetic theory has played a significant part in these studies.

The problem of exact solutions to the full non-linear Boltzmann equation has until recently provoked little interest. In an isolated paper, Truesdell (1956) gave an exact solution for a special shear flow type problem, but the greatest stimulus has undoubtedly derived from a model studied by Krook & Wu (1976,1977) who found an exact (similarity) solution for a homogeneous gas of Maxwell molecules. This solution which was also found independently by Bobylev (1976b) has been generalised to n-dimensions, and been shown to be a solution for a number of other models by Ernst (1979a,b).

To produce their solution Krook & Wu choose a particularly simple form of the differential scattering cross section (characteristic of Maxwell molecules (see e.g. Kogan (1969))

$$I(g,\chi) = \frac{k\,\phi(\chi)}{g} \tag{1.6}$$

so that the angular integration can be carried out exactly. This resulted in a particularly simple form of the moment equations which were then transformed into the non-linear partial differential equation,

$$\frac{\partial^2 u}{\partial x\,\partial \tau} + \frac{\partial u}{\partial x} + u^2 = 0 \tag{1.7}$$

by the use of a moment generating function. A particular solution of this equation was then quoted using the method of similarity theory (Bluman & Cole (1974)). This solution which relies on the variables x and τ being combined in a certain unique way was then inverted to give a closed expression for $f(\underline{v},t)$. Other solutions of (1.7) found by Tenti & Hui (1978) were shown to correspond to the presence of sources and sinks and that the Krook-Wu solution was the only one to preserve all of the conservation conditions.

Bobylev (1976a) examined the invariance of the Boltzmann equation (for a spatially homogeneous system of Maxwell molecules) to a one parameter semi-group of transformations (a central point in similarity theory) and in a later paper (Bobylev (1976b)) with knowledge of this invariance found the same solution as Krook & Wu (1977) although in a more straightforward fashion. The latter part of his method is the same as the one that is used throughout this thesis. Essentially he assumed a solution of the form,

$$f(\underline{v},t) = \left(A(t) + B(t)\,\underline{v}^2 \right) \exp^{-C(t)\,\underline{v}^2} \tag{1.8}$$

and found the values of A, B and C by use of the conservation laws and direct substitution into the Boltzmann equation. The solution was then generalised by a method due to Nikol'skii (1964) to produce a solution to the non-isotropic case. This was also used by Tenti & Hui (1978) to find solutions for the non-isotropic case in the presence of sources and sinks.

Subsequently Barnsley & Cornille (1979) have examined the Sonine moments of the Krook-Wu model and given an expression, although not in closed form, for the general solution. Barnsley & Turchetti (1979) have computed this Fourier series and found that good convergence to the exact solution is obtained by using relatively few terms.

The exact solution of Krook & Wu has also provoked some interest in a few secondary matters. Ray (1979) showed that the moment equations imply a unique convergence to the equilibrium maxwellian without reference to an H-Theorem, whilst Rouse & Simons (1976) have used the model to give further support to their conjecture about the sign of the nth time derivative of entropy (S),

$$(-)^n \frac{d^n S}{dt^n} \leq 0 \tag{1.9}$$

Hoare (1979) has investigated the properties of a general class of scalar models whose evolution is governed by a scalar Boltzmann equation of the form,

$$\frac{\partial P(x,t)}{\partial t} = \int_x^\infty du \int_0^u dy \left\{ K(x,y;u)\, P(y,t)\, P(u-y,t) - K(y,x;u)\, P(x,t)\, P(u-x,t) \right\} \tag{1.10}$$

whilst the existence and uniqueness of solutions of such equations has been investigated by Melzak (1957).
Ernst (1979a) showed that the n-dimensional generalisation of the Krook-Wu model is described by equation (1.10) with,

$$K(x,y;u) = \frac{\Gamma(n)}{\Gamma(n/2)^2} \cdot \frac{x^{n/2-1}\,(u-x)^{n/2-1}}{u^{n-1}} \tag{1.11}$$

thus making a definite connection between the classical Boltzmann equation (1.1) and the scalar equation (1.10).

This model was investigated numerically by Tjon & Wu (1979) for the case n=2 to give support to the conjecture, " An arbitrary initial state tends first to relax to the similarity solution; the subsequent stage of the relaxation is essentially represented by the similarity solution with appropriate phase." More recently Tjon (1979) has shown that there exist certain classes of initial states which relax towards equilibrium in a way quantitatively different from the Krook-Wu solution.

Finally the kernel (1.11) has also been deduced as a result of the collision between two molecules, each with p internal degrees of freedom (where p = d/2). An exact solution for this model and the corresponding one with discrete energy states has been found by Futcher , Hoare, Hendriks & Ernst (1979a,b). These models are the subject matter of Chapters 3 and 4 whilst the general properties of systems described by equations such as (1.10) are proved in Chapter 2.

In search of general solutions of (1.10) Ernst & Hendriks (1979) have examined the case of

$$K(x,y;u) = 1 \tag{1.12}$$

and found the general solution to within a Laplace transform.

$$P(x,t) = \mathcal{L}^{-1}\left\{ \frac{\phi(z+t) + (z-1)e^{-t}}{(z+1)\phi(z+t) - e^{-t}} \right\} \tag{1.13}$$

where the arbitrary function ϕ is determined by the initial distribution.

The discrete version of this model was solved by Rouse & Simons (1978) and was repeated in a somewhat shorter manner by Ernst & Hendriks (1979). The choice of this simplified model and the ensuing general solution enabled Ernst & Hendriks to draw a few important conclusions. 1. The inadequacy of the linearised Boltzmann equation in describing the relaxation phenomena in the high energy tail of the distribution function. 2. They also found the transient overpopulation in the high energy tail first found by Krook & Wu (1977) and later on by Tjon (1979) in numerical work.

Perhaps the most simple model for which a general solution has been obtained is one due to McKean (1967) who considered an ensemble of particles with velocities of ±1 only. Kac (1955) gave a general solution in series form of another model which is a generalised form of McKean's. These models were reviewed and the entropy production studied by Henin & Prigogine (1974).

There is also a small literature on the relaxation of baths of harmonic oscillators. Much of the work has been from the Master equation approach, considering an ensemble of oscillators interacting with a heat bath (Montroll & Shuler (1957)). However Shuler (1960) studied the problem of an isolated ensemble of oscillators with Landau-Teller transition probabilities, which effectively linearised the problem. The same problem was also considered by Rankin & Light (1967) who gave their solution in terms of a generating function. These solutions were the first ones for a system with discrete state variables and it is in this context that the discrete models are presented later in this thesis.

CHAPTER TWO : PROPERTIES OF THE SCALAR BOLTZMANN EQUATION

2.1 Introduction

In this chapter we study the properties of a scalar transport equation (1.10) describing the relaxation of a microcanonical ensemble of subsystems towards equilibrium. The structure of this equation is similar to that of the kinetic theory Boltzmann equation (1.1) and hence it is termed a Boltzmann-like equation, and in the following work is more loosely described as a Boltzmann equation since there is no confusion with the kinetic theory one which is not used. The sub-systems are invariably termed molecules and the interactions between them collisions, although various alternative descriptions are discussed in the following sections. The general model is then formulated before the transport equation is derived and it's properties proved.

2.2 Scalar Models

The previous chapter dealt with the classical Boltzmann equation (1.1) and how, in the case of Maxwell molecules at least, it could be related to a scalar Boltzmann equation (1.10). It is the purpose of this chapter to prove the properties of this scalar equation which describes the relaxation towards equilibrium of certain idealised, closed systems. These properties can be shown to hold for either a discrete or continuous state variable. Although both types of system are considered in this thesis only the proofs for the latter type are given, since to give the proofs for the discrete variable case would simply be a repetition of the continuous variable proof with the replacement of integral signs by summation ones.

The basic model is defined by several postulates, viz.

(1) In the system there are a total of N molecules which is a conserved quantity.

(2) These molecules interact through binary collisions and the exchanged quantity (energy) is conserved at each collision. This implies that the energy of the system as a whole is conserved.

(3) The state of each element is described by a single, positive, scalar variable, (the state variable). This point is the first departure from the classical Boltzmann equation (1.1) where a particle's state is traditionally described by a velocity $\underline{v}$ and a position $\underline{r}$.

(4) The interactions are statistical and governed by a transition kernel K(y,x;u)dy (in the discrete case this is the transition matrix K(j,i;k)) which describes the probability density for the transition from x to dy about y, given that there is a total energy u in the collision complex.

(5) Finally the number of elements is large and so it is reasonable to consider the global state of the system which is described by a probability density P(x,t), only defined for positive values of x.

There are two natural simplifications of the transition kernel, the first is when the final state becomes independent of the initial state and depends only on the total energy in the collision complex (i.e. K(y,x;u) $\longrightarrow$ K(y;u)). This type of interaction is one between molecules of diffuse scattering type, and the molecules have no memory of their previous states. The second simplification which can be for molecules of either diffuse or persistent scattering type is that the collision number is independent of state. There are thus four subclasses of kernels and we differentiate between them as,

$$\int_0^u K(y,x;u)\,dy = \int_0^u K(y;u)\,dy = \text{constant} \tag{2.1a}$$

$$\int_0^u K(y,x;u)\,dy = \int_0^u K(y;u)\,dy = Z(u) \tag{2.1b}$$

$$\int_0^u K(y,x;u)\,dy = \text{constant} \tag{2.1c}$$

$$\int_0^u K(y,x;u)\,dy = Z(x,u) \tag{2.1d}$$

There are of course another four which all have discrete variables but which are otherwise indistinguishable as sub-classes. Models a and b are of the diffuse scattering type whilst c and d are of the persistent scattering type.

Types b and d produce a singular transport equation, however we are only concerned with the sub-classes a and c, and the general properties of these models only will be proved. Many of the properties can also be shown to hold for the singular types of model (b,d) (see Hoare (1979)). Examples of types a and c will be given later in this thesis whilst a model of type b has been solved completely (Ernst & Hendriks (1979), with K(y;u)=1). There are no known models of type d.

All of these kernels must have the necessary interactional symmetry,

$$K(x,y;u) = K(u-x,u-y;u) \tag{2.2}$$

In addition since only positive values of the state variables are allowed this implies that the kernel K(y,x;u) is only defined if the state variables x and y are on the range (0,u), or alternatively the kernel has the following step fuctions associated with it, H(u), H(y), H(u-y), H(x), H(u-x) where H is the standard Heaviside step function. These implicit step functions make the interchange of integrals a much easier task in the later work.

The quantity which is of interest in continuous systems is the probability density P(x,t) where,

$$P(x,t)dx = \Pr\left\{\begin{array}{l}\text{a particle has an energy between } x \text{ and}\\ x+dx \text{ at a time } t.\end{array}\right\}$$

the corresponding discrete probability distribution is written in the same way P(i,t) and defined in a similar way,

$P(i,t)=\Pr\left\{\text{a particle has an energy } i \text{ at a time } t\right\}$. To distinguish between discrete and continuous state variables the set of letters $\{i,j,k,l,m,n\}$ will be reserved for the discrete state variables and all others will be availiable for the continuous state variables.

2.3 Internal State Models

Much of the emphasis of the previous work has been on the kinetic theory Boltzmann equation. In this thesis this is shifted to examine the relaxation of sub-systems with internal energy states (or degrees of freedom) in a microcanonical ensemble with a specified total energy. The resulting transport equation is one of the Tjon-Wu type (Tjon & Wu (1979)) which they and others have shown to be equivalent to the classical Boltzmann equation for a homogeneous, isotropic system of Maxwell molecules.

A simple example of the type of model to be considered would be the relaxation of vibrational energy in a closed system of molecules interacting via binary collisions at constant collision number. By considering this, the transition to a discrete set of state variables is a natural extension to that of quantum transfer, which would be highly artificial in the case of velocities.

In this context, examples of soluble non-linear oscillator relaxation are presented (with both diffuse and persistent scattering) in which multiple degrees of freedom are allowed for and where a discrete or continuous state space may be assumed with equal facility. The connection of these models to those of Krook & Wu (1977), Tjon & Wu (1979) and the linear distributive models for a test particle in a heat bath (Cooper & Hoare (1979),Cooper, Hoare & Rahman (1977), and Hoare & Rahman (1979)) are discussed and the interrelationships between the various models are also studied. Exact similarity solutions are given for each model, and the moment equations are studied with a view to obtaining a general solution.

2.4 Economic and Biological Systems

In the previous section the context was one of oscillator relaxation in isolated systems, and indeed this will be the terminology for most of the future work. However the overall formulation of these non-linear systems is sufficiently general to allow for systems other than physical ones to be considered. An example of this is given in Appendix E where a kernel irrelevant to Physics leads to a general solution of a problem which can only be discussed under the guise of an economic system.

In the possibility of economic systems an elementary and perhaps naive approach would be to consider a collective of N players, where now the state variable represents the wealth of each player, playing two person zero-sum games (binary interactions) with their opponents being chosen at random. The crux of a physical system is the principle of microscopic reversibility, or the existence of the reverse collision, however in a non-physical system such as this there is no need for restrictions such as these, thus admitting a far wider range of systems to be studied.

Whilst the formalism is not immediately applicable to biological systems, the problem of interacting populations does have some connection. It is found that the systems of equations for moment evolution (see e.g. equation (2.40)) are identical to those for a number of a particular species in a world of competing species (see e.g. Goel, Maitre & Montroll (1971)). This aspect of the present work has not been investigated, but it appears that the solutions of the moments equations will also provide solutions for similar population equations given suitable boundary conditions and transition probabilities.

2.5 The Transport Equation

The interactions are described pictorially in Fig. 2.1. From this it can be seen that the balance of flux of a state x is given by,

$$\frac{\partial P(x,t)}{\partial t} = \omega \int_x^\infty du \int_0^u dy \; P(y,t)\, P(u-y,t)\left[k(x,y;u) + k(x,u-y;u)\right]$$
$$- \omega \int_x^\infty du \int_0^u dy \; P(x,t)\, P(u-x,t)\left[k(y,x;u) + k(y,u-x;u)\right] \qquad (2.3)$$

where ω is some collision rate. We note that inherent in this equation are the usual assumptions made in

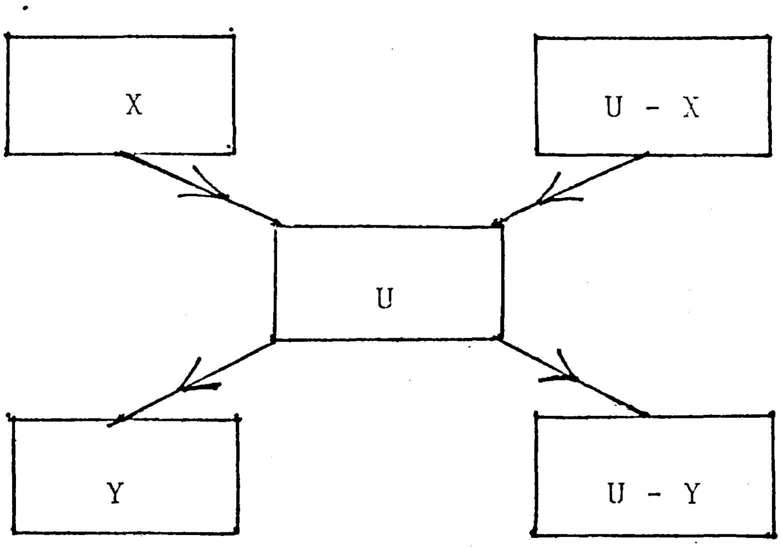

Fig. 2.1

deriving the Boltzmann equation which have been discussed in the previous chapter. For the second integral in the first bracket we have,

$$\omega\int_{x}^{\infty}du\int_{0}^{u}dy\; P(y,t)\,P(u-y,t)\;K(x,u-y;u)$$

$$=\omega\int_{x}^{\infty}du\int_{0}^{u}dy\; P(u-y,t)\,P(y,t)\;K(x,y;u) \qquad (2.4)$$

on making the transformation y = u-y. By making a similar transformation to the second integral in the second bracket we get,

$$\frac{\partial P(x,t)}{\partial t}=2\omega\int_{x}^{\infty}du\int_{0}^{u}dy\; P(y,t)\,P(u-y,t)\;K(x,y;u)$$

$$-2\omega\int_{x}^{\infty}du\int_{0}^{u}dy\; P(x,t)\,P(u-x,t)\;K(y,x;u) \qquad (2.5)$$

The factor 2ω may be scaled into the time giving,

$$\frac{\partial P(x,t)}{\partial t} = \int_x^\infty du \int_0^u dy \Big\{ P(y,t)\,P(u-y,t)\,K(x,y;u) - P(x,t)\,P(u-x,t)\,K(y,x;u) \Big\} \tag{2.6}$$

This is then the most general scalar equation that we need to consider. The second integral over y and u may be performed explicitly noting that

$$\int_0^u K(y,x;u)\,dy = Z(x,u) \tag{2.7}$$

where Z(x,u) is the collision number. Although all of the proofs in the rest of the chapter can be shown to hold for a general Z (Hoare (1979)), we restrict ourselves to the subset of models where Z(x,u) = 1. At first sight this appears to be a very severe restriction, but as we shall see later all of the models that we consider here fall into this class; indeed in the context of internal state relaxation this is the natural assumption to make. On using this the transport equation can be written as,

$$\left(\frac{\partial}{\partial t} + N\right) P(x,t) = \int_x^\infty du \int_0^u dy \; P(y,t)\,P(u-y,t)\,K(x,y;u) \tag{2.8}$$

where N is given by,

$$\int_0^\infty P(x,t)\,dx = N \tag{2.9}$$

It is then obvious that the time may be scaled such that the distribution is properly normalised.

$$\int_0^\infty P(x,t)\,dx = 1 \tag{2.10}$$

This is the condition for conservation of probability (or number), and it will be shown that this is a natural consequence of the form of the scalar transport equation (2.6). Thus with the probability distribution so normal-ised the transport equation becomes,

$$\left(\frac{\partial}{\partial t}+1\right)P(x,t) = \int_x^\infty du \int_0^u dy\, P(y,t)\,P(u-y,t)\,K(x,y;u) \tag{2.11}$$

and this will be the starting point of most of the future work.

2.6 Number Conservation

One of the premises that we used in the construction of these models was that the number of particles in the system is a conserved quantity. This can be seen to be a natural result due to the form of equation (2.6). The number is defined by equation (2.9) and hence the rate of change of number is found by directly integrating equation (2.6) with respect to x. This gives,

$$\begin{aligned}\frac{dN}{dt} + N^2 &= \int_0^\infty dx \int_x^\infty du \int_0^u dy\, P(y,t)\,P(u-y,t)\,K(x,y;u)\\ &= \int_0^\infty du\, P(u,t) \int_0^\infty dy\, P(y,t)\\ &= N^2\end{aligned}$$

which of course implies that dN/dt = 0, and hence number is conserved. Putting N=1 is equivalent to scaling the time by a factor N, this along with the factor 2 which was scaled in earlier means that the time is scaled by one collision time since at each collision two particles are relaxed.

2.7 Energy Conservation

Another basic assumption that was made, was to assume that the total energy of the system is conserved. Like the conservation of number this is also a natural consequence of the form of the transport equation. The total energy is defined as,

$$\int_0^\infty x\, P(x,t)\, dx = N\varepsilon \tag{2.12}$$

and so to find the temporal change of this quantity we multiply equation (2.6) by x, and integrate it with respect to x,

$$\frac{d\varepsilon}{dt} + N\varepsilon = \int_0^\infty x\, dx \int_x^\infty du \int_0^u dy\, P(y,t)\, P(u-y,t)\, K(x,y;u) \tag{2.13}$$

We note that if this proved for the persistent scattering case then it is also proved for the diffuse scattering case, and although the diffuse scattering case provides a few simplifications in the proof it will not be proved separately here. It is first necessary to prove a subsidiary result here which is given in full since the result will be required elsewhere.

$$\int_0^\infty dx \int_x^\infty du \int_0^u dy \; x \, K(x,y;u) \, P(y,t) \, P(u-y,t)$$

$$= \int_0^\infty dx \int_x^\infty du \int_0^u dy \; x \, K(u-x,u-y;u) \, P(y,t) \, P(u-y,t)$$

$$= \int_0^\infty du \int_0^u dx \int_0^u dy \; (u-x) K(x,y;u) \, P(y,t) \, P(u-y,t)$$

$$= \frac{1}{2} \int_0^\infty du \int_0^u dy \; u \, P(y,t) \, P(u-y,t)$$

$$= \frac{1}{2} \left(N\varepsilon + N\varepsilon \right) = N\varepsilon . \qquad (2.14)$$

Thus using this result the right hand side of equation (2.13) is easily evaluated and it becomes,

$$\frac{d\varepsilon}{dt} + N\varepsilon = N\varepsilon$$

and thus $d\varepsilon/dt = 0$ and the energy is conserved. We note that again there is no restriction as to the actual value of the energy and that the state variable x may be scaled by the energy ε without any loss of generality. This is the first important departure from the discrete case where the energy is not an entirely redundant parameter. In the discrete formalism the conservation of energy is written as,

$$\varepsilon_0 \sum_{i=1}^{\infty} i \, P(i,t) = \varepsilon \qquad (2.15)$$

where ε_0 is the quantum size and ε the total energy. We further note that one of these parameters is not needed since the two always occur in the combination $\varepsilon/\varepsilon_0$ which may be replaced by a single parameter. However for easy comparison between the continuous and discrete models these constants are left explicit in all of the future work.

2.8 Positivity of P(x,t)

For the scalar Boltzmann equation to make any physical sense it must preserve the postivity of the distribution function P(x,t). This is standard bookwork for the classical Boltzmann equation (see e.g. Resibois & de Leener (1977)), and in the present notation the proof is as follows.

Conjecture - If the initial distribution is positive for all x, then this positivity is preserved for all time at all x.

The first (necessary) assumption is that,

$$P(x,0) \geqslant 0 \qquad \forall x \tag{2.16}$$

Suppose that there is a point x_0 where, in the course of time the function first becomes negative. This occurs at a time t_0 such that,

$$P(x_0,t_0) < 0 \tag{2.17}$$

By continuity at a slightly earlier time $t_0 - \varepsilon$ the distribution at x_0 was zero.

$$P(x_0, t_0-\varepsilon) = 0 \tag{2.18}$$

We evaluate equation (2.11) at the time $t = t_0 - \varepsilon$ and at the point x_0.

$$\left.\frac{\partial P(x_0,t)}{\partial t}\right|_{t=t_0-\varepsilon} = \int_{x_0}^{\infty} du \int_0^u dy\, K(x_0,y;u)\, P(y,t_0-\varepsilon)\, P(u-y,t_0-\varepsilon) \geqslant 0 \tag{2.19}$$

(since $P(y,t_0-\varepsilon)$ and $P(u-y,t_0-\varepsilon)$ are both zero or positive and the kernel K is positive.) The result (2.18) together with the result (2.19) disprove the assumed result (2.17) by contradiction.

2.9 Equilibrium and Detailed Balance

For real closed systems it is reasonable to assume that there is only one solution $P_\infty(x)$ satisfying the equilibrium solution,

$$\int_x^\infty du \int_0^u dy \left\{ P_\infty(y) P_\infty(u-y)\, K(x,y;u) - P_\infty(x)\, P_\infty(u-x)\, K(y,x;u) \right\} = 0 \tag{2.20}$$

The detailed balance condition is the stronger one that the integrand also vanishes, and it's existence is a requirement on the kernel K. Thus for systems with detailed balance,

$$\frac{P_\infty(y)\,P_\infty(u-y)}{P_\infty(x)\,P_\infty(u-x)} = \frac{K(y,x;u)}{K(x,y;u)} \tag{2.21}$$

This says that at equilibrium the flux out of a volume of phase space is equal to the flux into that volume. The analogue of (2.21) for discrete systems is

$$\frac{P_\infty(j)\,P_\infty(k-j)}{P_\infty(i)\,P_\infty(k-i)} = \frac{K(j,i;k)}{K(i,j;k)} \tag{2.22}$$

2.10 Entropy and The H-Theorem

2.10.1 Entropy

The usual definition of entropy (S) is,

$$S = -k\int_0^\infty P(x,t)\,\ln\left[P(x,t)\right]\,dx. \tag{2.23}$$

However since we are dealing with molecules with internal energy states this must be modified to,

$$S = -k\int_0^\infty P(x,t)\,\ln\left[\frac{P(x,t)}{P_\infty(x)}\right]dx \tag{2.24}$$

or an equivalent form,

$$S = -k\int_0^\infty P(x,t)\,\ln\left[\frac{P(x,t)}{g(x)}\right]dx \tag{2.25}$$

where g(x) is the density of states function (see e.g.

Tolman (1938) or van Kampen (1959)). These two forms can be seen to be equivalent to within an additive constant by substituting in the definition of density of states in equation (2.24)

$$g(x) = Z(\beta)\, e^{\beta x}\, P_{\infty}(x) \tag{2.26}$$

Using the form (2.25) the entropy naturally splits into two parts σ_1 and σ_2, defined as,

$$\sigma_1 = -k\int_0^{\infty} P(x,t)\ln\left[P(x,t)\right]dx$$

$$\sigma_2 = +k\int_0^{\infty} P(x,t)\ln\left[g(x)\right]dx \tag{2.27}$$

where σ_2 can be seen to be the result of the multiple internal states in each subsystem. The total entropy is the sum of these two component parts,

$$S = \sigma_1 + \sigma_2 \tag{2.28}$$

2.10.2 Entropy Production

The total entropy production is given by,

$$\frac{dS}{dt} = -k\int_0^{\infty} \frac{\partial P(x,t)}{\partial t}\ln\left[\frac{P(x,t)}{P_{\infty}(x)}\right] \tag{2.29}$$

Using (2.6) in (2.29) gives,

$$k^{-1}\frac{dS}{dt} = -\int_0^{\infty}du\int_0^{u}dy\int_0^{u}dx\,\Big\{P(x,t)P(u-x,t)K(y,x;u) - P(y,t)P(u-y,t)K(x,y;u)\Big\}\ln\left[\frac{P(x,t)}{P_{\infty}(x)}\right] \tag{2.30}$$

and we note that the variables x and y may be interchanged to give,

$$k^{-1}\frac{dS}{dt} = -\int_0^\infty du \int_0^u dy \int_0^u dx \,\Big\{P(x,t)\,P(u-x,t)\,K(y,x;u) - P(y,t)\,P(u-y,t)\,K(x,y;u)\Big\} \ln\left[\frac{P(y,t)}{P_\infty(y)}\right]$$

$$= \frac{1}{2}\int_0^\infty du \int_0^u dy \int_0^u dx \,\Big\{P(x,t)P(u-x,t)K(y,x;u) - P(y,t)P(u-y,t)K(x,y;u)\Big\} \cdot \ln\left[\frac{P(u-x,t)\,P_\infty(u-y)}{P_\infty(u-x)\,P(u-y,t)}\right]$$

$$= \frac{1}{4}\int_0^\infty du \int_0^u dy \int_0^u dx \,\Big\{P(x,t)P(u-x,t)K(y,x;u) - P(y,t)P(u-y,t)K(x,y;u)\Big\} \cdot \ln\left[\frac{P(x,t)\,P(u-x,t)\,P_\infty(y)\,P_\infty(u-y)}{P_\infty(x)\,P_\infty(u-x)\,P(y,t)\,P(u-y,t)}\right] \qquad (2.31)$$

Defining a transformation,

$$h(x,t) = \frac{P(x,t)}{P_\infty(x)} \qquad (2.32)$$

gives,

$$k^{-1}\frac{dS}{dt} = \frac{1}{4}\int_0^\infty du \int_0^u dy \int_0^u dx \,\Big\{h(x,t)\,h(u-x,t)\,P_\infty(x)P_\infty(u-x)\,K(y,x;u) - h(y,t)\,h(u-y,t)\,P_\infty(y)\,P_\infty(u-y)\,K(x,y;u)\Big\} \ln\left[\frac{h(x,t)\,h(u-x,t)}{h(y,t)\,h(u-y,t)}\right] \qquad (2.33)$$

Finally using the detailed balance condition (2.21),

$$\frac{dS}{dt} = \frac{k}{4}\int_0^\infty du \int_0^u dy \int_0^u dx \; P_\infty(x)\, P_\infty(u-x)\; K(y,x;u)$$

$$\cdot \left\{ h(x,t)\, h(u-x,t) - h(y,t)\, h(u-y,t) \right\} \ln\left[\frac{h(x,t)\; h(u-x,t)}{h(y,t)\; h(u-y,t)}\right]$$

$$\geqslant 0 \tag{2.34}$$

and hence the H-Theorem is proved in general for the class of systems considered here. We note that no definite sign can be obtained for the higher derivatives of S for the general system, although these have been examined for specific models.

2.11 Moments

Due to the inherent difficulty of this type of non-linear problem it is often useful to obtain information about the solution from the moments of the probability distribution function. The moments are defined as,

$$m_n(t) = \int_0^\infty x^n \; P(x,t)\, dx \tag{2.35}$$

although it will also be of use to define the 'normalised' moments,

$$\mu_n(t) = \frac{1}{n!}\int_0^\infty x^n \; P(x,t)\, dx \tag{2.36}$$

The problem of inverting these power moments is an old one (see Zernike (1926)), and can be circumvented by using suitable polynomial moments, since one is then expanding

P(x,t) in a complete orthogonal set. In classical kinetic theory these are traditionally Sonine Polynomials (see e.g. Chapman & Cowling (1970)) or generalised Laguerre polynomials, and it is found that these and their discrete counterparts (the Meixner Polynomials - see Appendix C) are also suitable for the scalar models considered in later chapters.

The zeroth moment $\mu_0(t) = 1$, since that is just the conservation of probability condition, and the first moment $\mu_1(t) = \mathcal{E}$ (with the appropriate change for the discrete case), because of the conservation of energy. The second moment is the most important one since it describes the width of the distribution and has the longest relaxation time. For this reason we study the relaxation of the second moments of both the diffuse and persistent scattering systems in general.

2.11.1 Diffuse Scattering Case

The moments of the kernel are,

$$\int_0^\infty x^n K(x;u)\,dx = c_n u^n \tag{2.37}$$

This result is argued on purely dimensional grounds, and although it excludes the possibility of terms such as u^{n+1}/kT the resultant class of kernels is large and contains all that are examined here. It should also be noted that the work in this section is valid only for the continuous models and that there is no such general formalism for the discrete models. On taking the n'th moment of equation (2.11) for a diffuse scattering kernel we get,

$$\begin{aligned}\left(\frac{d}{dt}+1\right)\mu_n(t) &= \int_0^\infty \frac{x^n}{n!}\,dx \int_x^\infty du\; K(x;u)\int_0^u P(y,t)\,P(u-y,t)\,dy \\ &= \int_0^\infty du \int_0^u dy\; P(y,t)P(u-y,t)\; c_n \frac{u^n}{n!} \\ &= c_n \sum_{k=0}^{n} \int_0^\infty \frac{u^k}{k!} P(u,t)\,du \int_0^\infty \frac{y^{n-k}}{(n-k)!} P(y,t)\,dy \\ &= c_n \sum_{k=0}^{n} \mu_k(t)\,\mu_{n-k}(t)\end{aligned} \tag{2.38}$$

As is well known in the case of kinetic theory and the classical Boltzmann equation the result is a set of equations for the moments which can be solved sequentially. This set of equations represents a general solution to the scalar Boltzmann equation for diffuse scattering molecules; the only variant arising from the moments of the kernel in the form of the constants c_n. As mentioned this idea of finding the moments is not new and was first hinted at by Maxwell (1866) when he formulated his theory of Maxwell molecules. The second and third moments μ_2 and μ_3 are calculated explicitly in Appendix D, but it can be seen that the results rapidly become cumbersome and difficult to calculate. There have been several attempts to find the solutions of these moment equations for specific models and these will be considered more deeply when similar models are solved in later chapters.

2.11.2 Persistent Scattering Case

The n'th moment of a persistent scattering kernel does not necessarily have such a nice form as that in the diffuse scattering case; however assuming that the kernel is a convolution of distributions each of which has proportional moments then the moments of the persistent scattering kernel are of the form,

$$\int_0^{u+y} x^n K(x,y;u+y)\,dx = \sum_{k=0}^{n} \binom{n}{k} a_{n,k}\, u^k y^{n-k} \tag{2.39}$$

(Note the shift in u for convenience). This means that whilst the general moment equations can be written down, the class of systems to which they apply is smaller than that in the diffuse scattering case. Taking moments of equation (2.11) for a persistent scattering kernel gives,

$$\left(\frac{d}{dt}+1\right)\mu_n(t) = \int_0^\infty \frac{x^n}{n!}\,dx \int_x^\infty du \int_0^u dy\; P(y,t)\,P(u-y,t)\,K(x,y;u)$$

$$= \sum_{k=0}^{n} a_{n,k} \int_0^\infty \frac{u^k}{k!} P(u,t)\,du \int_0^\infty \frac{y^{n-k}}{(n-k)!} P(y,t)\,dy$$

$$= \sum_{k=0}^{n} a_{n,k}\, \mu_k(t)\, \mu_{n-k}(t) \tag{2.40}$$

Again these equations have the same boundary conditions as those in the diffuse scattering case and can be solved sequentially. The equation for the second moment is similar to that in the diffuse scattering case, viz.,

$$\mu_2(t) - \mu_2(\infty) = (\mu_2(0) - \mu_2(\infty)) e^{-\lambda_2 t} \tag{2.41}$$

where,

$$\lambda_2 = 1 - a_{2p} - a_{22} \tag{2.42}$$

$$\mu_2(\infty) = \frac{a_{21}\varepsilon^2}{\lambda_2} \tag{2.43}$$

The higher moments are not considered since the algebra becomes prohibitively cumbersome.

2.12 The Linearised Equation

As already mentioned the underlying difficulty of the full non-linear equation prompts one to consider various approximations to it. For distributions or systems which are everywhere close to equilibrium, the equation may be linearised by the substitution,

$$P^L(x,t) = P_\infty(x) + h(x,t) \tag{2.44}$$

where h(x,t) is, in some sense, small everywhere. The alternative linearisation procedure of putting,

$$\bar{P}^L(x,t) = P_\infty(x)\left(1 + \bar{h}(x,t)\right) \tag{2.45}$$

can easily be recovered at any stage in the future working by putting,

$$h(x,t) = \bar{h}(x,t)\, P_\infty(x)$$

(2.46)

Since P(x,t) has boundary conditions imposed upon it by equations (2.10) and (2.12) and $P_\infty(x)$ has the same conditions this implies the following boundary conditions for h(x,t),

$$\int_0^\infty h(x,t)\,dx = 0$$

$$\int_0^\infty x\,h(x,t)\,dx = 0$$

(2.47)

and the asymptotic condition,

$$h(x,\infty) = 0$$

(2.48)

Substituting equation (2.44) in equation (2.11) gives,

$$\left(\frac{\partial}{\partial t}+1\right) h(x,t) + P_\infty(x)$$

$$= \int_x^\infty du \int_0^u dy \left[P_\infty(y)+h(y,t)\right]\cdot\left[P_\infty(u-y) + h(u-y,t)\right]\cdot K(x,y;u)$$

$$\simeq \int_x^\infty du \int_0^u dy\, P_\infty(y)\, P_\infty(u-y)\, K(x,y;u)$$

$$+ \int_x^\infty du \int_0^u dy \left\{P_\infty(y)\, h(u-y,t) + P_\infty(u-y)\, h(y,t)\right\} K(x,y;u)$$

(2.49)

Using the detailed balance property, the first integral becomes $P_\infty(x)$, whilst exchanging the variables in the first part of the bracket yields,

$$\left(\frac{\partial}{\partial t} + 1\right) h(x,t) = \int_0^{\infty} dy \, A(x,y) \, h(y,t) \tag{2.50}$$

where,

$$A(x,y) = \int_{\max(x,y)}^{\infty} du \; P_{\infty}(u-y) \left\{ K(x,y;u) + K(x,u-y;u) \right\}. \tag{2.51}$$

In the case of diffuse interactions A is more simply defined as,

$$A(x,y) = 2 \int_{\max(x,y)}^{\infty} du \; P_{\infty}(u-y) \, K(x,u) \tag{2.52}$$

For the case of a discrete state variable these equations become,

$$\left(\frac{\partial}{\partial t} + 1\right) h(i,t) = \sum_{i=0}^{\infty} A(i,j) \, h(j,t) \tag{2.53}$$

$$A(i,j) = \sum_{k=\max(i,j)}^{\infty} P_{\infty}(k-j) \left\{ K(i,j;k) + K(i,k-j;k) \right. \tag{2.54}$$

$$A(i,j) = 2 \sum_{k=\max(i,j)}^{\infty} P_{\infty}(k-j) \; K(i;k) \tag{2.55}$$

respectively. Equation (2.50) is then the scalar linearised Boltzmann equation (note that h(x,t) can be replaced by $P^L(x,t)$ in (2.50)) which describes the relaxation of the system when it is close to equilibrium. In chapters three and four equations (2.50) and (2.53) have been solved exactly for the case of diffuse scattering molecules and the linearised solution compared to the exact one of the full non-linear equation.

2.13 The Fokker-Planck Equation

The Fokker-Planck equation is a partial differential equation, and is usually derived as an approximation to the Smoluchowski equation for Brownian motion (Wang & Uhlenbeck (1945) or Kittel (1958)) or to the Master equation (van Kampen (1960)). Both of these methods lead to a linear second order partial differential equation of the form,

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[A(x)\,P(x,t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[B(x)P(x,t)\right] \tag{2.56}$$

where A and B are the first and second transfer moments respectively of the transition kernel. It is used to describe the Brownian motion of a particle with the basic assumption that at each collision the step size in the state variable is small. In this section a non-linear Fokker-Planck equation will be derived starting from equation (2.6). This equation, when applied to the particular model of Chapter 5, reduces without further approximation to an equation linear in P(x,t), but with the coefficient B dependent on time as well as x.

The derivation of the equation will be given in full since it highlights some of the approximations made (which can also be considered as restrictions on the type of persistent scattering models to which this approximation can be applied). These approximations which appear to restrict severely the type of model to which the equation applies, are in fact only the conditions that the equation still conserves both energy and number; which it must if it is still to provide a realistic approximation to the system in question.

The essential idea behind the Fokker-Planck equation is that at each collision the change in the state varaible is small and so all relevant quantities in the equation (2.6) may be expanded as a Taylor series using this step as the small parameter. Only powers of this small parameter up to and including the second are retained in the approximation. Note that the assumption of a small step size must be justified by the existence of a small parameter. In the general derivation the existence of this small parameter is assumed.

Using a method parallel to that of Wang & Uhlenbeck (1945) we consider the average of an arbitrary function g(x). Using equation (2.6) the average is described by,

$$\frac{\partial}{\partial t}\int_0^\infty g(x)P(x,t)\,dx = \int_0^\infty g(x)\,dx\int_x^\infty du\int_0^u dy\,\Big\{P(y,t)P(u-y,t)K(x,y;u)$$

$$- P(x,t)\,P(u-x,t)\,K(y,x;u)\Big\}$$

$$= \int_0^\infty du\int_0^u dy\int_0^u dx\;P(x,t)P(u-x,t)K(y,x;u)\big(g(y)-g(x)\big)$$

(2.57)

Since the step size y-x is small, g(y) can be expanded about the point y=x using a Taylor expansion.

$$g(y) \simeq g(x) + (y-x)\frac{dg(x)}{dx} + \frac{1}{2}(y-x)^2\frac{d^2g(x)}{dx^2}$$

(2.58)

On defining the transfer moments of the kernel as,

$$A_n(x,u) = \int_0^{u+x} (y-x)^n \; K(y,x;u+x)\, dy \tag{2.59}$$

and substituting (2.58) and (2.59) in (2.57) the approximate form of (2.57) is,

$$\frac{\partial}{\partial t}\int_0^{\infty} g(x)\, P(x,t)\, dx = \int_0^{\infty} dx \int_0^{\infty} du \; P(x,t)\, P(u,t) \cdot \left\{ A_1(x,u)\frac{\partial g}{\partial x} + \frac{1}{2} A_2(x,u) \frac{\partial^2 g}{\partial x^2} \right\} \tag{2.60}$$

The two parts in the brackets may then be integrated by parts, the first once and the second twice to give,

$$\int_0^{\infty} g(x)\, \frac{\partial P(x,t)}{\partial t} = \int_0^{\infty} dx \int_0^{\infty} du \; g(x) \left\{ -\frac{\partial}{\partial x}\Big[A_1(x,u)\, P(x,t)\Big] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\Big[A_2(x,u)\, P(x,t)\Big] \right. \tag{2.61}$$

and since g(x) is an arbitrary function we can make the stronger assertion that,

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[P(x,t)\int_0^{\infty} du \; A_1(x,u)\, P(u,t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[P(x,t)\int_0^{\infty} du \; A_2(x,u)\, P(u,t)\right] \tag{2.62}$$

This is then the non-linear Fokker-Planck equation . When doing the integrations by parts and remembering that the function g(x) is entirely arbitrary two assumptions were made,

$$\int_0^\infty du\, P(u,t)\, P(x,t)\, A_1(x,u)\, g(x) \Big|_{x=0}^{x=\infty} = 0 \qquad (2.63)$$

$$\int_0^\infty du\, P(u,t) \frac{\partial}{\partial x}\Big[P(x,t)\, A_2(x,u)\, g(x) \Big] \Big|_{x=0}^{x=\infty} = 0 \qquad (2.64)$$

These are quoted without comment here, and it will be seen that these are precisely the conditions needed for (2.62) to conserve energy and number.They are equivalent to the two conditions,

$$P(x,t) \Big|_{x=0}^{x=\infty} = 0 \qquad (2.65)$$

$$\frac{\partial P(x,t)}{\partial x} \Big|_{x=0}^{x=\infty} = 0 \qquad (2.66)$$

For the Fokker-Planck equation to be a true representation of the system under examination it must preserve two important properties of that system; namely conservation of energy and of number.

2.13.1 Conservation of Number

Using equation (2.62) and integrating with respect to x gives,

$$\frac{dN}{dt} = -\int_0^\infty dx \frac{d}{dx}\Big\{ P(x,t) \int_0^\infty du\, P(u,t)\, A_1(x,u) \Big\} + \frac{1}{2}\int_0^\infty dx \frac{d^2}{dx^2}\Big\{ P(x,t) \int_0^\infty du\, P(u,t)\, A_2(x,u) \Big\}$$

$$= -P(x,t) \int_0^\infty du\, P(u,t)\, A_1(x,u) \Big|_{x=0}^{x=\infty} + \frac{1}{2}\frac{\partial}{\partial x}\left\{ P(x,t) \int_0^\infty du\, P(u,t)\, A_2(x,u) \right\} \Big|_{x=0}^{x=\infty}$$

$$= 0$$

and hence N is a constant. We note that this is dependent on the assumptions (2.65) and (2.66) which were made in the derivation of equation (2.62).

2.13.2 Conservation of Energy

A similar proof follows for the conservation of energy. We multiply both sides of equation (2.62) by x and integrate. Thus,

$$\frac{d\mathcal{E}}{dt} = I_1 + I_2 \tag{2.67}$$

where I_1 is given by,

$$I_1 = -\int_0^\infty dx\; x \cdot \frac{\partial}{\partial x}\left\{ P(x,t) \int_0^\infty du\, P(u,t)\, A_1(x,u) \right\}$$

$$= -x\, P(x,t) \left\{ \int_0^\infty du\, P(u,t)\, A_1(x,u) \right\} \Big|_{x=0}^{x=\infty} + \int_0^\infty dx\, P(x,t) \int_0^\infty du\, P(u,t)\, A_1(x,u)$$

$$= \int_0^\infty dx\, P(x,t) \int_0^\infty du\, P(u,t) \int_0^{u+x} dy\, (y-x)\, K(y,x;u+x).$$

Using the proof given by equation (2.14) this becomes,

$$= \int_0^\infty dx\, P(x,t) \int_0^\infty du\, P(u,t) \int_0^{u+x} dy \left(\frac{u-x}{2}\right) K(y,x;u+x) = 0 \tag{2.68}$$

and where I_2 is given by,

$$I_2 = \frac{1}{2}\int_0^\infty x \frac{\partial^2}{\partial x^2}\left\{P(x,t)\int_0^\infty du\, P(u,t)\, A_2(x,u)\right\}dx$$

$$= \frac{1}{2} x \frac{\partial}{\partial x}\left\{P(x,t)\int_0^\infty du\, P(u,t)\, A_2(x,u)\right\}\Bigg|_{x=0}^{x=\infty}$$

$$-\frac{1}{2}\int_0^\infty dx \frac{\partial}{\partial x}\left\{P(x,t)\int_0^\infty du\, P(u,t)\, A_2(x,u)\right\}$$

$$= -\frac{1}{2}\left\{P(x,t)\int_0^\infty du\, P(u,t)\, A_2(x,u)\right\}\Bigg|_{x=0}^{x=\infty} = 0$$

(2.69)

Hence $d\mathcal{E}/dt=0$ and energy is conserved.

2.13.3 'Conservation' of the Second Moment

The second moment is defined as,

$$m_2(t) = \int_0^\infty x^2 P(x,t)\, dx$$

(2.70)

and using the scalar Boltzmann equation (2.11) the relaxation of the second moment is described by,

$$\left(\frac{d}{dt}+1\right) m_2(t) = \int_0^\infty x^2 dx \int_x^\infty du \int_0^u dy\, K(x,y;u)\, P(y,t) P(u-y,t)$$

(2.71)

Using the Fokker-Planck equation (2.62) and taking the second moment of each side gives,

$$\frac{dm_2(t)}{dt} = I_1 + I_2$$

(2.72)

where,

$$I_1 = -x^2 \left\{ P(x,t) \int_0^\infty du\, P(u,t)\, A_1(x,u) \right\} \Bigg|_{x=0}^{x=\infty}$$

$$+2 \int_0^\infty dx \int_0^\infty du \int_0^{u+x} dy\, (y-x)x\, P(u,t)\, P(x,t)\, K(y,x;u+x)$$

$$= 2 \int_0^\infty dx \int_x^\infty du \int_0^u dy\, y(x-y)\, P(u-y,t)\, P(y,t)\, K(x,y;u)$$

(2.73)

and,

$$I_2 = \tfrac{1}{2} x^2 \frac{\partial}{\partial x} \{2.\} \Bigg|_{x=0}^{x=\infty} - \int_0^\infty dx\, x \frac{\partial}{\partial x} \{2.\}$$

$$= -x \{2.\} \Bigg|_{x=0}^{x=\infty} + \int_0^\infty dx \int_0^\infty du\, P(u,t) P(x,t)\, A_2(x,u) \cdot$$

$$= \int_0^\infty dx \int_x^\infty du \int_0^u dy\, P(u-y,t)\, P(y,t)\, (x-y)^2\, K(x,y;u)$$

(2.74)

Thus adding these two parts together and inserting them back in (2.72) produces,

$$\frac{dm_2}{dt} = \int_0^\infty dx \int_x^\infty du \int_0^u dy\, P(u-y,t)\, P(y,t)\, k(x,y;u)\, (x^2-y^2)$$

$$= \int_0^\infty dx \int_x^\infty du \int_0^u dy\, P(u-y,t)\, P(y,t)\, x^2 K(x,y;u) - m_2(t)$$

(2.75)

Thus it is seen that the equation for the relaxation of the second moment as derived from the scalar Boltzmann equation (2.71) is exactly the same as that derived from the Fokker-Planck equation.

2.14 Mixtures of Molecules

Until now all of the molecules in the system have been of the same type and therefore indistinguishable. More generally, however one may be concerned with the relaxation of a closed system when two or more types of molecule are present. This section deals with the problem of two interacting species, but is readily extended to a general composition of molecule types.

There are two types of particles which we shall label p and q types. An obvious example would be to have two sorts of oscillators, one with p degrees of freedom and one with q, but for the moment these systems will be treated quite generally. Nominally there are four different transition kernels which we notate as A,B,C and D of which two are connected. They are all stochastic, so that,

$$\int_0^u A(y,x;u)\,dy = 1 \qquad \text{etc.} \tag{2.76}$$

These interactions and their corresponding transition kernels are described diagrammatically in fig 2.2. The probability distribution functions for the p and q type molecules are P(x,t) and Q(x,t) respectively. Since the number of particles is conserved for each particle type but the energy is only conserved for the system as a whole, the conservation laws are,

$$\int_0^\infty P(x,t)\,dx = N_p \tag{2.77}$$

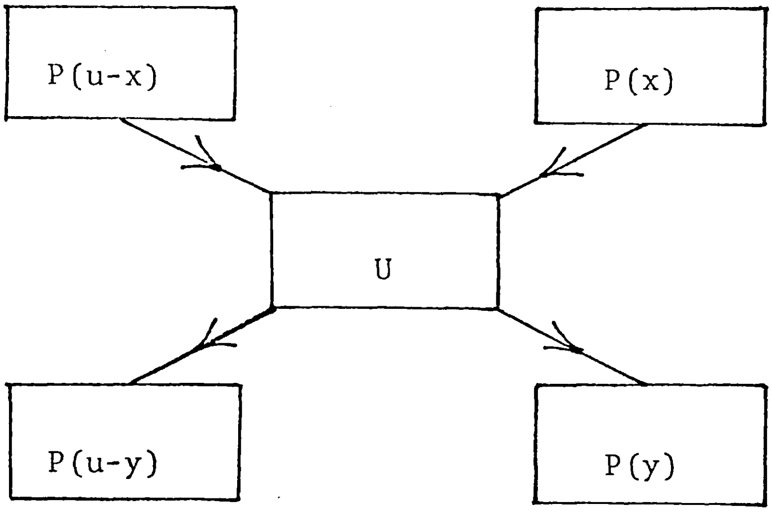

Fig 2.2a : Collision between two p type particles. $A(y,x;u) = A(u-y,u-x;u)$.

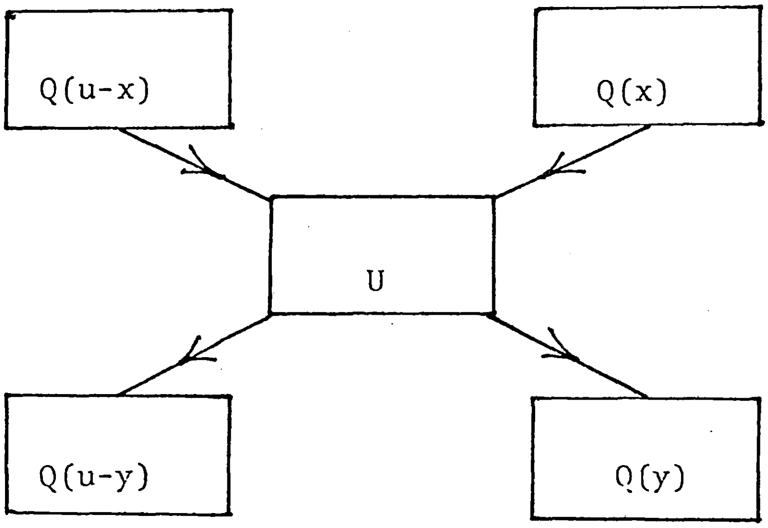

Fig 2.2b : Collision between two q type particles. $C(y,x;u) = C(u-y,u-x;u)$.

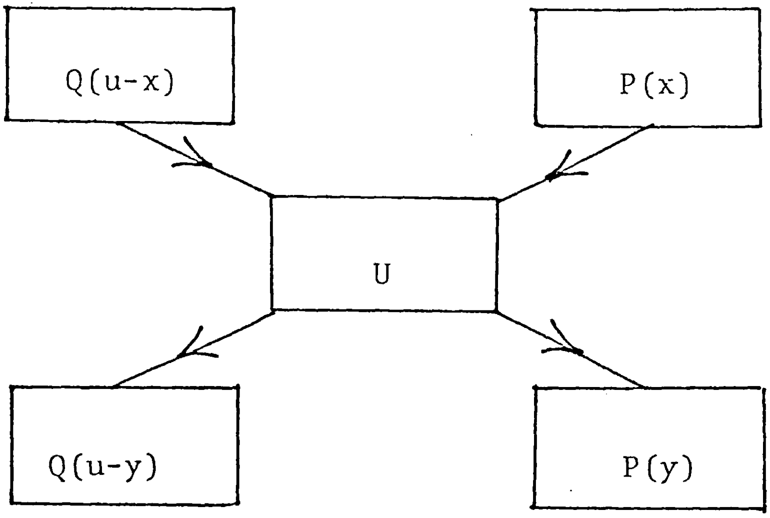

Fig 2.2c : Collision between p and q type particles . B(y,x;u) = D(u-y,u-x;u).

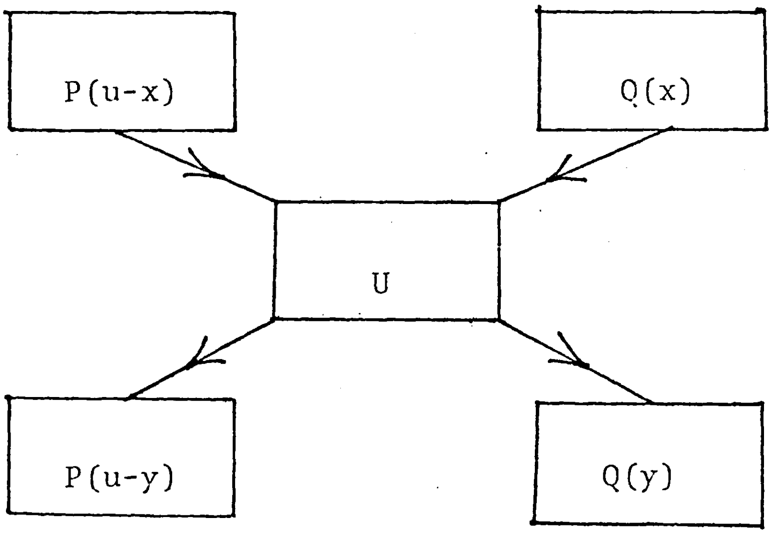

Fig 2.2d : Collision between p and q type particles. D(y,x;u) = B(u-y,u-x;u).

$$\int_0^\infty Q(x,t)\,dx = N_q$$

(2.78)

$$\int_0^\infty x\,\big(P(x,t) + Q(x,t)\big)\,dx = \mathcal{E}$$

(2.79)

The procedure of formulating the transport equations for these models is almost parallel to that for one type (see section 2.5). We consider the flux in x for the p type molecules; that for the q type can then be deduced without further analysis. A simple consideration of this change of flux for p type particles gives,

$$\begin{aligned}
\frac{\partial P(x,t)}{\partial t} &= \int_x^\infty du \int_0^u dy\; P(y,t)\,P(u-y,t)\big[A(x,y;u) + A(x,u-y;u)\big] \\
&\quad - \int_x^\infty du \int_0^u dy\; P(x,t)\,P(u-x,t)\big[A(y,x;u) + A(u-y,x;u)\big] \\
&\quad + \int_x^\infty du \int_0^u dy\; P(y,t)\,Q(u-y,t)\;B(x,y;u) \\
&\quad - \int_x^\infty du \int_0^u dy\; P(x,t)\,Q(u-x,t)\;B(y,x;u) \\
&= 2\int_x^\infty du \int_0^u dy\; P(y,t)\,P(u-y,t)\,A(x,y;u) - 2N_p P(x,t) \\
&\quad + \int_x^\infty du \int_0^u dy\; P(y,t)\,Q(u-y,t)\,B(x,y;u) - N_q P(x,t)
\end{aligned}$$

(2.80)

where a factor of ω (the nominal collision rate) has been scaled into the time.We note that unlike the case of one species the total number of a species cannot be scaled into the time without loss of generality. The relaxation of the q type molecules obeys the equation,

$$\frac{\partial Q(x,t)}{\partial t} = 2\int_x^{\infty} du \int_0^{u} dy\, Q(y,t)\, Q(u-y,t)\, C(x,y;u) - 2N_q\, Q(x,t)$$
$$+ \int_x^{\infty} du \int_0^{u} dy\, Q(y,t)\, P(u-y,t)\, D(x,y;u) - N_p\, Q(x,t) \qquad (2.81)$$

It can be shown in a manner completely analogous to that used in sections 2.6 and 2.7 that the conservation laws (equations (2.77),(2.78) and (2.79)) are also a natural consequence of these two equations.

Although a solution of these equations has not been attempted for a particular model a number of facts can be deduced quite generally from them. The only known solution of a pair of equations such as these is by Oppenheim, Shuler & Weiss (1967-8), where some of their results can be shown to arise from these equations without reference to a particular model.

2.14.1 Derivation of the Master Equation

The Master equation describes the relaxation of a test particle towards equilibrium due to collisions with a heat bath (which is always at equilibrium). In terms of the problem here this means that there is one type (say the p type) which is relatively few in number and not at equilibrium. Since they are sparsely distributed collisions between particles of that type are not considered (A=0). The other type of particle (q type) are numerous and at equilibrium ($Q(x,t)=Q_{\infty}(x)$). This equilibrium is not disturbed by the collisions with the test particles.

In these limits it is clearly seen that equation (2.80) becomes,

$$\frac{\partial P(x,t)}{\partial t} + N_q P(x,t) = \int_x^\infty du \int_0^u dy\, B(x,y;u)\, P(y,t)\, Q_\infty(u-y) \tag{2.82}$$

We now absorb the factor N_q into the time and define a new kernel,

$$B'(x,y) = \int_{\max(x,y)}^\infty du\; B(x,y;u)\; Q_\infty(u-y) \tag{2.83}$$

which gives the final form of the Master equation,

$$\frac{\partial P(x,t)}{\partial t} + P(x,t) = \int_0^\infty B'(x,y)\, P(y,t)\, dy. \tag{2.84}$$

We note that in the diffuse scattering case this is identical to the linearised equation apart from a different time scale.

2.14.2 Energy Flux Between Species

Although the total energy is conserved (equation (2.79)) there will be a flux of energy from one type of particle to the other. These energies are defined as,

$$\int_0^\infty x\, P(x,t)\, dx = \mathcal{E}_p(t) \tag{2.85a}$$

$$\int_0^\infty x\, Q(x,t)\, dx = \mathcal{E}_q(t) \tag{2.85b}$$

The conservation of energy now reads in this notation,

$$\mathcal{E}_p + \mathcal{E}_q = \mathcal{E} \tag{2.86}$$

Considering the special case of diffuse scattering molecules, the relaxation of these energies is given by,

$$\frac{d\mathcal{E}_p}{dt} + N_q \mathcal{E}_p (1-c_1) = c_1 N_p \mathcal{E}_q \tag{2.87}$$

where,

$$c_1 u = \int_0^x x B(x;u)\, dx \tag{2.88}$$

In common with the case of one species type the time is scaled to the total number of particles in the system. The mol fraction of p type particles is written as,

$$\gamma = \frac{N_p}{N_p + N_q} \tag{2.89}$$

and thus equation (2.87) becomes,

$$\frac{d\mathcal{E}_p}{dt} + (1-\gamma)(1-c_1)\,\mathcal{E}_p = c_1 \gamma \mathcal{E}_q \tag{2.90}$$

Using equation (2.86) this is seen to have the solution,

$$\mathcal{E}_p(t) - \mathcal{E}_p(\infty) = (\mathcal{E}_p(0) - \mathcal{E}_p(\infty))e^{-\lambda t} \tag{2.91}$$

where,

$$\lambda = (1-\gamma)(1-c_1) + c_1\gamma$$

$$\mathcal{E}_p(\infty) = \frac{c_1 \gamma \mathcal{E}}{\lambda} \tag{2.92}$$

The result (2.91) is quite general and was first obtained for the special case $c_1=\frac{1}{2}$ by Oppenheim, Shuler & Weiss (1967-8) for the case of harmonic oscillators with nearest neighbour interactions. The result for $\mathcal{E}_q$ is obtained by inserting (2.86) in (2.91),

CHAPTER. THREE : CONTINUOUS DIFFUSE SCATTERING MODEL

3.1 The Model

Consider a bath of molecules, each of which has p internal degrees of freedom, interacting via binary collisions. At each collision all of the degrees of freedom interact and hence all of the molecule's energy is 'scrambled' so that the molecule has no memory of it's previous state. (i.e. the molecule is of the diffuse scattering type.) The assumption that the mean collision time is long enough for all of the molecule's internal energy to be distributed amongst the internal energy states is implicit in this model and all of those considered later. In practice for dilute gases (an assumption in the derivation of the Boltzmann equation) this is easily realised.

The interaction is represented diagrammatically in fig. 3.1 which shows two molecules with energies x and u-x each with p degrees of freedom colliding to make a total collision complex of u in 2p degrees of freedom. The transition kernel is then obviously the probability that an energy in the range (y,y+dy) in p degrees of freedom arises from a total u in 2p degrees of freedom. This is the symmetric Beta distribution (see Appendix B).

$$K(y;u) = W_{pp}(y;u) = \frac{\Gamma(2p)}{\Gamma(p)^2} \frac{y^{p-1}(u-y)^{p-1}}{u^{2p-1}} \tag{3.1}$$

(The power moments for this are given in Appendix B, as is the derivation of the distribution.). In the case of p=1 this reduces to a uniform distribution $K(y;u)=u^{-1}$,

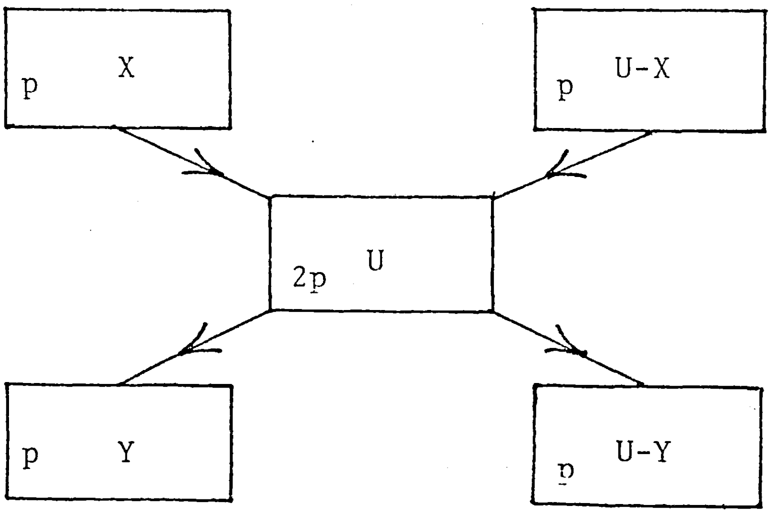

Fig. 3.1

which has been investigated by Tjon & Wu (1979) who showed that this model is equivalent to one investigated by Krook & Wu (1976,1977) and Bobylev (1976b), and by a similar method it will be shown that the general p kernel is exactly the same as the d-dimensional generalisation of the Krook-Wu-Bobylev model solved by Ernst (1979). The resulting Boltzmann equation is,

$$\left(\frac{\partial}{\partial t}+1\right)P(x,t) = \int_x^\infty du\, W_{pp}(x;u)\int_0^u dy\; P(y,t)\; P(u-y,t) \tag{3.2}$$

3.2 Equilibrium and Detailed Balance

The condition for detailed balance is,

$$K(y;u)\, P_\infty(x)\, P_\infty(u-x) = K(x;u)\, P_\infty(y)\, P_\infty(u-y) \tag{3.3}$$

or on replacing the kernel K with it's explicit form this is,

$$\frac{y^{p-1}(u-y)^{p-1}}{x^{p-1}(u-x)^{p-1}} = \frac{P_\infty(y)\,P_\infty(u-y)}{P_\infty(x)\,P_\infty(u-x)}$$

(3.4)

An obvious solution to this is of the form,

$$P_\infty(x) = a\,x^{p-1}\,e^{-bx}$$

(3.5).

The values of a and b are determined from the conditions of normalisation and conservation of energy. The normalisation condition gives,

$$\frac{a\,\Gamma(p)}{b^p} = 1$$

(3.6)

and the conservation of energy,

$$\frac{a\,\Gamma(p+1)}{b^{p+1}} = \mathcal{E}$$

(3.7)

These are solved to give,

$$b = p/\mathcal{E} \qquad , \qquad a = (p/\mathcal{E})^p\,\Gamma(p)^{-1}$$

(3.8)

and thus the equilibrium distribution is,

$$P_\infty(x) = (p/\mathcal{E})^p\,\Gamma(p)^{-1}\,x^{p-1}\,e^{-\frac{px}{\mathcal{E}}}$$

(3.9)

We note that the state variable x can be scaled in terms of the total energy $\mathcal{E}$ and the number of degrees of freedom p, thus there is no loss of generality in the future work by putting $\mathcal{E}$ =p, or $\mathcal{E}$ =1.

However the energy dependence will be left explicit in most of the future work to facilitate easy comparison with the discrete case where the energy cannot be scaled out.

3.3 Moments

3.3.1 Power Moments

In section 2.11.1 it was shown that the moment equations of all diffuse scattering models are the same to within an arbitrary constant c_n (defined in equation (2.37)). This constant is a funcion of the kernel and in the present case is,

$$c_n = \frac{(p)_n}{(2p)_n} \tag{3.10}$$

(see Appendix B for the moments of the symmetric Beta distribution). Thus the moments of the probability distribution function are given by the infinite set of moment equations,

$$\left(\frac{d}{dt} + 1\right) \mu_n(t) = \frac{(p)_n}{(2p)_n} \sum_{k=0}^{n} \mu_k(t)\, \mu_{n-k}(t) \tag{3.11}$$

The boundary conditions for these equations are,

$$\mu_0(t) = 1 \quad , \quad \mu_1(t) = \varepsilon \qquad , \forall t \tag{3.12}$$

and the asymptotic conditions,

$$\mu_n(\infty) = (\varepsilon/p)^n \, \frac{(p)_n}{n!} \tag{3.13}$$

In the case of p=1 and ε =1 the equations reduce to the simpler set of equations,

$$\left(\frac{d}{dt}+1\right)\mu_n(t) = \frac{1}{n+1}\sum_{k=0}^{n} \mu_k(t)\,\mu_{n-k}(t) \tag{3.14}$$

where now,

$$\mu_0' = 1\ ,\ \mu_1 = 1\ ,\quad \mu_n(\infty) = 1 \tag{3.15}$$

This set of equations (3.14) is exactly the same as that obtained by Krook & Wu (1977). for a class of Maxwell molecules. They obtained the solution,

$$\mu_n(t) = K^{n-1}(n-(n-1)K) \tag{3.16}$$

where,

$$K = 1 - e^{-t/6} \tag{3.17}$$

to these equations for a restricted class of initial distributions. Krook & Wu's work was in two dimensions and more recently Ernst (1979) has shown that the d-dimensional case can be identified the equations (3.11) using the relationship,

$$p = d/2 \tag{3.18}$$

thus making a definite connection between the p internal state oscillator model and the d-dimensional Maxwell molecule.

3.3.2 Polynomial Moments

Although the equations (3.11) can in theory be solved, due to the non-linearity of the problem the algebra rapidly becomes cumbersome, and as explained earlier it is by no means easy, having found the moments to find the explicit form of the distribution function (see Zernike (1926)).For this reason polynomial moments have been used since they are easily inverted to give the distribution function in terms of a series involving these moments and they provide a faster convergence to the actual function.

As shown previously the equilibrium distribution is the gamma function and thus it becomes natural to expand the distribution in terms of the Laguerre polynomials. These are identical to the Sonine polynomials which are traditionally used in kinetic theory and the classical Boltzmann equation.(Chapman & Cowling (1970)). The equilibrium distribution is given by (3.9) and hence we use the particular set of Laguerre polynomials $\left\{ L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right)\right\}$ as the basis set with the equilibrium distribution as the weight function. Expanding the probability distribution function in terms of the above set gives,

$$P(x,t) = (p/\varepsilon)^p x^{p-1} e^{-\frac{px}{\varepsilon}} \sum_{n=0}^{\infty} \gamma_n(t) L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) \frac{n!}{\Gamma(p+n)} \tag{3.19}$$

where the time dependent coefficients are the Laguerre moments of the probability distribution function.

$$\gamma_n(t) = \int_0^{\infty} L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) P(x,t)\, dx \tag{3.20}$$

It is worth noting the different boundary and asymptotic conditions from the case of power moments viz.,

$$\gamma_0(t) = 1 \quad , \quad \gamma_1(t) = 0 \qquad \forall t \tag{3.21}$$

The second of these follows immediately from the fact that $L_1^{(p-1)}\left(\frac{px}{\varepsilon}\right) = p\left(1 - \frac{x}{\varepsilon}\right)$ For the asymptotic behaviour as t ⟶ 0 we have,

$$\begin{aligned} \gamma_n(\infty) &= 1 \quad , \quad n = 0 \\ \gamma_n(\infty) &= 0 \quad , \quad n \neq 0 \end{aligned} \tag{3.22}$$

To find the $\gamma_n(t)$ explicitly, one multiplies (3.2) by $L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right)$ and integrates over all x to obtain

$$\left(\frac{d}{dt} + 1\right)\gamma_n(t) = \int_0^\infty L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right)\int_x^\infty du\, W_{pp}(x;u)\int_0^u dy\, P(y,t)\, P(u-y,t) \tag{3.23}$$

On rearranging the orders of integration on the right hand side (RHS) the x integral is,

$$\int_0^u L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) W_{pp}(x;u)\, dx = \frac{(p)_n}{(2p)_n}\, L_n^{(2p-1)}\left(\frac{pu}{\varepsilon}\right) \tag{3.24}$$

which is a standard integral (see e.g. Gradshteyn & Ryshik (1965)). On shifting the variable u to u+y and using the addition formula for Laguerre polynomials (equation(C.9})we have,

$$\left(\frac{d}{dt} + 1\right)\gamma_n(t) = \frac{(p)_n}{(2p)_n}\sum_{k=0}^{n}\int_0^\infty L_n^{(p-1)}\left(\frac{pu}{\varepsilon}\right) P(u,t)\, du$$

$$\cdot \int_0^\infty L_n^{(p-1)}\left(\frac{py}{\varepsilon}\right) P(y,t)\, dy$$

$$= \frac{(p)_n}{(2p)_n} \sum_{k=0}^{n} \gamma_k(t)\,\gamma_{n-k}(t) \tag{3.25}$$

These equations take exactly the same form as those for the ordinary power moments (3.11) but of course the boundary (3.21) and asymptotic conditions (3.22) are different to those for the power moments (3.12) and (3.13). Again these equations can be solved recursively to give,

$$\gamma_2(t) = \gamma_2(0)\, e^{-\frac{pt}{2p+1}} \tag{3.26}$$

$$\gamma_3(t) = \gamma_3(0)\, e^{-\frac{3pt}{2(2p+1)}} \tag{3.27}$$

and in general the n$^{\text{th}}$ moment will contain only sums of pure exponentials with no constant terms. (This is obvious from the form of the moment equations but can also be shown by induction.) In turn this implies that in the limit $t \rightarrow \infty$ all of the moments apart from the first will vanish, and hence any initial distribution (or at least one that can be expanded in terms of Laguerre polynomials) will tend to the weight function, i.e. the gamma function. This proof is without reference to the H- Theorem which was shown to hold in general for this class of systems (section 2.10.2) and avoids the tedious analysis given by Ray (1979) where the ordinary moments are used and one needs to extract the constant term from each of the moments.

3.4 The Similarity Solution

3.4.1 Introduction

Although having found the moment equations which can be solved sequentially one has essentially solved the problem exactly for an arbitrary initial distribution it is possible to find a class of exact solutions which can be expressed in closed form. It has been seen that the moment equations (and hence the solution of them) are identical to those found by Krook & Wu. For p=1 at least their solution could be copied line for line, however for arbitrary p there is no such proof availiable and so to find the solution for arbitrary p we turn to a method discussed by Bobylev in one of his papers (1976b) on these problems. Essentially he assumes a solution of the form (1.8) where A, B and C are time dependent 'constants' which he finds by direct substitution and use of the conservation laws.

3.4.2 The Solution

Bearing in mind that we are dealing with energy coordinates one might be tempted to assume a solution of the form,

$$P(x,t) = (A + Bx)e^{-Cx}$$

however since the function must contain the equilibrium distribution in some form we choose a trial solution of the form,

$$P(x,t) = (\alpha + \beta x)\, x^{p-1}\, e^{-\psi x}$$

(3.28)

where $\alpha(t)$, $\beta(t)$ and $\psi(t)$ are all time dependent functions. The conservation of energy and normalisation (equations (2.12) and (2.10)) enable α and β to be written as functions of ψ. Conservation of number gives,

$$\alpha + \frac{\beta p}{\psi} = \frac{\psi^{p}}{\Gamma(p)}$$

(3.29)

and conservation of energy,

$$\alpha + \frac{\beta(p+1)}{\psi} = \frac{\psi^{p+1}}{\Gamma(p+1)}\,\varepsilon$$

(3.30)

These are easily solved to give,

$$\alpha = \frac{\psi^{p}}{\Gamma(p)}\,(1 + p - \varepsilon\psi)$$

(3.31)

and

$$\beta = \frac{\psi^{p+1}}{\Gamma(p+1)}\,(\varepsilon\psi - p)$$

(3.32)

Equation (3.28) is then substituted directly into equation (3.2) to give,

$$\left(\frac{\partial}{\partial t} + 1\right)\left[(\alpha + \beta x)\, x^{p-1} e^{-\psi x}\right]$$
$$= \int_x^{\infty} du\, W_{pp}(x;u)\, e^{-\psi u} \int_0^{u} dy\, y^{p-1}(u-y)^{p-1}(\alpha + \beta y)(\alpha + \beta(u-y))$$

(3.33)

Using the detailed balance condition (3.3) the right hand side (RHS) becomes,

$$(\mathrm{RHS}) = x^{p-1}\int_x^{\infty} du\,(u-x)^{p-1} e^{-\psi u}\int_0^u (\alpha+\beta y)(\alpha+\beta(u-y))\,W_{pp}(y;u)\,dy$$

(3.34)

The inner integral involves moments of the kernel and the u integral gamma functions and powers.

$$(\mathrm{RHS}) = e^{-\psi x} x^{p-1}\int_0^{\infty} du\; u^{p-1} e^{-\psi u}\int_0^{u+x} dy\; W_{pp}(y;u+x)$$

$$\cdot\left\{\alpha^2 + \alpha\beta(u+x) + \beta^2(u+x)y - \beta^2 y^2\right\}$$

$$= e^{-\psi x} x^{p-1}\int_0^{\infty} du\; u^{p-1} e^{-\psi u}\left\{\alpha^2 + \alpha\beta(u+x) + \lambda\beta^2(u+x)^2\right\}$$

$$= e^{-\psi x} x^{p-1}\,\Gamma(p)\,\psi^{-p-2}\left\{(\alpha^2+\alpha\beta x + x^2\beta^2\lambda)\psi\right.$$

$$\left. + p\psi(\alpha\beta + 2\beta^2\lambda x) + \beta^2\lambda p(p+1)\right\}$$

(3.35)

where,

$$\lambda = \frac{p}{2(2p+1)}$$

(3.36)

Thus equating left and right hand sides gives,

$$\left(-x\frac{d\psi}{dt} + \frac{\partial}{\partial t} + 1\right)(\alpha+\beta x)$$

$$= \frac{\Gamma(p)}{\psi^{p+2}}\left\{\left[\alpha^2\psi^2 + \alpha\beta p\psi + \beta^2 p(p+1)\lambda\right]\right.$$

$$\left. + \left[\alpha\beta\psi^2 + 2\beta^2 p\,\psi\lambda\right]x + \beta^2\lambda\psi^2 x^2\right\}$$

(3.37)

For the trial solution to actually be a solution of the Boltzmann equation (3.2) the coefficients of x^0, x and x^2 must all be equal, and lead to a unique equation for ψ. After much algebra this is indeed, surprisingly perhaps, found to be the case; the coefficient of each of these powers gives rise to,

$$\frac{d\psi}{dt} = -\lambda\left(\frac{\varepsilon\psi}{p} - 1\right)\psi \tag{3.38}$$

This is easily solved to give,

$$\psi(t) = p/\varepsilon\left[1 - \eta e^{-\lambda t}\right]^{-1} \tag{3.39}$$

where η is an arbitrary constant which determines the form of the initial distribution, or expresses the fact that the solution is invariant with respect to time translation. Writing the solution in explicit form gives,

$$P^s(x,t) = \frac{\psi^p}{\Gamma(p)}\left[1 + p - \varepsilon\psi + \psi\left(\frac{\varepsilon}{p}\psi - 1\right)x\right]x^{p-1}e^{-\psi x} \tag{3.40}$$

where ψ is given by equation (3.39).

3.4.3 Why Similarity Solution ?

The method of similarity solution of a partial differential equation is a way by which the number of independent variables is reduced by one. (This method, which does not only apply to partial differential equations, is comprehensively covered by Bluman & Cole (1974)). The integro-differential equation Boltzmann equation (3.2) can be reduced by partial differentiation with respect to x into a non-linear partial differential equation with two independent variables. This is the method by which Krook & Wu solved the p=1 case of equation (3.2). The two independent variables x and t are combined in a certain fixed way to form a similarity variable. This combination follows from finding two invariant transformations of the partial differentia-equation which leave the boundary conditions unchanged.

This unique combination of the variables x and t is then carried right through to the final answer and is easily seen in equation (3.40) to be ψ x after noting that $\psi\varepsilon$ can be written as, $\int_0^\infty (\psi x) P(x,t)\,dx$. For this reason the solution is termed a similarity solution even though the methods of similarity theory have not been used directly.

3.4.4 Range of Solutions

In solving equation (3.38) an arbitrary parameter η arose, which parameterises the range of possible initial conditions. Hence the initial distribution is parameterised by ψ(0) where,

$$\psi(0) = P/\varepsilon\,(1-\eta)^{-1} \tag{3.41}$$

On physical grounds the solution must be positive for all x $\geqslant$ 0 and all t $\geqslant$ 0. This implies that both α and β must be positive so that ψ is restricted by,

$$P/\varepsilon \leqslant \psi(t) \leqslant \frac{1+P}{\varepsilon}$$

3.42)

in turn implying that the possible range of values for η is,

$$0 \leqslant \eta \leqslant (p+1)^{-1} \tag{3.43}$$

It is also obvious that for some non-physical distribution with $\eta > (1+p)^{-1}$ the distribution will become positive after a time τ where,

$$\tau = \lambda^{-1} \ln[\eta(p+1)] \tag{3.44}$$

Considering just ψ it is obvious that the value of $\psi(0) = (1+p)/\varepsilon$ corresponds to the value of the initial distribution which is furthest from the equilibrium distribution (3.9). In figs. 3.2 to 3.4 these most extreme initial distributions are plotted in comparison with the equilibrium distribution. It will be seen that although they are disappointingly close to equilibrium they are still outside the linear regime. These diagrams are also consistent with what equation (3.42) suggests, that as p increases the range of possible initial distributions decreases.

It is perhaps more meaningful to consider the ratio of the initial and final (equilibrium) distributions. Scaling the energy into the state variable we have for the initial distribution,

$$P^{s}(x,0) = \frac{(1+p)^{p+1}}{\Gamma(p+1)} x^{p} e^{-(p+1)x} \tag{3.45}$$

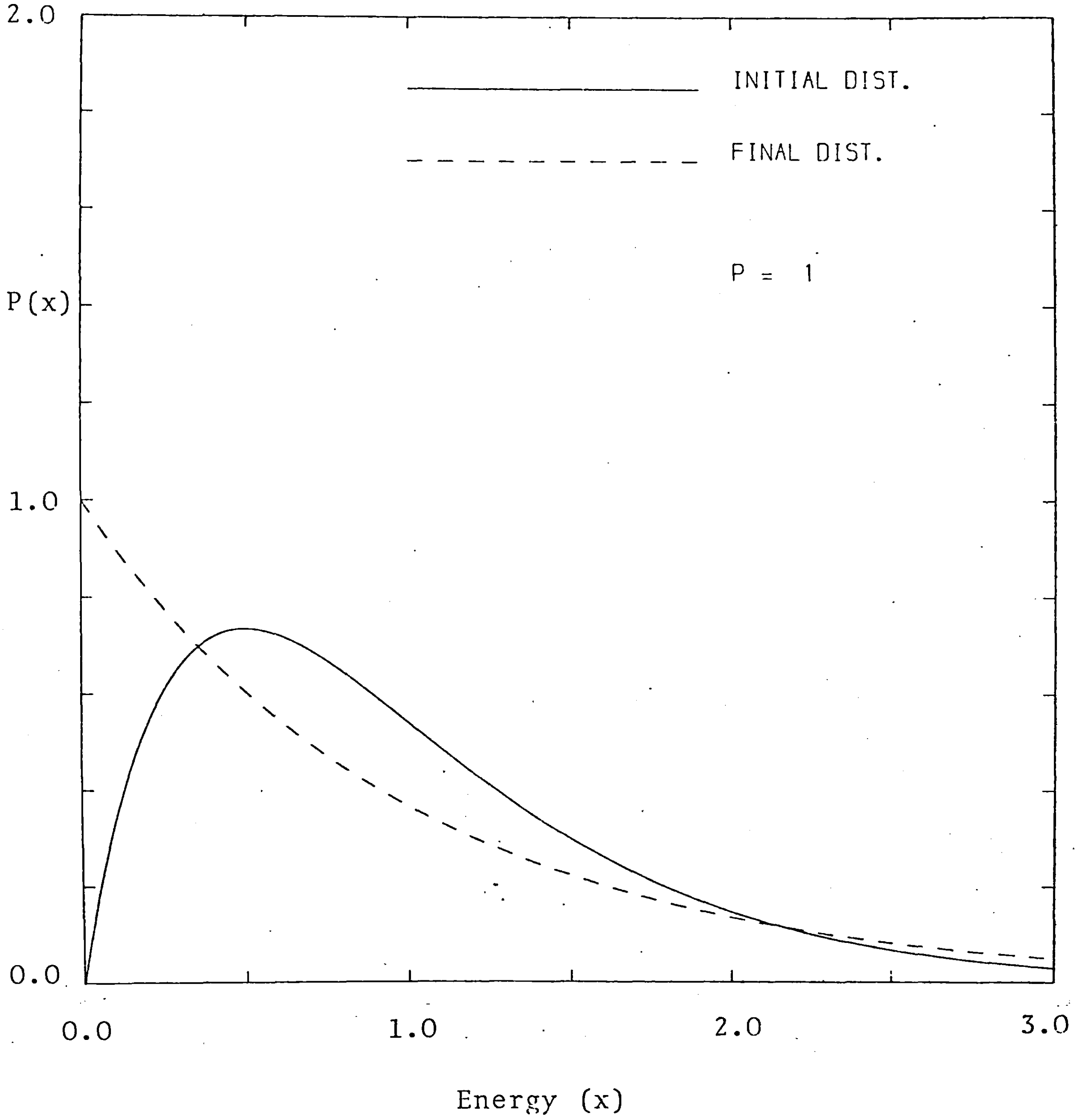

Fig. 3.2 : Comparison of Initial and Final Distributions.

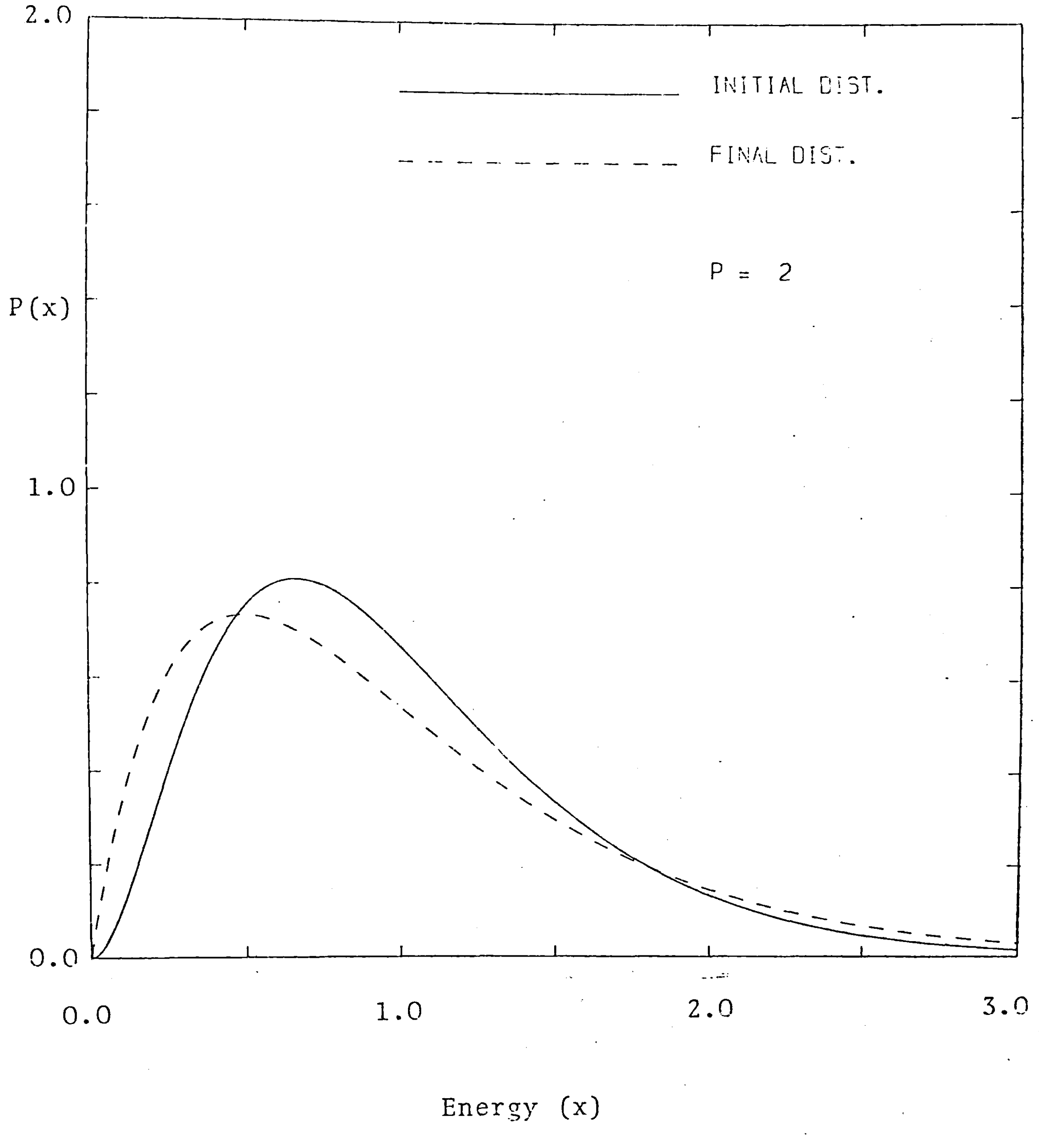

Fig. 3.3 : Comparison of Initial and Final Distributions

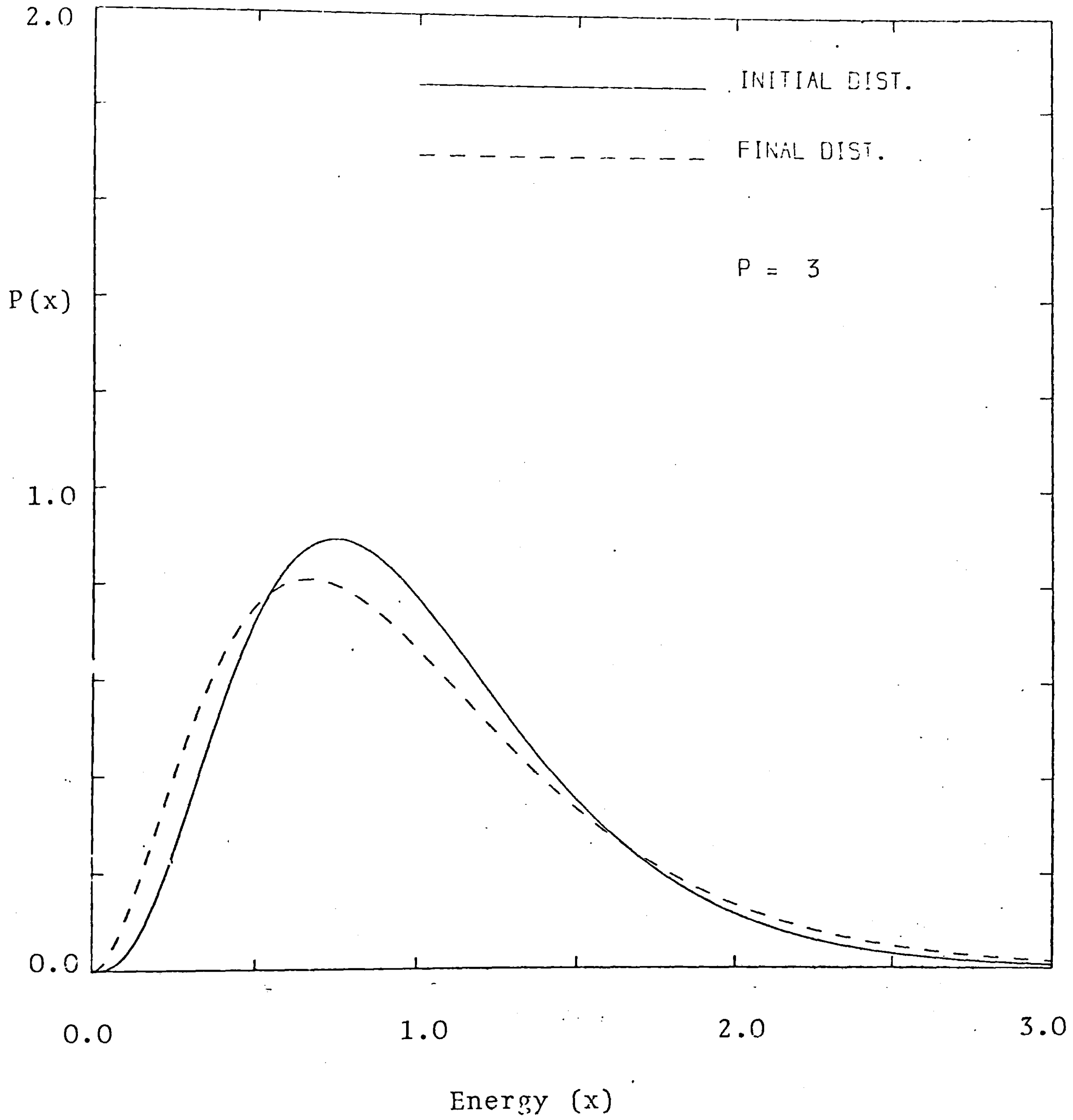

Fig. 3.4 : Comparison of Initial and Final Distributions.

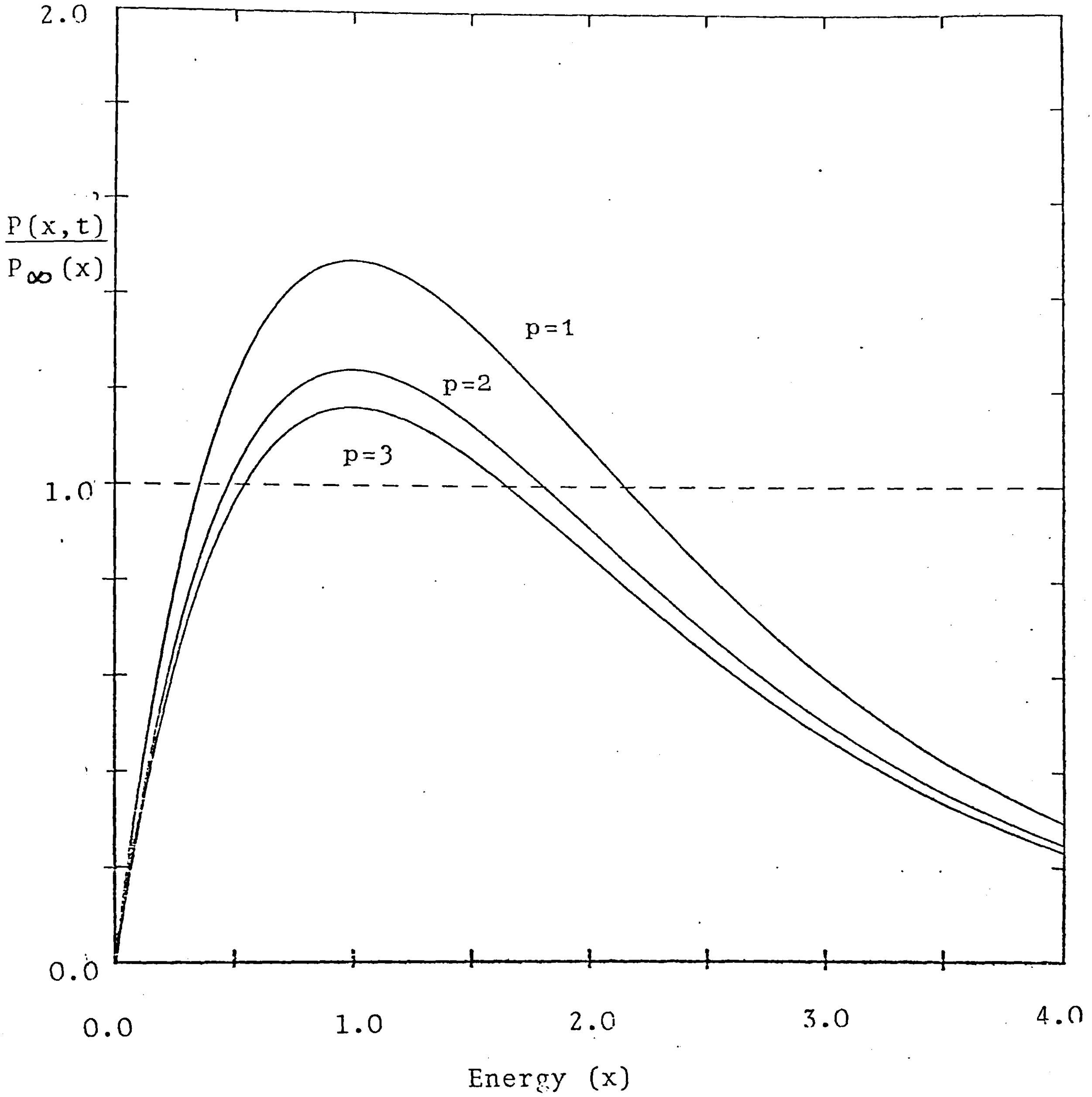

Fig 3.5 : Ratio of Initial and Final Distributions.

and for the final distribution,

$$P_\infty(x) = \frac{(p)^p}{\Gamma(p)} x^{p-1} e^{-px} \tag{3.46}$$

Thus the ratio is,

$$\frac{P^s(x,0)}{P_\infty(x)} = \left(1+\frac{1}{p}\right)^{p+1} x e^{-x} \tag{3.47}$$

Thus it can be seen (fig. 3.5) that all of the curves are of the same shape being merely scaled by a p dependent factor which can vary between 4 and e. Furthermore as x increases the deviation from the equilibrium also increases hence suggesting that the use of these similarity solutions is in studying the relaxation in the high energy tail and not at thermal energies.

3.4.5 Similarity Moments

Having found an exact solution to the problem we can construct exact solutions to the corresponding moment equations (3.11,3.25). In addition the polynomial moments will be needed to facilitate comparison of the exact solution with the solution of the corresponding Master or Linearised equation.

Power Moments

These are defined by equation (2.36) and are,

$$\begin{aligned}\mu_n^s(t) &= \int_0^\infty \frac{x^n}{n!} P^s(x,t)\,dx \\ &= \frac{1}{n!}\left[\frac{\alpha\,\Gamma(p+n)}{\psi^{p+n}} + \beta\frac{\Gamma(p+n+1)}{\psi^{p+n+1}}\right] \\ &= \frac{(p)_n}{\psi^n n!}\left(1+n\left(\frac{\varepsilon\psi}{p}-1\right)\right)\end{aligned} \tag{3.48}$$

Polynomial Moments

The polynomial moments are defined by equation (3.20) and using the form (3.28) for the similarity solution we can write them as,

$$\gamma_n^s(t) = \int_0^\infty L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right)(\alpha+\beta x)\,x^{p-1}e^{-\psi x}\,dx$$

$$= \left(\alpha-\beta\frac{\partial}{\partial\psi}\right)\int_0^\infty L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right)x^{p-1}e^{-\psi x} \qquad (3.49)$$

Using the standard integral,

$$\int_0^\infty e^{-st}\,t^{\alpha}L_n^{\alpha}(t)\,dt = \frac{\Gamma(\alpha+n+1)(s-1)^n}{n!\;s^{\alpha+n+1}}$$

$$[\mathrm{Re}\,\alpha>-1\,,\ \mathrm{Re}\,s>0] \qquad (3.50)$$

(see e.g. Gradshteyn & Ryshik (1965)) this becomes,

$$\gamma_n^s(t) = (p/\varepsilon)^n\,(n+1)_{p-1}\left(\alpha-\beta\frac{\partial}{\partial\psi}\right)\left[\frac{\left(\frac{\varepsilon\psi}{p}-1\right)^n}{\psi^{p+n}}\right]$$

After some algebra this reduces to the rather simple form,

$$\gamma_n^s(t) = \frac{(p)_n}{n!}\left(1-\frac{p}{\varepsilon\psi}\right)^n(1-n) \qquad (3.51)$$

and when the particular form of ψ is inserted (3.39) it further reduces to,

$$\gamma_n^s(t) = \frac{(p)_n}{n!}\,\eta^n\,(1-n)\,e^{-\lambda_n^s t} \qquad (3.52)$$

where,

$$\lambda_n^s = \frac{np}{2(2p+1)} \qquad (3.53)$$

3.5 Entropy

It has been shown in section 2.10.2 that the H-Theorem is satisfied in general for the class of scalar systems considered. Furthermore it has also been shown that the second time derivative of entropy (S) satisfies the inequality,

$$\frac{d^2S}{dt^2} \leqslant 0 \tag{3.54}$$

for several isolated systems and in particular for the Krook-Wu model (Rouse & Simons (1976), and the references in Simons (1979) for other systems.)

However as shown in section 2.10.1 the entropy can be split into two different parts σ_1 and σ_2. Unless the system has degenerate energy states or internal degrees of freedom the latter of these is zero (since the density of states is a constant), but in this model we can examine the temporal change of σ_2 during the passage to equilibrium. Monte Carlo calculations (see next chapter) indicate that,

$$\frac{d\sigma_2}{dt} \leqslant 0 \ , \ \frac{d\sigma_1}{dt} \geqslant 0 \ , \ \frac{dS}{dt} \geqslant 0 \tag{3.55}$$

The last of these has been proved in general (H-Theorem) and it is thus sufficient to merely prove the first of these inequalities. σ_2 is defined as,

$$\sigma_2 = +k\int_0^\infty P(x,t)\ \ln g(x)\ dx. \tag{3.56}$$

to within an arbitrary additive constant, where g(x) is the density of states function,

$$g(x) = x^{p-1}$$

(3.57)

Inserting (3.28) and (3.57) into (3.56) gives,

$$\frac{\sigma_2}{k(p-1)} = \int_0^\infty (\alpha+\beta x)\, x^{p-1} e^{-\psi x} \ln x \, dx$$

(3.58)

The integral is standard (see e.g. Gradshteyn & Ryshik (1965)) giving the result,

$$\frac{\sigma_2}{k(p-1)} = \Omega_{p-1} - \ln\psi + \left(\frac{\varepsilon\psi}{p} - 1\right)$$

(3.59)

where $\Omega_n = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} - 0{\cdot}577\ldots$.

Differentiating with respect to time and inserting the value of $d\psi/dt$ (3.38) gives,

$$\frac{d\sigma_2}{dt} = -\lambda k(p-1)\left(\frac{\varepsilon}{p}\psi - 1\right)^2 \leqslant 0$$

(3.60)

To find the sign of higher derivatives we note that,

$$\left(\frac{\varepsilon}{p}\psi - 1\right)^2 = \left(\frac{\eta e^{-\lambda t}}{1-\eta e^{-\lambda t}}\right)^2$$

$$= \sum_{n=0}^{\infty} (n+1)\, e^{-(n+2)\lambda t}\, \eta^{n+2}$$

(3.61)

All of the terms in this series are positive and when differentiated with respect to time they change sign, thus the sign of the summation and hence the sign of σ_2 changes on each occasion that the time derivative is taken.

This can be written as,

$$(-)^n \frac{d\hat{\sigma}_2}{dt^n} \geqslant 0 \quad . \quad \forall n \tag{3.62}$$

and one may be tempted to conjecture that such a relationship holds for all systems with internal energy states in line with the similar relationship proposed by Simons (1979, and the references therin) for the total entropy. A simple extension of this proof shows that the same relationship holds for all of the models considered in this thesis.

3.6 The Linearised Equation

In the previous chapter the formulation of the linearised equation was given, and the final equation is (see equation (2.50)),

$$\left(\frac{\partial}{\partial t} + 1\right) h(x,t) = \int_0^\infty K(x,y)\, h(y,t)\, dy \tag{3.63}$$

where in this case the kernel is given by,

$$K(x,y) = 2\int_{\max(x,y)}^\infty W_{p,p}(x;u)\, P_\infty(u-y)\, du \tag{3.64}$$

and where the equilibrium distribution $P_\infty(u)$ is the gamma function (equation (3.9)). Several avenues are open to solve this equation but it is simplest if we note that the spectral representation of the kernel defined by (3.64) has been determined elsewhere (Cooper &Hoare (1979)), thus effectively solving the equation (3.63). The kernel K(x,y) can be written as,

$$K(x,y) = \omega\left(\frac{px}{\varepsilon}\right)\sum_{n=0}^{\infty} \Lambda_n L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) L_n^{(p-1)}\left(\frac{py}{\varepsilon}\right) \tag{3.65}$$

where w(x) is the weight function (gamma function, or the equilibrium distribution) and Λ_n the eigenvalues of the linear problem are,

$$\Lambda_n = \frac{(p)_n}{(2p)_n} \tag{3.66}$$

Without further analysis we can write the solution as a series of Laguerre polynomials,

$$h(x,t) = \sum_{n=2}^{\infty} \zeta_n(0)\, L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) e^{-\lambda_n^L t} \tag{3.67}$$

and hence the linearised solution as,

$$P^L(x,t) = P_\infty(x)\left\{1 + \sum_{n=}^{\infty} b_n L_n^{(p-1)}\left(\frac{px}{\varepsilon}\right) e^{-\lambda_n^L t}\right\} \tag{3.68}$$

where,

$$\lambda_n^L = 1 - \frac{2(p)_n}{(2p)_n} \tag{3.69}$$

The same result could also have been obtained by taking Laguerre moments of (3.63) or more simply by linearising the moment equations (3.25) by,

$$\gamma_n(t) = \gamma_n(\infty) + \zeta_n(t) \tag{3.70}$$

where $\gamma_n(\infty)$ is given by (3.22). Inserting this (3.70) in equations (3.25) and ignoring terms in ζ^2 one immediately gets,

$$\left(\frac{d}{dt}+1\right)\zeta_n(t) = \frac{2(p)_n}{(2p)_n}\,\zeta_n(t) \tag{3.71}$$

which have the solution,

$$\zeta_n(t) = \zeta_n(0)\,e^{-\lambda_n^L t} \tag{3.72}$$

where λ_n^L is again given by (3.69). These values can then be put into (3.19) to give the same equation as (3.68) for the linearised solution.

3.6.1 Comparison of Exact and Linearised Solutions

The linearisation of the Boltzmann equation certainly produces a more tractable equation, but it's domain of validity remains uncertain (see Cercignani (1975)). Since we have an exact solution to both the non-linear and linearised Boltzmann equations it is possible to examine exactly where the two solutions differ. The first two terms in the Fourier expansion are obviously equal (equilibrium distribution and zero) , and the decay constants of the third and fourth terms are also equal

$$\lambda_2^L = \lambda_2^S = \frac{p}{2p+1}$$

$$\lambda_3^L = \lambda_3^S = \frac{3p}{2(2p+1)} \tag{3.73}$$

For higher terms it can be seen that they diverge rapidly confirming the commonly held belief that the differences come in the higher rather than the lower moments and that the higher moments in the linearised case decay slower than in the non-linear case. Furthermore when the range of solutions was investigated it was seen that the similarity solution was only close to equilibrium at thermal energies and hence any comparison must also be restricted to that range.

CHAPTER FOUR : DISCRETE DIFFUSE SCATTERING MODEL

4.1 The Model

As in the previous chapter we consider a bath of diffuse scattering molecules each with p internal degrees of freedom ; except that now the molecule's states are restricted to a discrete space. The interaction is represented diagrammatically in fig. 4.1 and shows two molecules with energies i and k-i interacting to form a total collision complex of energy k. The post collisional energies are j and k-j. If each of the molecules has p internal energy states then the collision complex has 2p and the transition kernel is the probability that an amount j in p degrees of freedom arises from a total k in 2p degrees of freedom. This is then the symmetric Negative Hypergeometric (NHG) distribution.(see Appendix B)

$$K(j;k) = W_{pp}(j;k) = \frac{\Gamma(2p)}{\Gamma(p)^2} \frac{(j+1)_{p-1}(k-j+1)_{p-1}}{(k+1)_{2p-1}} \qquad (4.1)$$

Where $(a)_n$ is the rising Pochhammmer function (see Appendix A).

4.2 The Transport Equation

In chapter 2 a general class of scalar models with continuous state variables was examined. All of the results obtained there can be translated into a formulation with discrete variables but it is necessary to quote a few of the corresponding results here for

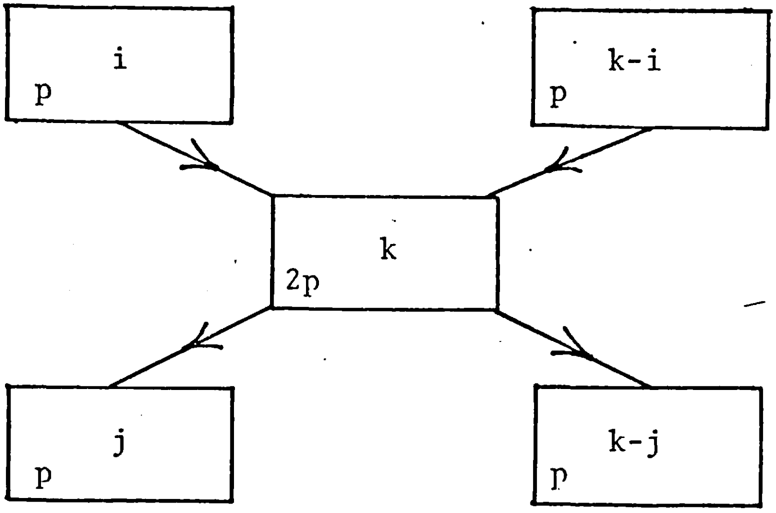

Fig. 4.1.

the sake of clarity. The transport equation for diffuse scattering molescules analogous to (3.2) is,

$$\left(\frac{\partial}{\partial t}+1\right) P(i,t) = \sum_{k=i}^{\infty} W_{pp}(i;k) \sum_{j=0}^{k} P(j,t)\, P(k-j,t) \tag{4.2}$$

An important distinction to draw here is with the probability distribution function in the continuous case. In the continuous case P(x,t) is a probability density (P(x,t) is the probability of finding a molecule with an energy in the range x to x+dx at a time t.), however in the discrete case P(i,t) is the probability of finding a molecule with an energy i at a time t. Similarly the kernel $W_{pp}(x;u)$ is a probability density whereas the discrete kernel is a matrix of transition probabilities per unit time.

The conservation of number gives,

$$\sum_{i=0}^{\infty} P(i,t) = 1 \tag{4.3}$$

and of energy,

$$\varepsilon_0 \sum_{i=1}^{\infty} i\, P(i,t) = \varepsilon \tag{4.4}$$

Equation (4.3) implies that a factor N has been scaled into the time. It is worth noting that although in the continuous case the parameter ε is in someways redundant since it can always be scaled into the state variable x, the two variables ε and ε_0 are not both redundant (although they always occur in the combination $\varepsilon / \varepsilon_0$.)

To obtain the continuous limit of the discrete model it is necessary to take the constrained limit

$$\begin{aligned} i &\to \infty \\ \varepsilon_0 &\to 0 \\ i\varepsilon_0 &= x \end{aligned} \tag{4.5}$$

and note that,

$$\varepsilon_0 \Delta i = dx \tag{4.6}$$

The other properties which are proved for the continuous case are not proved here since as already mentioned the proofs follow a one to one relationship with those for the continuous case.

4.3 Detailed Balance and Equilibrium

The detailed balance condition in the discrete formalism is,

$$K(j;k)\,P_\infty(i)\,P_\infty(k-i) = K(i,k)\,P_\infty(j)\,P_\infty(k-j)$$

(4.7)

On substituting the symmetric NHG distribution (equation (4.1)) for the kernel this becomes,

$$\frac{P_\infty(i)\;P_\infty(k-i)}{P_\infty(j)\;P_\infty(k-j)} = \frac{(i+1)_{p-1}\;(k-i+1)_{p-1}}{(j+1)_{p-1}\;(k-j+1)_{p-1}}$$

(4.8)

where the use of the Pochhammer symbol brings out the striking resemblance with the continuous case (see equation (3.4)). This relationship is solved by $P_\infty(i)$ in the form,

$$P_\infty(i) = a\,(i+1)_{p-1}\;b^i \quad .$$

(4.9)

where again the constants a and b are determined by the conservation of number,

$$a\sum_{i=0}^{\infty} (i+1)_{p-1}\,b^i = 1$$

(4.10)

and the conservation of energy conditions,

$$a\varepsilon_0 \sum_{i=1}^{\infty} i\,(i+1)_{p-1}\,b^i = \varepsilon$$

(4.11)

The first of these summations is evaluated by the normalisation of the Negative Binomial distribution (see Appendix B for the normalisation and the moments of the Negative Binomial distribution.) to give,

$$a = (1-b)^{p} \, \Gamma(p)^{-1} \tag{4.12}$$

The second is found by using the first moment of the Negative Binomial distribution to give,

$$\mathcal{E} = \frac{\mathcal{E}_o p b}{1-b} \tag{4.13}$$

These are easily solved, and upon substitution in equation (4.9) we arrive at the equilibrium distribution which is a Negative Binomial distribution with p degrees of freedom and mean $\mathcal{E}/\mathcal{E}_0$.

$$P_\infty(i) = \Gamma(p)^{-1} \left(\frac{\mathcal{E}_o p}{\mathcal{E}+\mathcal{E}_o p}\right)^{p} (i+1)_{p-1} \left(\frac{\mathcal{E}}{\mathcal{E}+\mathcal{E}_o p}\right)^{i} \tag{4.14}$$

The appropriate moments of this distribution are,

$$\bar{m}_n(\infty) = \sum_{i=0}^{\infty} (i)^{(n)} P_\infty(i) \tag{4.15}$$

(where $(a)^{(n)}$ is now the falling factorial function (see Appendix A)), and can be evaluated to give,

$$\bar{m}_n(\infty) = (p)_n \left(\mathcal{E}/\mathcal{E}_o\right)^{n} \tag{4.16}$$

Of interest later will be the corresponding normalised moments,

$$\bar{\mu}_n(\infty) = \frac{\bar{m}_n(\infty)}{n!} = \frac{(p)_n}{n!} \left(\mathcal{E}/\mathcal{E}_o\right)^{n} . \tag{4.17}$$

For these moments to be adequately compared with those in the last chapter (which were defined by equation

(3.13)) these discrete moments $\bar{\mu}_n$ should be multiplied by a factor $\mathcal{E}_0^n$ to give them the dimensions of (energy)^n. It is then obvious that these are exactly comparable with those in the continuous case.

The limiting process which transforms the discrete distributions into the continuous ones is central to the theme of this work, and it is easily demonstrated that upon taking the constrained limit (4.5) the stationary distribution in the discrete case becomes the gamma function, or equilibrium distribution of the continuous case. (equation (3.9)). Since the correspondence between the discrete and continuous models is so important and to demonstrate that the continuous analogue of a discrete model can always be determined by taking the appropriate limit the transformation will be given in full. Using the limit (4.5) means that the gamma distribution can be written as,

$$P_\infty(x)\,dx = \lim_{\begin{bmatrix} i\to\infty \\ \mathcal{E}_0\to 0 \\ i\mathcal{E}_0 = x \end{bmatrix}} P_\infty(i)\,\Delta i \tag{4.18}$$

where Δi=1 and noting that $\mathcal{E}_0\Delta$i=dx we get,

$$\begin{aligned} P_\infty(x)\,dx &= \lim_{[\;]} \Gamma(p)^{-1}\left(\tfrac{p}{\varepsilon}\right)^p \mathcal{E}_0^p\,(i+1)_{p-1}\left(1+\frac{\mathcal{E}_0 p}{\varepsilon}\right)^i \frac{dx}{\mathcal{E}_0} \\ &= \Gamma(p)^{-1}\left(\tfrac{p}{\varepsilon}\right)^p x^{p-1} \lim_{i\to\infty}\left[\frac{(i+1)_{p-1}}{i^{p-1}}\cdot\left(1+\frac{px}{\varepsilon i}\right)^i\right]dx \\ &= \Gamma(p)^{-1}\left(\tfrac{p}{\varepsilon}\right)^p x^{p-1} e^{-\frac{px}{\varepsilon}}\,dx \end{aligned} \tag{4.19}$$

or the gamma function with mean ε which has already been shown to be the equilibrium distribution for the Beta kernel of the last chapter.

It can be shown by a proof completely similar to that given in section 2.10.2 that the general scalar model with a discrete state variable (and hence this one with an NHG kernel) satisfies an H-Theorem, which in turn implies that there is a unique equilibrium distribution. This fact can also be shown (for this particular model) by considering the discrete equivalent of the Laguerre moments (Meixner moments) and using the same arguments as those in section 3.3.2 .

4.4 The Similarity Solution

As in the previous model we use the term similarity solution by virtue of the general form of the answer and not because any intricasies of similarity theory are used in the solution of the problem. However unlike the result in the previous chapter where the combination of x and t is a prominent feature of the solution the corresponding connection between i and t is somewhat more disguised. It will however be shown that the two solutions are equivalent and that the continuous solution can be found by taking the appropriate limit of the discrete one. Furthermore it will also be shown how, in theory at least, the discrete solution can be constructed from the continuous one.

4.4.1 The Solution

The literature on differential-sum equations such as (4.2) is very limited , and so starting from a similar viewpoint to that in the continuous case we assume a solution of the form,

$$P^{s}(i,t) = (A + Bi)(i+1)_{p-1}\,(1-\Psi)^{i} \tag{4.20}$$

where again A(t), B(t) and Ψ(t) are all time dependent functions. This type of solution is chosen by analogy with the continuous case where the solution is of the form of a first order polynomial (in the energy) multiplied by the equlibrium distribution with a time dependent temperature. These constants in (4.20) are to be compared with α , β and ψ in the continuous case but not to be definitely identified with them.

The method of finding the values of A, B and Ψ closely parallels that used in the previous chapter. Conservation of number gives,

$$\sum_{i=0}^{\infty} (A+Bi)(i+1)_{p-1}\,(1-\Psi)^{i} = 1 \tag{4.21}$$

and of energy

$$\mathcal{E}_0 \sum_{i=1}^{\infty} i\,(A+Bi)\,(i+1)_{p-1}\,(1-\Psi)^{i} = \mathcal{E} \tag{4.22}$$

The first is evaluated from the normalisation and first moment of the Negative Binomial distribution whilst the second one involves the first and second moments of the Negative Binomial distribution when i(A+iB) is written as (A+B)i + Bi(i-1). Upon doing these summations we obtain,

$$A + Bp\,\frac{1-\Psi}{\Psi} = \frac{\Psi^{p}}{\Gamma(p)} \qquad (4.23)$$

and,

$$A+B + B(p+1)\,\frac{1-\Psi}{\Psi} = \frac{\varepsilon}{\varepsilon_0}\,\frac{\Psi^{p+1}}{(1-\Psi)\,\Gamma(p+1)} \qquad (4.24)$$

which are readily solved to give,

$$A = \frac{\Psi^{p}}{\Gamma(p)}\left(1+p-\left(\frac{\varepsilon}{\varepsilon_0}+p\right)\Psi\right) \qquad (4.25)$$

$$B = \frac{\Psi^{p+1}}{\Gamma(p+1)}\left[\left(\frac{\varepsilon}{\varepsilon_0}+p\right)\Psi - p\right](1-\Psi)^{-1} \qquad (4.26)$$

Proceeding as before we can substitute the trial solution (4.20) into equation (4.2) and this time equate the coefficients of i^{o}, i and i^{2}. The left hand side (LHS) of equation (4.2) becomes,

$$(LHS) = \left(\frac{\partial}{\partial t}+1\right)(A+Bi)(i+1)_{p-1}\,(1-\Psi)^{i}$$

$$= (i+1)_{p-1}\,(1-\Psi)^{i}\left(\frac{-i}{1-\Psi}\,\frac{d\Psi}{dt} + \frac{\partial}{\partial t} + 1\right)(A+Bi) \qquad (4.27)$$

Inserting (4.20) into the right hand side (RHS) of (4.2) gives,

$$(RHS) = \sum_{k=i}^{\infty} W_{pp}(i;k) \sum_{j=0}^{k} (A+Bj)(A+B(k-j))\,(1-\Psi)^k \cdot (j+1)_{p-1}\,(k-j+1)_{p-1} \tag{4.28}$$

On using the detailed balance property (4.7) and shifting the variable k to k+i this becomes,

$$(RHS) = (i+1)_{p-1}\,(1-\Psi)^i \sum_{k=0}^{\infty} (k+1)_{p-1}\,(1-\Psi)^k \cdot \sum_{j=0}^{k+i} (A+Bj)(A+B(k+i-j))\,W_{pp}(j;k+i) \tag{4.29}$$

When the brackets are multiplied out and the powers of j rearranged into falling Pochhammer functions the inner summation involves moments of the symmetric NHG distribution (4.1).

$$(RHS) = (i+1)_{p-1}\,(1-\Psi)^i \sum_{k=0}^{\infty} (k+1)_{p-1}\,(1-\Psi)^k \cdot \left\{\lambda B^2 (k)^{(2)} + (2\lambda B^2 i + AB)\,k + \lambda B^2 (i)^{(2)} + ABi + A^2\right\} \tag{4.30}$$

The k summation involves moments of the Negative Binomial distribution (equation (B.16)) and the resulting equation after equating left and right hand sides is,

$$\left(\frac{-i}{1-\Psi}\cdot\frac{d\Psi}{dt} + \frac{\partial}{\partial t} + 1\right)(A+Bi)$$
$$= \frac{\Gamma(p)}{\Psi^{p+2}}\left\{A^2\Psi^2 + pAB\Psi(1-\Psi) + p(p+1)B^2\lambda(1-\Psi)^2 + (AB\Psi^2 + 2p\lambda B^2\Psi(1-\Psi))\,i + \lambda B^2\Psi^2 i(i-1)\right\} \tag{4.31}$$

where λ is again given by,

$$\lambda = \frac{p}{2(2p+1)} \tag{4.32}$$

The time derivatives of A and B are readily evaluated in terms of $d\Psi/dt$ and hence we can equate the coefficients of i^0, i and i^2. After some algebra these are found to be the same and gives rise to a first order equation in Ψ viz.,

$$\frac{d\Psi}{dt} = -\lambda \Psi\left[\Psi\left(\frac{\varepsilon}{\varepsilon_0 p}+1\right)-1\right] \tag{4.33}$$

Since this is of the same form as (3.38) we can immediately write the solution as,

$$\Psi = \frac{\varepsilon_0 p}{\varepsilon+\varepsilon_0 p}\left[1-\eta e^{-\lambda t}\right] \tag{4.34}$$

where η again gives a parameterisation of the range of possible initial distributions. Thus the similarity solution is,

$$\begin{aligned} P^s(i,t) = {} & (i+1)_{p-1}\, \Psi^p (1-\Psi)^i\, \Gamma(p)^{-1} \\ & \cdot\left\{1+p-\left(\frac{\varepsilon}{\varepsilon_0}+p\right)\Psi+\frac{i\Psi}{1-\Psi}\left[\left(\frac{\varepsilon}{\varepsilon_0 p}+1\right)\Psi-1\right]\right\} \end{aligned} \tag{4.35}$$

4.4.2 Range of Validity of The Solution

Many of the remarks made in the last chapter also apply here. The conditions that the initial distribution is positive are,

$$A(0) \geqslant 0 \quad , \quad B(0) \geqslant 0 \tag{4.36}$$

i.e. that,

1.

$$\Psi(0)^{p}\left(1+p-\Psi(0)\left(\varepsilon/\varepsilon_0+p\right)\right) \geqslant 0$$

$$\eta \leqslant (1+p)^{-1} \tag{4.37}$$

2.

$$\Psi(0)^{p+1}\left(\left(\varepsilon/\varepsilon_0+p\right)\Psi(0)-p\right)\left(1-\Psi(0)\right)^{-1} \geqslant 0$$

$$0 \leqslant \eta \leqslant \frac{\varepsilon}{\varepsilon+\varepsilon_0 p} \tag{4.38}$$

Thus the possible range of values for η is,

$$0 \leqslant \eta \leqslant \min\left[\frac{1}{1+p} \, , \, \frac{\varepsilon}{\varepsilon+\varepsilon_0 p}\right] \tag{4.39}$$

In addition we note that if η is positive and outside of this range then the initial distribution will not be positive everywhere but will become so after a certain time τ where,

$$\tau = \lambda^{-1} \ln\left[\eta \max\left(1+p, \, 1+\frac{\varepsilon_0 p}{\varepsilon}\right)\right] \tag{4.40}$$

If however η is negative then the solution will remain negative on it's passage to equilibrium.

4.4.3 Limiting Cases of the Solution

Equilibrium Limit

It is evident that in the limit t $\longrightarrow \infty$

$$\Psi(t) \longrightarrow \frac{\varepsilon_0 p}{\varepsilon + \varepsilon_0 p} \tag{4.41}$$

and the solution (4.35) tends to a Negative Binomial distribution which is the requisite equilibrium distribution (4.14).

Continuous Limit

In section 4.3 we showed that the discrete equilibrium distribution (4.14) collapsed to the continuous equilibrium distribution (3.9) upon taking the constrained limit (4.5). Taking this limit of the discrete similarity solution (4.35) we get,

$$\lim_{\left[\begin{smallmatrix} i \to \infty \\ \varepsilon_0 \to 0 \\ i\varepsilon_0 = x \end{smallmatrix}\right]} \Delta i\, P^s(i,t) = \lim_{[\;]} (i+1)_{p-1}\, \Psi^p (1-\Psi)^i\, \Gamma(p)^{-1} \Delta i \cdot \left\{ 1+p - \left(\frac{\varepsilon}{\varepsilon_0}+p\right)\Psi + \left(\left(\frac{\varepsilon}{p\varepsilon_0}+1\right)\Psi - 1\right)\frac{i\Psi}{1-\Psi} \right\}$$

$$= \lim_{[\;]} (i+1)_{p-1}\, \Psi^p (1-\Psi)^i\, \Gamma(p)^{-1} \left\{ 1+p-\varepsilon\psi + \left(\frac{\varepsilon\psi}{p}-1\right)\frac{i\Psi}{1-\Psi} \right\} \Delta i$$

Noting that,

$$\lim_{[\;]} \frac{i\Psi}{1-\Psi} = x\psi$$

gives,

$$\underset{[\;\;]}{\mathrm{Lim}}\; P^s(i,t)\,\Delta i = \Gamma(p)^{-1}\left\{1+p-\varepsilon\psi+\left(\frac{\varepsilon\psi}{p}-1\right)x\psi\right\}$$

$$\cdot\underset{[\;\;]}{\mathrm{Lim}}\;(i+1)_{p-1}\,\Psi^p(1-\Psi)^i\,\Delta i$$

$$= \Gamma(p)^{-1}\left\{1+p-\varepsilon\psi+\left(\frac{\varepsilon\psi}{p}-1\right)x\psi\right\}\psi^p\underset{[\;\;]}{\mathrm{Lim}}\;(i+1)_{p-1}\,\varepsilon_0^p\,\Delta i\left(1-\frac{x\psi}{i}\right)^i$$

$$= \Gamma(p)^{-1}\left\{1+p-\varepsilon\psi+\left(\frac{\varepsilon\psi}{p}-1\right)x\psi\right\}\psi^p x^{p-1}e^{-\psi x}dx$$

$$= P^s(x,t)\,dx. \tag{4.42}$$

4.5 Moments

As in the previous chapter the only way of finding an exact solution of the problem for an arbitrary initial distribution is by considering the moments and the solution of the corresponding evolution equations. In considering the moments of the discrete distribution the correspondence with the continuous case becomes clear since there is no limiting procedure needed to transform one problem into the other.

4.5.1 Factorial Moments

As is obvious by now the analogue of the power of a continuous variable is the Pochhammer factorial function of the discrete variable. The most convenient ones are the falling factorial functions and we define the moments of the distribution as,

$$\bar{\mu}_n(t) = \frac{1}{n!} \sum_{i=n}^{\infty} (i)^{(n)} P(i,t) \tag{4.43}$$

We note that this sum may equally well run from 0 to ∞ since in that case the first n terms are zero due to the Pochhammer function. On taking falling factorial moments of equation (4.2) we get,

$$\left(\frac{d}{dt}+1\right)\bar{\mu}_n(t) = \frac{1}{n!} \sum_{i=0}^{\infty} (i)^{(n)} \sum_{k=i}^{\infty} W_{pp}(k;i) \cdot \sum_{j=0}^{k} P(j,t)\, P(k-j,t)$$

$$= \frac{1}{n!} \sum_{k=0}^{\infty} \sum_{j=0}^{k} P(j,t)\, P(k-j,t) \sum_{i=0}^{k} (i)^{(n)} W_{pp}(i;k) \tag{4.44}$$

The inner sum involves the moments of the symmetric NHG distribution to give,

$$\left(\frac{d}{dt}+1\right)\bar{\mu}_n(t) = \frac{(p)_n}{(2p)_n \cdot n!} \sum_{k=0}^{\infty} \sum_{j=0}^{k} P(j,t)\, P(k-j,t)\, (k)^{(n)}$$

$$= \frac{(p)_n}{(2p)_n\, n!} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} P(j,t)\, P(k,t)\, (k+j)^{(n)}$$

$$= \frac{(p)_n}{(2p)_n\, n!} \sum_{r=0}^{n} \binom{n}{r} \sum_{j=0}^{\infty} (j)^{(r)} P(j,t) \sum_{k=0}^{\infty} (k)^{(n-r)} P(k,t) \tag{4.45}$$

where the Pochhammer function has been expanded by,

$$(k+j)^{(n)} = \sum_{i=0}^{n} \binom{n}{i} (k)^{(i)} (j)^{(n-i)} \tag{4.46}$$

(Note that this is just a particular form of the normalisation of the NHG distribution). Thus the result is upon using (4.43),

$$\left(\frac{d}{dt}+1\right)\bar{\mu}_n(t) = \frac{(\rho)_n}{(2\rho)_n}\sum_{k=0}^{n} \bar{\mu}_k(t)\,\bar{\mu}_{n-k}(t) \tag{4.47}$$

These equations are exactly the same as equations (3.11) with the similar boundary conditions,

$$\begin{aligned} \bar{\mu}_0(t) &= 1. \\ \bar{\mu}_1(t) &= \mathcal{E}/\mathcal{E}_0 \qquad \forall\, t \end{aligned} \tag{4.48}$$

and the asymptotic condition,

$$\bar{\mu}_n(\infty) = \frac{(\rho)_n}{n!}\left(\frac{\mathcal{E}}{\mathcal{E}_0\,\rho}\right)^n \tag{4.49}$$

The fact that the equilibrium distribution is a solution of the equations (4.47) is readily observed by using the addition property of the Pochhammer function (4.46).

4.5.2 Polynomial Moments

As mentioned when Laguerre moments were considered in the previous chapter for the continuous model, the problem of inverting the moment expression (4.43) can be circumvented if a suitable set of polynomials can be found which have the equilibrium distribution as the weight function. In this case the appropriate set is the Meixner Polynomials. The definition and properties of these polynomials are described in detail in Appendix B.

The Meixner moments of the distribution are defined as,

$$\bar{\gamma}_n(t) = \frac{(p)_n}{n!} \sum_{i=0}^{\infty} M_n(i,p,c)\, P(i,t) \tag{4.50}$$

where now c is given by,

$$c = \frac{\varepsilon}{\varepsilon + p\varepsilon_0} \tag{4.51}$$

Since

$$M_0(i,p,c) = 1 \tag{4.52}$$

and,

$$M_1(i,p,c) = 1 + \frac{i}{p}\left(1 - \frac{1}{c}\right) \tag{4.53}$$

the boundary conditions on the $\bar{\gamma}_n(t)$ are,

$$\begin{aligned} \bar{\gamma}_0(t) &= 1 \\ \bar{\gamma}_1(t) &= 0 \qquad \forall t \end{aligned} \tag{4.54}$$

The asymptotic condition is clearly the same as for the Laguerre moments, viz.,

$$\begin{aligned} \bar{\gamma}_n(\infty) &= 1 \qquad n = 0 \\ &= 0 \qquad n \neq 0 \end{aligned} \tag{4.55}$$

The expression (4.50) can be inverted to give,

$$P(i,t) = P_\infty(i) \sum_{n=0}^{\infty} M_n(i,p,c)\, \bar{\gamma}_n(t) \tag{4.56}$$

where $P_\infty(i)$ is the equilibrium distribution (4.14). To find the temporal change of these moments we multiply equation (4.2) by $M_n(i,p,c)$ and sum over all i, which gives,

$$\left(\frac{d}{dt}+1\right)\bar{\gamma}_n(t) = \frac{(p)_n}{n!}\sum_{k=0}^{\infty}\sum_{j=0}^{k} P(k-j,t)\,P(j,t) \cdot \sum_{i=0}^{k} M_n(i,p,c)\,W_{pp}(i;k) . \tag{4.57}$$

The inner summation is evaluated by using the Meixner addition formula (C.14) and noting (4.52) to give,

$$\sum_{i=0}^{k} M_n(i,p,c)\,W_{pp}(i;k) = M_n(k,2p,c) \tag{4.58}$$

Thus it is also seen that the NHG is the ladder operator for the raising of the second parameter of a Meixner Polynomial. Using this property, (4.57) becomes,

$$\left(\frac{d}{dt}+1\right)\bar{\gamma}_n(t) = \frac{(p)_n}{n!}\sum_{k=0}^{\infty}\sum_{j=0}^{k} P(k-j,t)\,P(j,t)\,M_n(k,2p,c)$$

$$= \frac{(p)_n}{n!}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} P(k,t)\,P(j,t)\,M_n(k+j,2p,c) \tag{4.59}$$

Using the addition formula for Meixner Polynomials (C.14) this can be written as,

$$\left(\frac{d}{dt}+1\right)\bar{\gamma}_n(t) = \frac{\Gamma(2p)(p)_n}{\Gamma(p)^2 n!\,(n+1)_{2p-1}} \cdot \sum_{r=0}^{n} (n-r+1)_{p-1}\,(r+1)_{p-1}$$

$$\cdot \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} P(k,t)\,P(j,t)\,M_{n-r}(k,p,c)\,M_r(j,p,c)$$

and upon noting that,

$$(n-r+1)_{p-1}\,(r+1)_{p-1} = \frac{(p)_{n-r}\,(p)_r\,\Gamma(p)^2}{(n-r)!\;r!} \tag{4.60}$$

this gives the final result,

$$\left(\frac{d}{dt}+1\right)\bar{\gamma}_n(t) = \frac{(p)_n}{(2p)_n}\sum_{r=0}^{n}\bar{\gamma}_r(t)\,\bar{\gamma}_{n-r}(t) \tag{4.61}$$

These equations are the same as those for the factorial moments (but with different boundary and asymptotic conditions), and are also the same as those for the Laguerre moments in the continuous case (3.25).

This last point is interesting since it means that having found a solution for either the discrete or continuous model then one can immediately construct the corresponding solution for the other one (By taking Laguerre/Meixner moments of the known solution these are also the polynomial moments of the unknown solution).

4.6 The Linearised Equation

As before the knowledge of an exact solution gives one a rare opportunity to compare the solution of the linearised equation with the exact solution of the full non-linear equation. Following an identical procedure to that in the previous chapter we can linearise the moment equations (4.61) and immediately write down the solution to the linearised equation (2.53) as,

$$P^L(i,t) = P_\infty(i)\left\{1 + \sum_{n=2}^{\infty} \bar{\zeta}_n(0)\, M_n(i,p,c)\, e^{-\lambda_n^L t}\right. \tag{4.62}$$

where,

$$\lambda_n^L = 1 - \frac{2(p)_n}{(2p)_n} \tag{4.63}$$

$\zeta_n(0)$ characterises the initial distribution and c is given by (4.51). We note that the eigenfunctions and eigenvalues of the linearised kernel defined by (2.55) with (4.1) have been found elsewhere (Hoare & Rahman (1979)) and that this provides an alternative method for finding the solution to the linearised equation.

4.6.1 Comparison of Exact and Linearised Solutions

The solution of the linearised equation given above is completely general and may be applied to any initial distribution which can be expanded in Meixner Polynomials, although it's domain of validity is restricted to the linear regime ,close to equilibrium. To compare the linearised solution with the exact solution we must write the similarity solution in a form similar to (4.62) and hence we need to find the Meixner moments of the similarity solution. These are,

$$\bar{\gamma}_n^S(t) = \frac{(p)_n}{n!} \sum_{i=0}^{\infty} M_n(i,p,c)\; P^S(i,t)$$

$$= \frac{(p)_n}{n!} \sum_{i=0}^{\infty} M_n(i,p,c)\,(A+Bi)\,(i+1)_{p-1}\,(1-\Psi)^i$$

$$= \frac{(p)_n}{n!} \sum_{\nu=0}^{\infty} \frac{(-n)_\nu}{(p)_\nu\, \nu!} \left(1-\frac{1}{c}\right)^\nu \cdot \sum_{i=0}^{\infty} \left\{ (-i)_\nu\, (A+Bi)(i+1)_{p-1}\, (1-\Psi)^i \right\}$$

(4.64)

The inner summation is evaluated by using the moments of the Negative Binomial distribution (B.16) to give,

$$\sum_{i=0}^{\infty} \{\ \} = \left(A + B(1-\Psi)\frac{d}{d\Psi}\right) \sum_{i=0}^{\infty} (-1)^\nu (i)^{(\nu)} (i+1)_{p-1}\, (1-\Psi)^i$$

$$= (-1)^\nu \frac{\Gamma(p)\,(p)_\nu\, (1-\Psi)^\nu}{\Psi^{p+\nu+1}} \left\{ A\Psi + Bp(1-\Psi) + B\nu \right\}$$

Thus,

$$\bar{\gamma}_n^s(t) = \frac{\Gamma(p+n)}{n!} \sum_{\nu=0}^{\infty} \frac{(-n)_\nu}{\nu!} (-1)^\nu \left(\frac{1-\Psi}{\Psi}\right)^\nu \left\{ A\Psi + Bp(1-\Psi) + B\nu \right\}$$

(4.65)

The ν summation involves only the binomial theorem and it's derivative, viz.,

$$\sum_{\nu=0}^{\infty} \frac{(-n)_\nu}{\nu!} x^\nu = {}_1F_0[-n, ; x] = (1-x)^n$$

(4.66)

and

$$\sum_{\nu=0}^{\infty} \nu \frac{(-n)_\nu}{\nu!} x^\nu = x\frac{\partial}{\partial x}\left\{ {}_1F_0[-n, ; x] \right\} = -nx(1-x)^{n-1}$$

(4.67)

Giving for (4.65)

$$\bar{\gamma}_n^s(t) = \eta^n (1-n) \frac{(p)_n}{n!}\, e^{-\lambda_n^s t}$$

(4.68)

where, ,

$$\lambda_n^S = \frac{np}{2(2p+1)} \tag{4.69}$$

Thus the similarity solution can be written as,

$$P^S(i,t) = P_\infty(i)\left\{1+\sum_{n=2}^{\infty}\eta^n(1-n)\frac{(p)_n}{n!}M_n(i,p,c)\,e^{-\lambda_n^S t}\right. \tag{4.70}$$

On comparing the terms in this series with those in (4.62) (the solution of the linearised equation) the first terms are both equal to the equilibrium distribution and the second terms (n=1) are both zero. (note that this is a general result arising from the form of $M_1(i,p,c)$). It can also be seen that the third and fourth terms in the series are also equal since,

$$\lambda_2^S = \lambda_2^L = \frac{p}{2p+1}$$

$$\lambda_3^S = \lambda_3^L = \frac{3p}{2(2p+1)} \tag{4.71}$$

and that after this the terms diverge increasingly, with the moments of the exact solution decaying faster than those of the linearised case. This is in full agreement with the results of the continuous model studied in the previous chapter.

4.7 Computer Simulation

We have shown that the Boltzmann equation may be solved exactly for only a small range of initial distributions. To find a solution for other initial conditions one inevitably has to turn to the computer for help, and it's aid may be applied in several ways.

Tjon & Wu (1979) examined the relaxation towards equilibrium in the high energy tail of the p=1 kernel of the previous chapter. They discretised the model (although in a different way to which we have) and 'solved' the problem by direct iteration of the non-linear Boltzmann equation. This method however is very time consuming and presents a number of difficulties.

In section 4.5.2 an algorithm was given for solving the model using the polynomial moments. This has also been investigated for the Krook-Wu model (Barnsley & Cornille (1979)) and more recently Barnsley & Turchetti (1979) have shown that 25 terms in the series (4.56) are enough to provide good convergence for a variety of initial distributions.

Finally Koura (1974) and Borgnakke & Larsen (1973,1974) have examined the more general problem of the relaxation of a gas with internal degrees of freedom using Monte Carlo techniques. Borgnakke & Larsen studied the relative relaxation of translational and rotational energy whilst Koura studied the problem of internal energy relaxation. Their methods produce a good description of the relative speeds of relaxation of various systems whilst using relatively little computer time. It is however not applicable for examining the relaxation in the high energy tail as the other methods are. A method along similar lines to that used by Koura has been developed to examine the relaxation of the system from various initial conditions for different values of the parameter p.

The model was simulated using Monte Carlo techniques as follows. Two molecules with energies i_1 and i_2 are chosen at random from the total ensemble of 1000 molecules. Then a random number k from the NHG distribution is generated on the range $(0,i_1+i_2)$. Molecule number 1 has it's energy i_1 replaced by k and molecule number 2 has it's energy i_2 replaced by i_1+i_2-k . Thus at each collision the total energy is conserved and in only a few seconds of computer time the relaxation of an initial distribution can be examined over several collision times. (One collision time is equivalent to 500 iterations of the above cycle, since at each collision two molecules are affected.)

These simulations were repeated for several values of the parameter p and for the mean energy $\mathcal{E}=5$, and the distributions at successive collision times plotted on microfilm. A selection of the results are shown in figures (4.2) and (4.3). At each stage of the simulation the entropy, variance and the mean energy were calculated to give a more definite characterisation of the distribution.

The relaxation was examined for several different initial conditions but the conclusions drawn from the delta function initial distribution include any others that have been made. It was found that the greater the number of degrees of freedom of each molecule then the longer the system takes to relax to equilibrium.

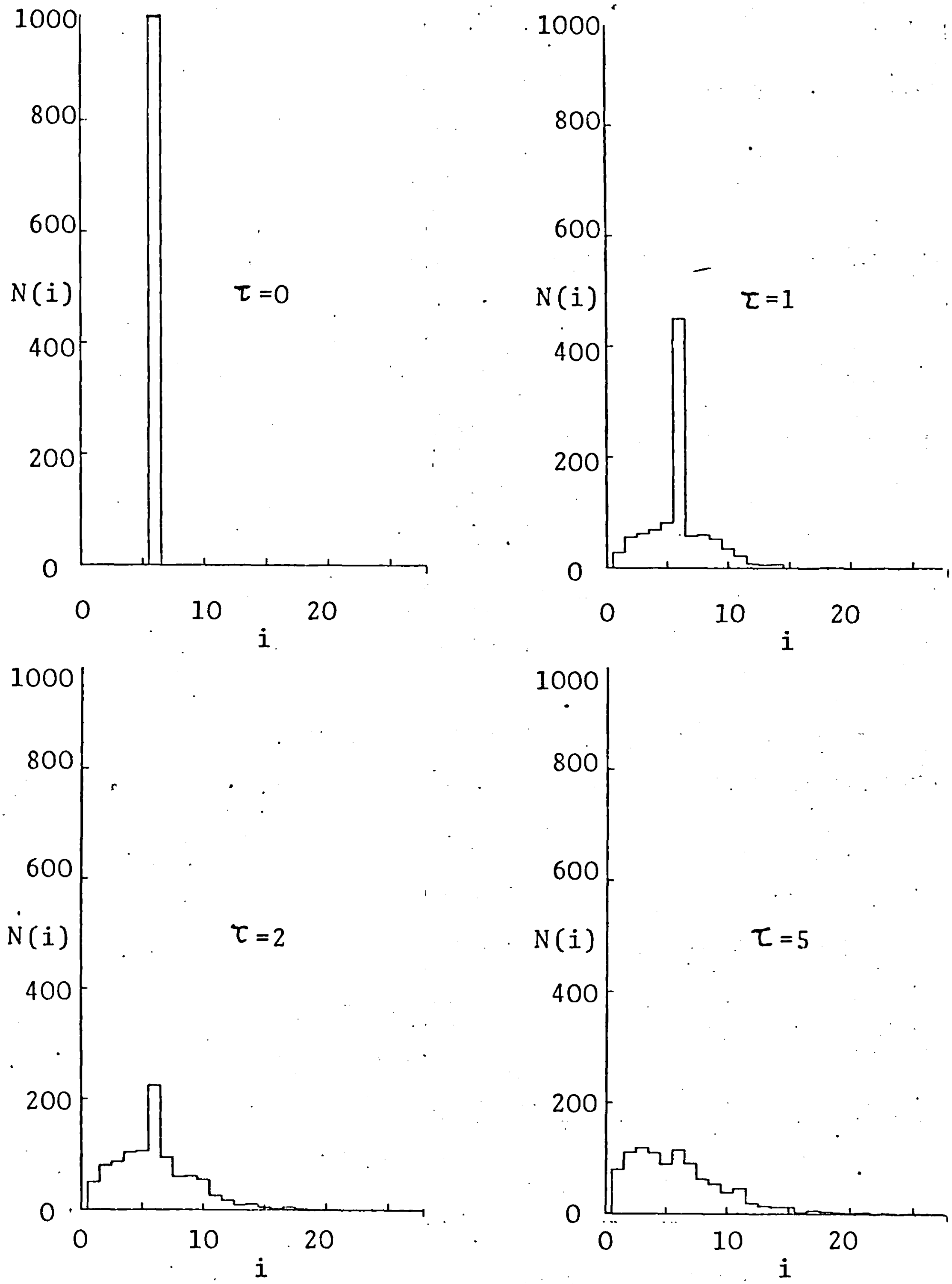

Fig. 4.2 : Computer simulation of Diffuse scattering system (p=2).

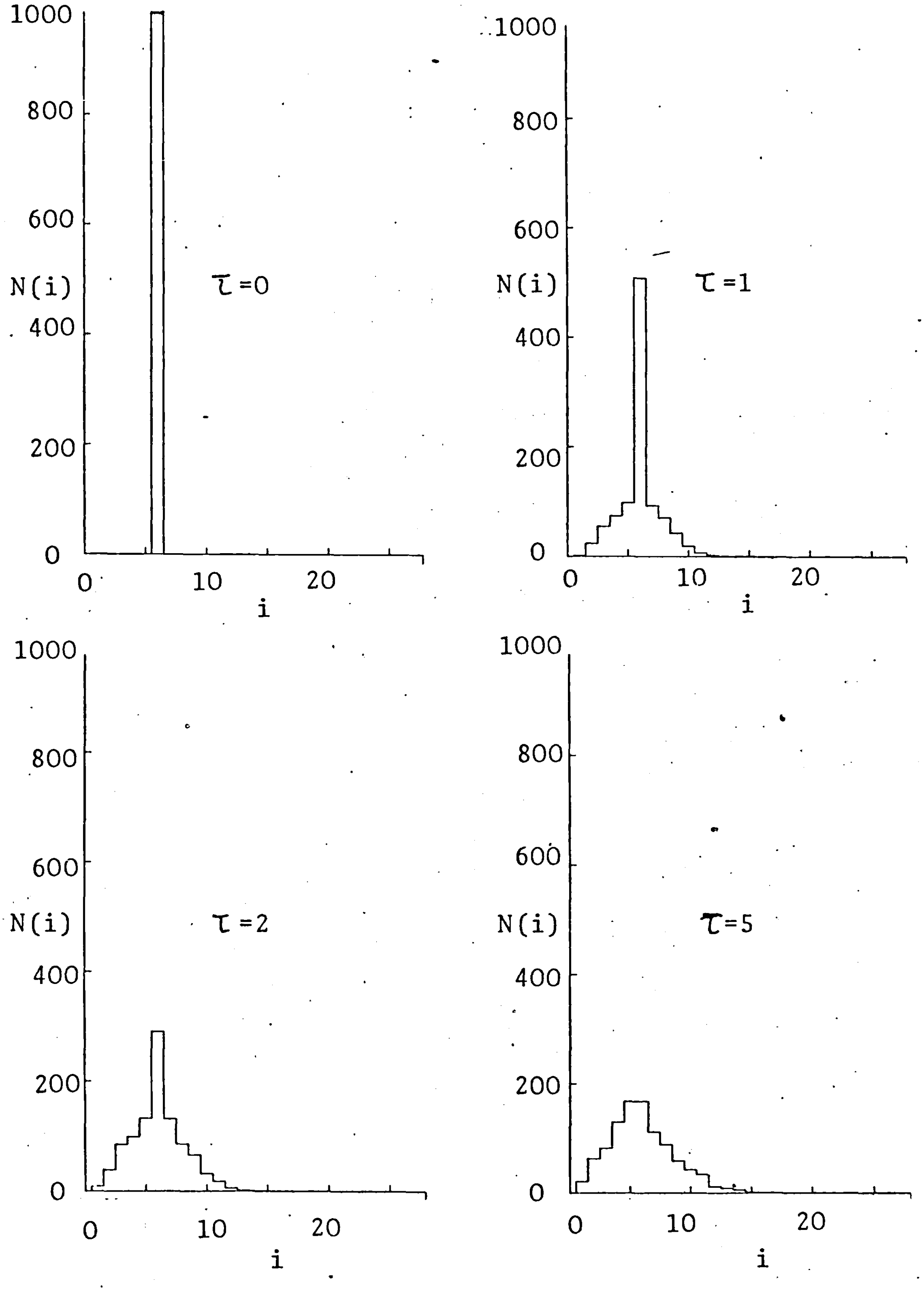

Fig. 4.3 : Computer simulation of diffuse scattering system (p=10).

However even for p=10 the system was effectively at equilibrium after 5 collision times, thus agreeing with the results of Koura (1974) who also found that the 'Maxwellisation time' depended weakly on p and was of the order of 5 collision times. No conclusions can be drawn about the relaxation in the high energy tail. The results are however best compared with those obtained for the persistent scattering model (see Chapter 6) and any more conclusions will be left until then.

CHAPTER FIVE : CONTINUOUS PERSISTENT SCATTERING MODEL

5.1 Introduction

In the previous two chapters the emphasis has been on diffuse scattering models. They have one unfortunate defect when applied to physical systems in that the interaction between them is too 'hard' since all of the molecule's energy is 'scrambled' at each collision, and there is no persistence of state. This point has not only been made in the literature on Maxwell molecules (to which our diffuse scattering molecules are related) but also in the work on the computer simulation of this type of system (Koura(1974)). It seems therefore essential to formulate some models which only allow some of their energy to interact with each other, with the non-interacting part giving a persistence of state character.

Models which have this property have already been discussed in the literature, (Cooper & Hoare (1979) (continuous) and Hoare & Rahman (1979) (discrete) and a more generalised one of these Rahman (1976a,b)) in the context of linear distributive processes. The relevant models in these papers have been formulated and the eigenfunctions and eigenvalues of their transition kernels have been found. Since we are dealing with closed systems the models in these papers are too general for our purposes and it is necessary to choose a simpler (symmetrical) form of them.

In this chapter the work of the previous two chapters is extended. It is seen how this persistent scattering model (the continuous one in this chapter and the discrete one in the next) are generalised forms of the diffuse scattering models, and how the latter can be derived as a limit of the former. A similarity solution of the Krook-Wu type has been found for these models and the moment equations are found to have a similar structure to (although not so concise as) the diffuse scattering ones. The linearised equation leads to an unsolved third order process, however the Fokker-Planck approximation can be studied and the existence of a small parameter shown.

5.2 The Model

This model is best described pictorially (see Fig 5.1) . The closed system contains molecules each with a total of p+q degrees of freedom of which q are allowed to interact and p do not interact at each collision. The energies of the two colliding molecules are x and u-x and so the first stage of the interaction is to examine how the energy x (and also the energy u-x) is distributed amongst the p+q degrees of freedom. More specifically we want the probability that there is an energy v in p degrees of freedom given that there is a total of x in p+q degrees of freedom. This is obviously the asymetric Beta distribution (see Appendix B). This is also multiplied by the probability of finding an energy u-w in p degrees of freedom given that there is a total of u-x in p+q. (again a Beta distribution).

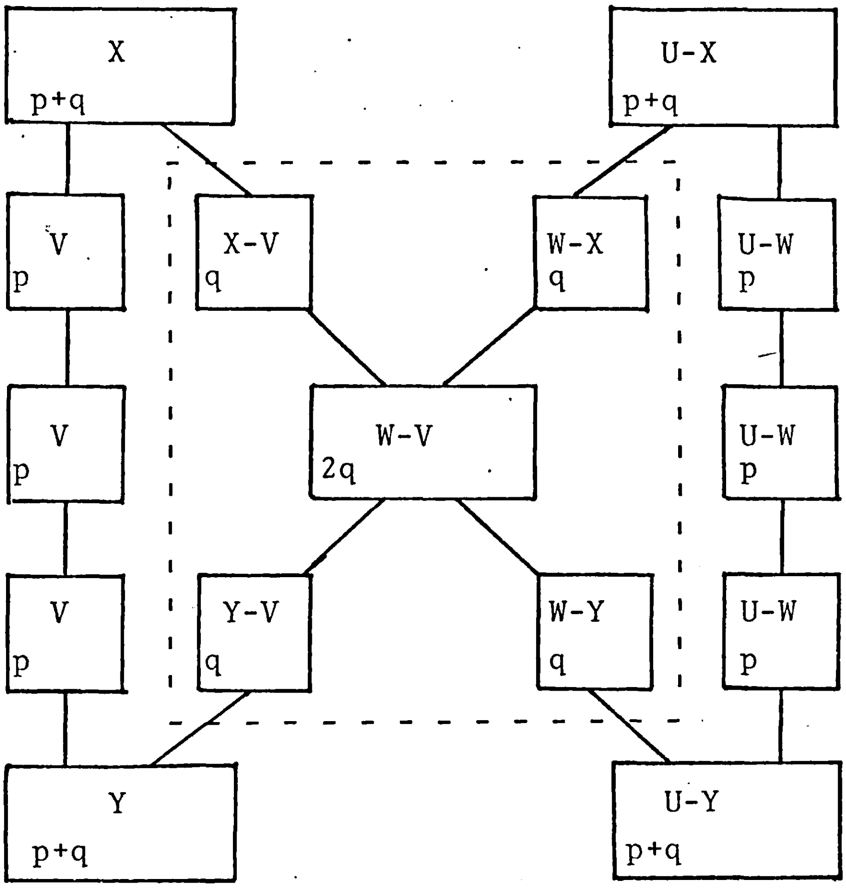

Fig. 5.1 .

At this stage there are two energies x-v and w-x which are going to interact (each in q degrees of freedom) , and so this part of the collision process is just a first order process (enclosed by a dotted line in fig. 5.1)), similar to the diffuse scattering problem of Chapter 3. The final stage is that an energy y-v in q degrees of freedom arises from w-v in 2q degrees of freedom. This is determined by the symmetric Beta distribution . Thus the resultant transition kernel describing the transition probability from x to dy about y is the convolution of the previously mentioned Beta distributions integrated over all w and v.

Three dimensional plots of the persistent scattering kernel

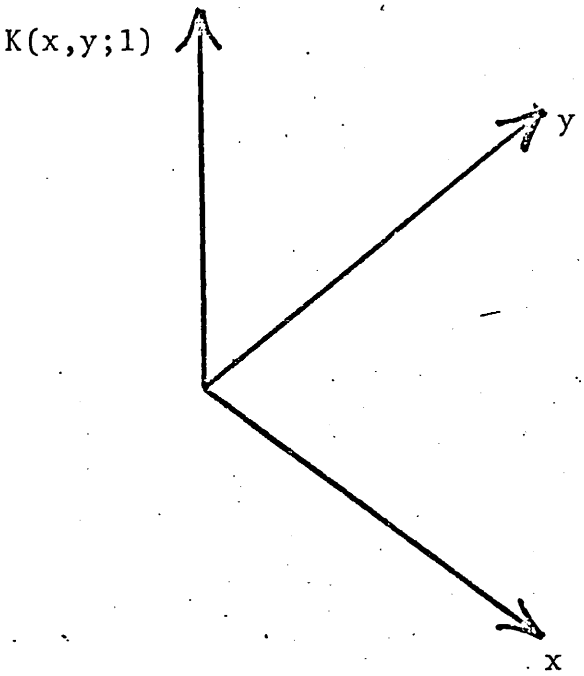

Fig. 5.2 Plan of 3-D plot.

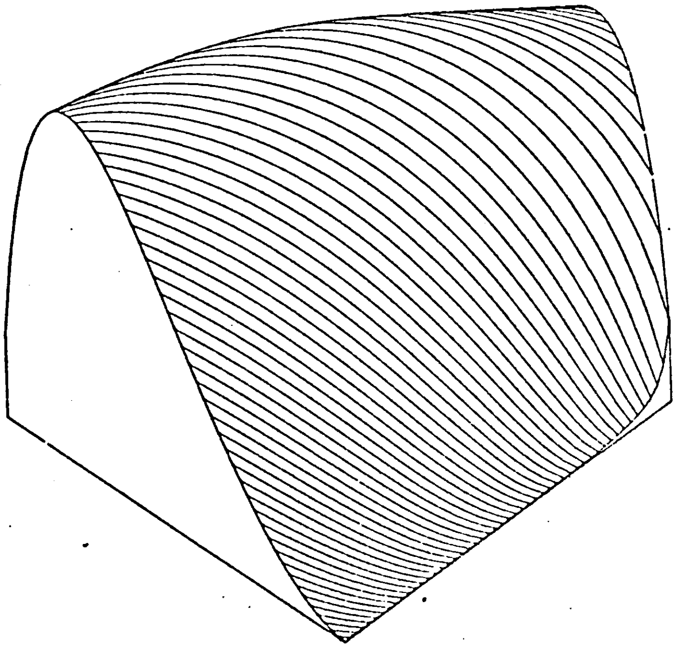

Fig. 5.3 : Persistent scattering kernel (p=1,q=2)

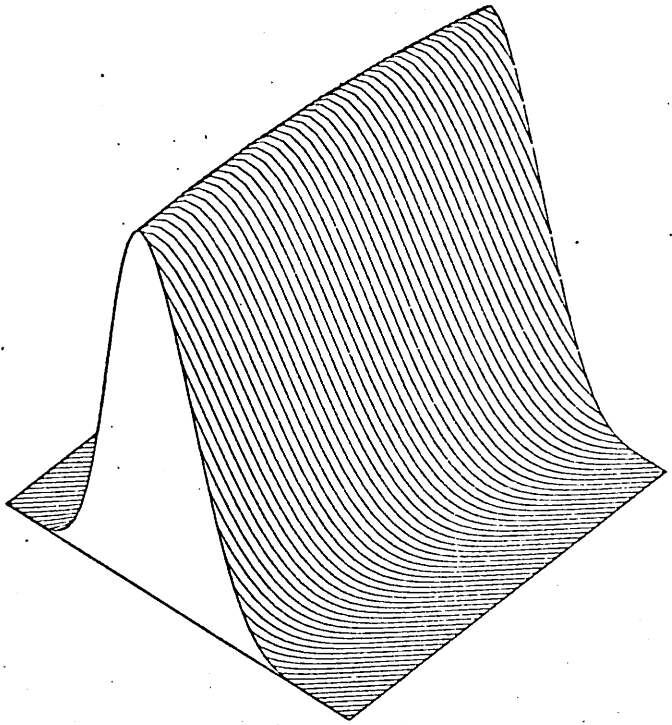

Fig 5.4 : Persistent scattering kernel (p=1,q=10)

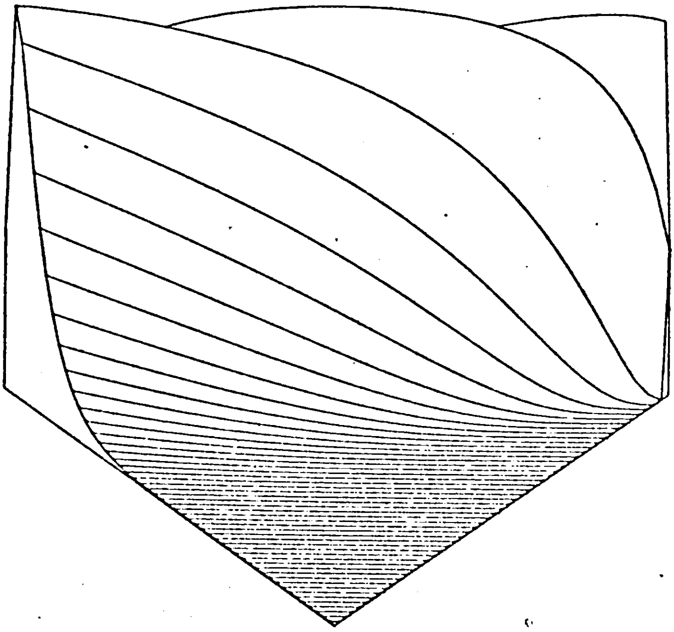

Fig. 5.5 : Persistent scattering kernel (p=10,q=2)

$$K(y,x;u) = \int_0^{\min(x,y)} dv\, W_{pq}(v;x) \int_{\mathrm{MAX}(x,y)}^{u} dw\, W_{qp}(w-x;u-x)\, W_{qq}(y-v;w-v) \tag{5.1}$$

This is the symmetric form of the pqrs kernel given by Cooper & Hoare (1979). Written out explicitly the kernel becomes,

$$K(y,x;u) = \frac{\Gamma(p+q)^2\,\Gamma(2q)}{\Gamma(p)^2\,\Gamma(q)^4\, x^{p+q-1}(u-x)^{p+q-1}}$$

$$\cdot \int_0^{\min(x,y)} dv\, v^{p-1}(x-v)^{q-1}(y-v)^{q-1} \int_{\max(x,y)}^{u} dw\, \frac{(w-x)^{q-1}(u-w)^{p-1}(w-y)^{q-1}}{(w-v)^{2q-1}} \tag{5.2}$$

The fact that the kernel is stochastic i.e. that,

$$\int_0^u K(y,x;u)\, dy = 1 \tag{5.3}$$

is readily observed by exchanging the orders of integration and doing the y integration first, using of course the normalisation of the Beta distribution (see Appendix B). The eigenfunctions and eigenvalues of this kernel have been given by Cooper & Hoare (1979) and also by Rahman (1976a,b) and it suffices simply to convert their notation into ours and write down these properties without giving the proofs (which are rather involved; see Rahman (1976b) for further details).

5.3 Equilibrium and Detailed Balance

The equilibrium distribution which ensures that the kernel and system satisfies detailed balance can be derived by a method akin to that in Chapter 3, but to avoid repetition it is simply quoted here,

$$P_\infty(x)\,dx = \left(\frac{p+q}{\varepsilon}\right)^{p+q}\Gamma(p+q)^{-1}\,x^{p+q-1}\,e^{-(p+q)x/\varepsilon}\,dx \tag{5.4}$$

This equilibrium distribution is a gamma distribution in p+q degrees of freedom with a mean ε and it is easily seen that the detailed balance condition

$$K(y,x;u)\;P_\infty(x)\,P_\infty(u-x) = K(x,y;u)\,P_\infty(y)\,P_\infty(u-y) \tag{5.5}$$

is satisfied for (5.2) and (5.4). The moments of the equilibrium distribution are,

$$\begin{aligned}\mu_n(\infty) &= \int_0^\infty \frac{x^n}{n!}P_\infty(x)\,dx \\ &= \frac{1}{n!}(p+q)_n\left(\frac{\varepsilon}{p+q}\right)^n\end{aligned} \tag{5.6}$$

5.4 Eigenvalues and Eigenfunctions

The eigenfunctions and eigenvalues are defined by,

$$\int_0^u K(y,x;u)\,\phi_n(x/u)\,dx = \lambda_n\,\phi_n(y/u) \tag{5.7}$$

or,

$$\int_0^u \psi_n(y/u)\,K(y,x;u)\,dy = \lambda_n\,\psi_n(x/u) \tag{5.8}$$

where the two types of eigenfunctions are connected by the relationship,

$$\psi_n(x/u)\, P_\infty(x)\, P_\infty(u-x) = \phi_n(x/u) \tag{5.9}$$

The eigenfunctions and eigenvalues are (see Cooper Hoare (1979)),

$$\psi_n(x) = J_n(2p+2q-1;\, p+q;\, x) \tag{5.10}$$

$$\lambda_n = {}_4F_3\left[\begin{matrix} -n,\, n+2p+2q-1,\, q,\, q \\ p+q,\, p+q,\, 2q \end{matrix};\, 1\right] \tag{5.11}$$

and the equilibrium distribution $P_\infty(x)$ is given by (5.4). The orthogonality relationship of the J_n is given in Appendix C and hence we can write the kernel in it's spectral representation as,

$$K(y,x;u) = u^{-1}\sum_{n=0}^{\infty} \omega_n(y/u)\, J_n(2p+2q-1;\, p+q;\, x/u) \cdot J_n(2p+2q-1;\, p+q;\, y/u) \tag{5.12}$$

where the weight function is,

$$\omega_n(x) = \frac{x^{p+q-1}(1-x)^{p+q-1}}{n!\ \Gamma(p+q)^2}\,(2p+2q+2n-1)\,\Gamma(2p+2q+n-1) \tag{5.13}$$

5.5 Special Cases of the Kernel

1. p=0. We note that,

$$\lim_{p \to 0} W_{pq}(x;u) = \delta(x) \tag{5.14}$$

and hence it is obvious that,

$$\lim_{p \to 0} K(y,x;u) = W_{qq}(x;u) \tag{5.15}$$

where K(y,x;u) is given by (5.1). Thus to obtain the diffuse scattering model of Chapter 3 the limit p → 0 is taken in the following work.

2. p=q=1. Apart from the above case this is the only other non-trivial case when the integrals in (5.1) can be evaluated exactly. The integrals are all elementary although care must be taken with the limits of them. The result is,

$$K(y,x;u) = [x(u-x)]^{-1}\Big\{ |x-y| \ln|x-y| + u \ln u - (u-\min(x,y))\ln(u-\min(x,y)) - \max(x,y)\ln(\max(x,y))\Big\} \tag{5.16}$$

3. q=0. In this case the kernel becomes the trivial one of a delta function,

$$K(y,x;u) = \delta(y-x) \tag{5.17}$$

where there are no interacting parts of the molecule and so this system does not relax from the initial distribution.

It will be seen that the exact solution obtained in section 7 of the present chapter has properties (1) and (3) intrinsically associated with it whilst (2) does not provide any appreciable simplification in the answer.

5.6 Moments of The Kernel

They are defined as,

$$m_n(x,u) = \int_0^u K(y,x;u+x)\, y^n\, dy \tag{5.18}$$

The shift in the variable u is for convenience only, and does not represent any appreciable simplification in the algebra when they are evaluated. Rewriting (5.18) by inserting the full form of the kernel (5.2) gives,

$$m_n(x,u) = \int_0^u y^n dy \int_0^{\min(x,y)} dv\, W_{pq}(v;x) \int_{\max(x,y)}^{u} dw\, W_{qp}(w-x;u)\, W_{qq}(y-v;w-v)$$

$$= \int_0^x dv\, W_{pq}(v;x) \int_x^{u+x} dw\, W_{qp}(w-x;u) \int_v^w dy\, y^n\, W_{qq}(y-v;w-v) \tag{5.19}$$

Although the moments can be evaluated generally in this form an easier method to find the n^{th} moment is to use the spectral representation of the kernel (5.12). However to find the first and second moments of the kernel the above method is not too cumbersome and produces the explicit form of the moments which is not so apparent in the other method.

5.6.1 First Moment (n=1)

$$m_1(x,u) = \int_0^x dv\, W_{pq}(v;x) \int_x^{u+x} dw\, W_{qp}(w-x;u) \cdot \int_0^{w-v} (y+v) W_{qq}(y;w-v)\, dy$$

$$= \frac{1}{2}\int_0^x dv\, W_{pq}(v;x) \int_x^{u+x} dw\, (w+v) W_{qp}(w-x;u)$$

$$= \frac{1}{2}\int_0^x dv\, W_{pq}(v;x) \int_0^u dw\, (v+w+x) W_{qp}(w;u)$$

$$= \frac{1}{2}\int_0^x dv\, W_{pq}(v;x) \left[\frac{q}{p+q}u + v + x\right]$$

$$= \frac{qu + (2p+q)x}{2(p+q)} \qquad (5.20)$$

In the notation of equation (2.40) this is,

$$m_1(x,u) = a_{10}x + a_{11}u \qquad (5.21)$$

where of course,

$$a_{10} = \frac{2p+q}{2(p+q)} \qquad (5.22)$$

and

$$a_{11} = \frac{q}{2(p+q)} \qquad (5.23)$$

Note that on putting p=0 the first moment becomes,

$m_1(x,u)=\frac{1}{2}(u+x)$ agreeing with the result for the diffuse scattering case.

5.6.2 Second Moment (n=2)

The working is essentially the same as for the first moment but involves more complicated algebra.

$$m_2(x,u)=\int_0^x dv\, W_{pq}(v;x)\int_x^{u+x} d\omega\, W_{qp}(\omega-x;u)\int_0^{\omega-v}(y+v)^2\, W_{qq}(y;\omega-v)\,dy$$

$$=\int_0^x dv\, W_{pq}(v;x)\int_x^{u+x} d\omega\, W_{qp}(\omega-x;u)\left\{\varrho(\omega-v)^2+\omega v\right\}$$

where ϱ has been used as an abbreviation for the expression

$$\varrho = \frac{1}{2}\left(\frac{q+1}{2q+1}\right)$$

$$m_2(x,u)=\int_0^x dv\, W_{pq}(v,x)\int_0^u d\omega\, W_{qp}(\omega,u)\left\{\varrho(\omega+x-v)^2+v(\omega+x)\right\}$$

(5.24)

The two integrations are now independent and we note that upon executing them the following transformations are effected,

$$\omega \rightarrow \frac{qu}{p+q} \qquad \omega^2 \rightarrow \frac{q(q+1)u^2}{(p+q)(p+q+1)}$$

$$v \rightarrow \frac{px}{p+q} \qquad v^2 \rightarrow \frac{p(p+1)x^2}{(p+q)(p+q+1)}$$

(5.25)

This gives for the second moment,

$$m_2(x,u) = a_{20}x^2 + 2a_{21}xu + a_{22}u^2 \tag{5.26}$$

where,

$$a_{20} = \frac{(p+q+1)(q^2+3pq+p+q) + p(p+1)(q+1)}{2(p+q)(p+q+1)(2q+1)} \tag{5.27}$$

$$a_{21} = \frac{q(2pq+p+q^2+q)}{2(2q+1)(p+q)^2} \tag{5.28}$$

$$a_{22} = \frac{q(q+1)^2}{2(p+q)(p+q+1)(2q+1)} \tag{5.29}$$

Note that on putting p=0,

$$a_{20} = a_{21} = a_{22} = \frac{q+1}{2(2q+1)}$$

and the second moment becomes,

$$m_2(x,u) = \frac{q+1}{2(2q+1)}(u+x)^2$$

agreeing with that for the diffuse scattering case.

5.6.3 N^th Moment

We define the n^th moment as,

$$m_n(x,u-x) = \int_0^u k(y,x;u)\, y^n\, dy \tag{5.30}$$

(i.e. without the shift in u). Using (5.12) this gives,

$$m_n(x,u-x) = u^{-1}\sum_{i=0}^{\infty} \lambda_i\, J_i(2p+2q-1;\, p+q;\, x/u)$$
$$\cdot \int_0^u y^n\, \omega_i(y/u)\, J_i(2p+2q-1;\, p+q;\, y/u)\, dy$$

$$= u^n \sum_{i=0}^{\infty} \lambda_i\, J_i(2p+2q-1;\, p+q;\, x/u) \cdot \frac{(2p+2q+2i-1)\,\Gamma(2p+2q+i-1)}{i!\;\Gamma(p+q)^2}$$
$$\cdot \int_0^1 s^{n+p+q-1}(1-s)^{p+q-1}\, {}_2F_1[-i,\, i+2p+2q-1;\, p+q;\, s]\, ds$$

Using the following standard integral (see e.g. Gradshteyn & Ryzhik (1965)),

$$\int_0^1 x^{\varrho-1}(1-x)^{\beta-\gamma-n}\, {}_2F_1[-n,\beta;\gamma;x]\,dx = \frac{\Gamma(\gamma)\,\Gamma(\varrho)\,\Gamma(\beta-\gamma+1)\,\Gamma(\gamma-\varrho+n)}{\Gamma(\gamma+n)\,\Gamma(\gamma-\varrho)\,\Gamma(\beta-\gamma+\varrho+1)}$$

$$[n=0,1,2\ldots;\ \operatorname{Re}\varrho>0;\ \operatorname{Re}(\beta-\gamma)>n-1] \qquad (5.31)$$

we have for the nth moment,

$$m_n(x,u-x) = u^n \sum_{i=0}^{n} \lambda_i\, J_i(2p+2q-1;\, p+q;\, x/u)$$
$$\cdot (2p+2q+2i-1)\, \frac{\Gamma(2p+2q+i-1)\,(-n)_i\,\Gamma(n+p+q)}{i!\;\Gamma(p+q)\;\Gamma(i+n+2p+2q)}$$
$$= u^n \sum_{i=0}^{n} N_i\, J_i(2p+2q-1;\, p+q;\, x/u) \qquad (5.32)$$

where N_i is given by,

$$N_i = \lambda_i\,(2p+2q+2i-1)\, \frac{\Gamma(2p+2q+i-1)\,(-n)_i\,\Gamma(n+p+q)}{i!\;\Gamma(p+q)\,\Gamma(i+n+2p+2q)} \qquad (5.33)$$

(Note that the sum terminates at i=n due to the falling Pochhammer function in N_i). Expanding the Jacobi polynomial (by using equation (G.2)) and collecting up terms in x and u gives,

$$m_n(x,u-x) = \sum_{i=0}^{n} N_i \sum_{\nu=0}^{i} \frac{(-i)_\nu \, (n+2p+2q-1)_\nu}{(p+q)_\nu \; \nu!} \, x^\nu u^{n-\nu} \tag{5.34}$$

To put this finally in the same form as (2.59) requires a bit more algebra and the result is,

$$\begin{aligned} m_n(x,u) &= \sum_{\nu=0}^{n} \frac{(n+2p+2q-1)_\nu}{(p+q)_\nu \; \nu!} \sum_{k=0}^{n-\nu} \binom{n-\nu}{k} x^{n-k} u^k \sum_{i=\nu}^{n} (-i)_\nu N_i \\ &= \sum_{k=0}^{n} x^{n-k} u^k \sum_{\nu=0}^{n-k} \frac{(n+2p+2q-1)_\nu}{(p+q)_\nu \; \nu!} \binom{n-\nu}{k} \sum_{i=\nu}^{n} (-i)_\nu N_i \end{aligned} \tag{5.35}$$

This then justifies the use of the form (2.39) for the n^{th} moment at least for this particular model and means that all of the moments can be calculated sequentially and hence a general solution can be found in terms of these moments. The coefficient $a_{n,k}$ is very complicated but can be written in closed form and is,

$$a_{nk} = \frac{(n-k)!}{n!} \sum_{\nu=0}^{n-k} \frac{(n+2p+2q-1)_\nu \, (n-\nu)!}{(p+q)_\nu \; \nu! \, (n-\nu-k)!} \sum_{i=\nu}^{n} (-i)_\nu N_i \tag{5.36}$$

The limiting case of p → 0 (diffuse scattering)is surprisingly easy to take. Examining the form of λ_i for p=0,

$$\lambda_i \Big|_{p=0} = {}_4F_3\left[\begin{matrix}-i, i+2q-1, q, q \\ q, q, 2q\end{matrix}; 1\right]$$

$$= {}_2F_1\left[-i, i+2q-1; 2q; 1\right]$$

$$= \frac{(1-i)_i}{(2q)_i} \qquad (5.37)$$

The summation of the ${}_2F_1$ is by Vandermonde's theorem (see Slater (1966)). In addition we note that,

$$(1-i)_i = \delta_{i,0} \qquad (5.38)$$

and hence in equation (5.35) $\nu=0$ and $i=0$, so

$$N_i\Big|_{i=0} = \frac{(p)_n}{(2p)_n} \qquad (5.39)$$

and all of the other terms in (5.36) are either unity or cancel giving,

$$a_{n,k} = \frac{(p)_n}{(2p)_n} \qquad (5.40)$$

the diffuse scattering result.

5.6.4 Laguerre Moments

The n^{th} Laguerre moment can be calculated with the aid of (5.35) and writing $\mathcal{L}_n^{(p+q-1)}(x)$ as a series, but unfortunately the result cannot be written as a Laguerre polynomial, thus rendering it impossible to find the evolution equations corresponding to (2.40) for the Laguerre moments.

5.6.5 Relaxation of the Second Moment

In section 2.11.2 it was shown that the form of the second moment is,

$$\mu_2(t) - \mu_2(\infty) = (\mu_2(0) - \mu_2(\infty))\, e^{-\lambda_2 t} \tag{5.41}$$

where λ_2 and $\mu_2(\infty)$ are given by (2.42) and (2.43) respectively. We are now in a position to calculate these two exactly in terms of p and q. They are,

$$\begin{aligned} \lambda_2 &= 1 - a_{20} - a_{22} \\ &= \frac{q(2pq+p+q+q^2)}{(p+q)(p+q+1)(2q+1)} \end{aligned} \tag{5.42}$$

$$\begin{aligned} \mu_2(\infty) &= \frac{a_{21}\,\varepsilon^2}{\lambda_2} \\ &= \frac{p+q+1}{2(p+q)}\,\varepsilon^2 \end{aligned} \tag{5.43}$$

which is of course the same as that from (5.16). It is obvious that for p → 0 the diffuse scattering second moment (equation (D.8)) is immediately recovered.

5.7 The Similarity Solution

In line with the train of thought of the previous two chapters the term 'similarity solution' does not hold any deep rooted meaning arising from the use of similarity theory to solve the problem but rather from the unique combination of variables which occur in the solution. Using (3.28) as a prototype of the form of solution that we might expect we choose a solution of the form,

$$P(x,t) = (\alpha + \beta x)\, x^{p+q-1}\, e^{-\psi x} \tag{5.44}$$

where again $\alpha(t)$, $\beta(t)$ and $\psi(t)$ are time dependent functions. The process of constructing the solution from this point is similar to that used in Chapter 3 and indeed some of the results obtained in that chapter may be used here. Most particularly we note that the only difference between (3.28) and (5.44) is that p in (3.88) has been replaced by p+q in (5.44), which means that we can immediately write α and β in terms of ψ as,

$$\alpha = \frac{\psi^{p+q}}{\Gamma(p+q)}\,(1+p+q-\varepsilon\psi) \tag{5.45}$$

$$\beta = \frac{\psi^{p+q+1}}{\Gamma(p+q+1)}\,(\varepsilon\psi-p-q) \tag{5.46}$$

Again the left hand side (LHS) of the Boltzmann equation (2.11) can immediately be translated from (3.33) and is,

$$(LHS) = \left(\frac{\partial}{\partial t}+1\right)\left\{(\alpha+\beta x)\, x^{p+q-1}\, e^{-\psi x}\right\} \tag{5.47}$$

It is in the right hand side (RHS) of (2.11) that the differences occur. Inserting the trial solution (5.44) into the RHS of (2.11) gives,

$$(RHS) = \int_x^\infty du \int_0^u dy\, e^{-\psi u} K(x,y;u)\, y^{p+q-1}(u-y)^{p+q-1}(\alpha+\beta y)(\alpha+\beta(u-y)) \tag{5.48}$$

Using the detailed balance condition this becomes,

$$(RHS) = x^{p+q-1}\int_x^\infty du\, (u-x)^{p+q-1} e^{-\psi u}\int_0^u K(y,x;u)\, (\alpha+\beta y)(\alpha+\beta(u-y))\,dy \tag{5.49}$$

and equating left and right hand sides the Boltzmann equation becomes,

$$\left(\frac{\partial}{\partial t}+1\right)(\alpha+\beta x)\, e^{-\psi x}$$

$$= \int_x^\infty du\, (u-x)^{p+q-1} e^{-\psi u}\int_0^u dy\, K(y,x;u)(\alpha+\beta y)(\alpha+\beta(u-y)) \tag{5.50}$$

Expanding the brackets and using the previously found forms of the kernel moments the RHS becomes,

$$(RHS) = e^{-\psi x}\int_0^\infty du\, u^{p+q-1} e^{-\psi u}\int_0^{u+x} dy\, K(y,x;u+x)$$

$$\cdot\left\{\alpha^2+\alpha\beta(u+x)+\beta^2(u+x)y-\beta^2y^2\right\}$$

$$= e^{-\psi x}\int_0^\infty du\, u^{p+q-1} e^{-\psi u}\left\{\alpha^2+\alpha\beta x+\beta^2x^2(a_{10}-a_{20})\right.$$

$$\left.+\left(\alpha\beta+\beta^2(a_{10}+a_{11}-2a_{21})x\right)u \;+\beta^2(a_{11}-a_{22})u^2\right\}$$

$$= \frac{e^{-\psi x}\Gamma(p+q)}{\psi^{p+q+2}} \Big\{ \alpha^2\psi^2 + \alpha\beta(p+q)\psi + \beta^2(p+q)(p+q+1)(a_{11}-a_{22})$$
$$+ x\left(\alpha\beta\psi^2 + \beta^2(p+q)(a_{11}+a_{10}-2a_{21})\psi\right)$$
$$+ x^2\beta^2\psi^2(a_{10}-a_{20}) \Big\} \tag{5.51}$$

Thus,

$$\left(-x\frac{d\psi}{dt} + \frac{\partial}{\partial t} + 1\right)(\alpha+\beta x)$$
$$= \frac{\Gamma(p+q)}{\psi^{p+q+2}} \Big\{ \alpha^2\psi^2 + \alpha\beta(p+q)\psi + \beta^2(p+q)(p+q+1)(a_{11}-a_{22})$$
$$+ x(\alpha\beta\psi^2 + \beta^2(p+q)(a_{11}+a_{10}-2a_{21})\psi) + x^2\beta^2\psi^2(a_{10}-a_{20}) \Big\} \tag{5.51}$$

We are now in a position to compare the coefficients of x^o, x and x^2. They are after some algebra,

Coefficient of x^2,

$$\frac{d\psi}{dt} = \psi\left(\frac{\psi\varepsilon}{p+q} - 1\right)(a_{20} - a_{10}) \tag{5.53}$$

of x,

$$\frac{d\psi}{dt} = \psi\left(\frac{\psi\varepsilon}{p+q} - 1\right)\frac{p+q}{2(p+q+1)}(a_{10} + a_{11} - 2a_{21} - 1) \tag{5.54}$$

and of the constant term,

$$\frac{d\psi}{dt} = \psi\left(\frac{\psi\varepsilon}{p+q} - 1\right)(a_{22} - a_{11}) \tag{5.55}$$

If these three equations are all identical then the validity of the trial solution is guaranteed. This is in fact the case with,

$$a_{22} - a_{11} = \frac{p+q}{2(p+q+1)}\left(a_{10} + a_{11} - 2a_{21} - 1\right)$$

$$= a_{20} - a_{10}$$

$$= -\lambda = -\frac{q\left(q^2 + 2pq + p + q\right)}{2(p+q)(p+q+1)(2q+1)} \qquad (5.56)$$

Thus the resulting equation for ψ is,

$$\frac{d\psi}{dt} = -\lambda\psi\left(\frac{\varepsilon\psi}{p+q} - 1\right) \qquad (5.57)$$

where now

$$\lambda = \frac{q\left(q^2 + 2pq + p + q\right)}{2(p+q)(p+q+1)(2q+1)} \qquad (5.58)$$

This is of the same form as equation (3.38) and hence we can immediately write down the solution as,

$$\psi = \frac{p+q}{\varepsilon}\left(1 - \eta e^{-\lambda t}\right)^{-1} \qquad (5.59)$$

The constant η plays the same role as before in describing the range of initial distributions. The similarity solution can be written in full as,

$$P^S(x,t) = \frac{\psi^{p+q}}{\Gamma(p+q)}\left\{1 + p + q - \varepsilon\psi + \psi\left(\frac{\varepsilon\psi}{p+q} - 1\right)x\right\}x^{p+q-1}e^{-\psi x} \qquad (5.60)$$

Any remarks as to the range of validity of the solution are the same as those made for the diffuse scattering model and will not be repeated here.

Considering the decay constant given by (5.58) it is apparent that in the limit $p \to 0$ it becomes the same as that in the diffuse scattering case (equation (3.36)) and hence the solution (5.60) becomes identical to that one (3.40), thus confirming prediction 1 of section 5 of the present chapter. The other limit $q \to 0$ implies that ψ becomes time independent and hence there is no relaxation of the initial distribution.

Also worthy of note is that the decay constant of all parts of the solution involves only multiples of the decay constant of the second moment (see equation (5.42)). This is the same as in the diffuse scattering case but due to it's complexity is far more apparent here.

Given a certain initial distribution it is now obvious that the system will evolve through the same set of distributions irrespective of the type of molecules (diffuse or persistent scattering). The only variant will be the value of the decay constant λ which for diffuse scattering systems varies between 1/6 and 1/4 and for persistent scattering molecules 0 and 1/4. In general for a given total number of degrees of freedom the decay constant λ is smaller in the persistet scattering case than in the diffuse scattering case (say $p=1,q=1$ cf. $p=2$) hence implying that the persistent scattering system will take longer to reach a given state.

5.8 The Linearised Equation

It was shown in section 2.12 that the linearised kernel is given by (2.51). Since the equilibrium distribution is a gamma distribution and the persistent scattering kernel is a convolution of three Beta distributions the structure of the linearised kernel is,

$$(\text{Gamma}) * (\text{Beta}) * (\text{Beta}) * (\text{Beta}) \tag{5.61}$$

or a kernel representing a third order process. There is no easy option this time to find the solution of the linearised equation, however one might expect that it would be possible to find the Fourier representation in terms of a set of Laguerre polynomials since again the weight function is the equilibrium distribution.
In due course this involves the Laguerre moments of the kernel (5.1) which are not readily evaluated in a convenient form and hence it has not been possible to find the solution to the linearised equation. Because of this interest was shifted to the non-linear Fokker-Planck equation which was formulated in Chapter 2.

5.9 The Fokker-Planck Equation

In Chapter 2 the idea of a non-linear Fokker-Planck equation was proposed and it was shown that with certain restrictions on the model the equation preserved the nature of the first and zeroth moments (conservation of energy and probability). In addition it was also shown that the second moment is identical in both the non-linear Boltzmann equation and the Fokker-Planck approximation . Although the solution of (2.62) has not been found explicitly it is possible to evaluate the moments successively as one would expect to be able to do, and it is to this end that this section is devoted.

The transfer moments ($\bar{A}_n(x,u)$) of the kernel defined by (2.59) are connected to the ordinary moments ($m_n(x,u)$) by,

$$A_n(x,u) = \sum_{k=0}^{n} \binom{n}{k} (-1)^{n-k} m_k(x,u) x^{n-k} \tag{5.62}$$

$$= \sum_{k=0}^{n} b_{n,k} u^k x^{n-k} \tag{5.63}$$

In particular for the first two transfer moments,

$$\begin{aligned} A_1(x,u) &= m_1(x,u) - x \\ &= (a_{10}-1)x + a_{11}u \\ &= b_{10}x + b_{11}u \end{aligned} \tag{5.64}$$

and

$$\begin{aligned} A_2(x,u) &= m_2(x,u) - 2m_1(x,u)x + x^2 \\ &= (1-a_{20}-2a_{10})x^2 + 2(a_{21}-a_{11})ux + a_{22}u^2 \\ &= b_{20}x^2 + b_{21}xu + b_{22}u^2 \end{aligned} \tag{5.65}$$

The values of these constants are,

$$b_{10} = a_{10} - 1 = \frac{-q}{2(p+q)}$$

$$b_{11} = a_{11} = \frac{q}{2(p+q)}$$

$$b_{20} = 1 + a_{20} - 2a_{10} = \frac{q(q+1)^2}{2(p+q)(p+q+1)(2q+1)}$$

$$b_{21} = 2(a_{21} - a_{11}) = \frac{-q^3}{(p+q)^2(2q+1)}$$

$$b_{22} = a_{22} = \frac{q(q+1)^2}{2(p+q)(p+q+1)(2q+1)}$$

(5.66)

We note that until now the existence of a small parameter to justify truncating the expansion in (2.58) has been ignored. The obvious small parameter is q/p and it can be seen that the first transfer moment goes as q/p, the second as $(q/p)^2$ and it is expected that the n^{th} transfer moment goes as $(q/p)^n$, thus justifying the Fokker-Planck limit if this limit is also taken.

If we suppose that q=1 and that the small parameter is θ where,

$$\theta = \frac{1}{p} \ll 1$$

(5.67)

then the above coefficients reduce to,

$$b_{10} = -\theta/2 \quad , \quad b_{11} = \theta/2$$

$$b_{22} = b_{20} = 2\theta^2/3$$

$$b_{21} = -\theta^2/3$$

(5.68)

and thus,

$$A_1(x,u) = -\theta/_2\,(x-u)$$

$$A_2(x,u) = \theta^2/_3\,(2x^2-xu+2u^2)$$

(5.69)

If the values (5.69) are inserted into (2.62) the u integration can be done explicitly, so that the equation is now linear in P(x,t) but with both time and energy dependent coefficients.

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left\{-\frac{\theta P(x,t)}{2}\int_0^\infty du\,(x-u)\,P(u,t)\right\}$$

$$+\frac{1}{2}\frac{\partial^2}{\partial x^2}\left\{\frac{\theta\,P(x,t)}{3}\int_0^\infty du\,(2x^2-xu+2u^2)P(u,t)\right\}$$

$$= \frac{\partial}{\partial x}\left\{\frac{\theta P(x,t)}{2}\,(x-\varepsilon)\right\}$$

$$+\frac{1}{2}\frac{\partial^2}{\partial x^2}\left\{\frac{\theta P(x,t)}{3}\,(2x^2-x\varepsilon+4\hat{\mu}_2(t))\right\}$$

(5.70)

the $\hat{\mu}_2$ (t) is exactly the same as μ_2(t) in (5.41) which was calculated from the exact equation and which we have shown in section 2.13.3 is consistent with the Fokker-Planck equation . Despite the apparent simplification this equation is not immediately soluble , and one cannot convert it into an eigenvalue problem because of the time dependent coefficient. For these reasons we again examine the relaxation of the moments with a view to obtaining information about the solution.

5.9.1 Moments of the Fokker-Planck Equation

Taking power moments of (5.70) such that,

$$\hat{\mu}_n(t) = \frac{1}{n!}\int_0^\infty x^n P(x,t)\,dx \qquad (5.71)$$

(with the hat distinguishing the moments of the Fokker-Planck equation from those of the exact equation) gives,

$$\frac{d\hat{\mu}_n(t)}{dt} = \frac{-1}{n!}\int_0^\infty x^n \frac{\partial}{\partial x}\{1\}\,dx + \frac{1}{2}\cdot\frac{1}{n!}\int_0^\infty x^n \frac{\partial^2}{\partial x^2}\{2\}\,dx$$

$$= \frac{1}{n!}\int_0^\infty n x^{n-1}\{1\}\,dx + \frac{1}{2}\frac{n(n-1)}{n!}\int_0^\infty x^{n-2}\{2\}\,dx$$

$$= n\hat{\mu}_n\left[(n-1)\theta^2/3 - \theta/2\right] + \varepsilon\hat{\mu}_{n-1}\left[\theta/2 - (n-1)\theta^2/6\right] + \frac{2\theta^2}{3}\hat{\mu}_{n-2}\hat{\mu}_2 \; . \qquad (5.72)$$

The n^{th} moment of the similarity solution (5.60) can on using (3.48) be shown to be,

$$\mu_n^s(t) = \frac{(p+q)_n}{\psi^n\, n!}\left(1 + n\left(\frac{\varepsilon\psi}{p+q} - 1\right)\right) \qquad (5.73)$$

and it is a simple matter to show that for n=2 and 3 the moments are equal in the Fokker-Planck approximation and in the similarity solution. Furthermore it can be seen that the higher moments decay faster in the exact solution than in the Fokker-Planck approximation.

CHAPTER SIX : DISCRETE PERSISTENT SCATTERING MODEL

6.1 Introduction

This is the last model that is considered and is the discrete analogue of that solved in the last chapter. Much of the introduction to that model can equally well be applied to this one and the concept of discrete energy states has been dealt with in Chapter 4. It suffices therefore only to describe the model and it's solution as well as showing it's connections to the other models.

6.2 The Model

The construction and structure of this model is the same as that in the previous chapter and is described diagrammatically in Fig. 6.1 . (It is a symmetrical form of one investigated by Hoare & Rahman (1979) with reference to distributive processes in linear systems.) Two molecules with energies i and k-i (both in p+q degrees of freedom) interact giving a total energy k in the collision complex. The energy i splits into two parts m (the non-interacting part in p degrees of freedom) and i-m (the interacting part in q degrees of freedom) , the division being governed by the asymetric Negative Hypergeometric (NHG) distribution (see Appendix B).Similarly the energy k-i splits into two corresponding parts k-n and n-i, thereby creating a total energy n-m (in 2q degrees of freedom) which is interacting.

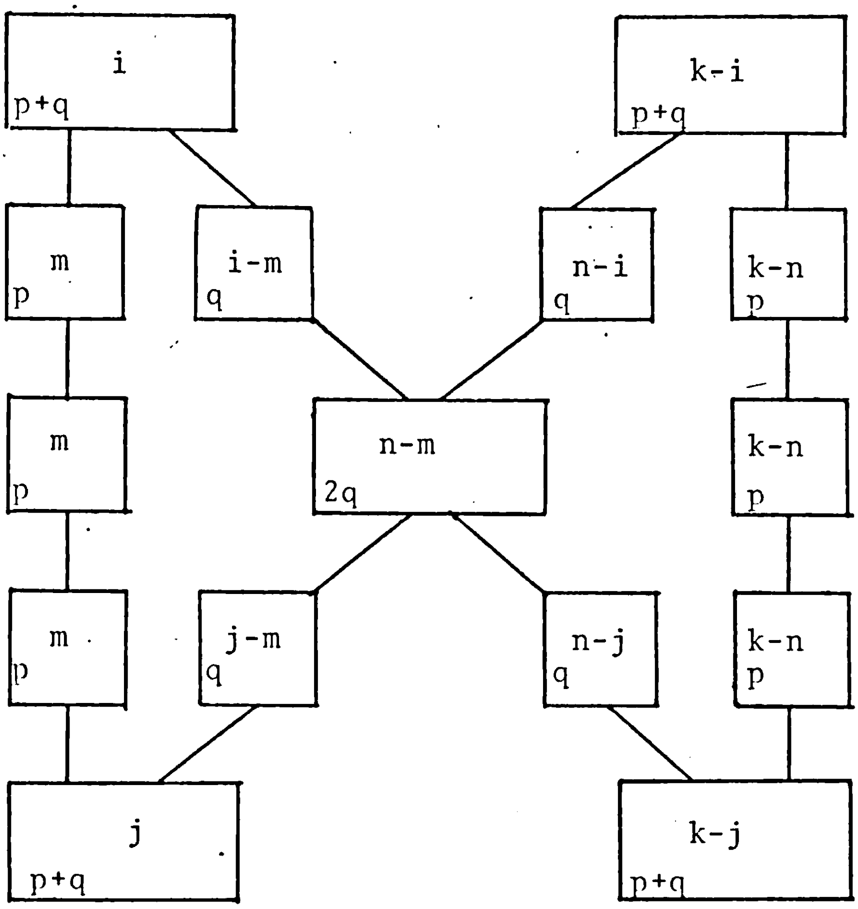

Fig. 6.1

This energy n-m splits into two parts, j-m and n-j each in q degrees of freedom which when recombined with the m and k-n give the final states as j and k-j. The transition kernel is the probability of going from a state i to a state j and is given by a convolution over three NHG distributions viz.,

$$K(j, i; k) = \sum_{r=0}^{\min(i,j)} W_{pq}(r;i) \sum_{s=\max(i,j)}^{k} W_{qp}(s-i; k-i)\, W_{qq}(j-r; s-r) \tag{6.1}$$

where $W_{pq}(i;k)$ is defined by equation (B.12).

6.3 Equilibrium and Detailed Balance

Writing the kernel explicitly gives,

$$K(j,i;k) = \frac{\Gamma(p+q)^2\,\Gamma(2q)}{\Gamma(p)^2\,\Gamma(q)^4} \cdot \frac{1}{(i+1)_{p+q-1}\,(N-i+1)_{p+q-1}}$$

$$\cdot \sum_{r=0}^{\min(i,j)} (r+1)_{p-1}\,(i-r+1)_{q-1}\,(j-r+1)_{q-1} \sum_{s=\max(i,j)}^{k} \frac{(s-i+1)_{q-1}}{(s-r+1)_{2q-1}}\,(k-s+1)_{p-1}\,(s-j+1)_{q-1} \qquad (6.2)$$

The detailed balance condition is,

$$K(j,i;k)\,P_\infty(i)\,P_\infty(k-i) = K(i,j;k)\,P_\infty(j)\,P_\infty(k-j) \qquad (6.3)$$

from which it is obvious that the equilibrium distribution is of the form,

$$P_\infty(i) = a\,(i+1)_{p+q-1}\,b^i$$

Using the same method as that in section 4.3 it can be shown that the equilibrium distribution is,

$$P_\infty(i) = \Gamma(p+q)^{-1} \left(\frac{\varepsilon_0(p+q)}{\varepsilon+\varepsilon_0(p+q)}\right) (i+1)_{p+q-1} \left(\frac{\varepsilon}{\varepsilon+\varepsilon_0(p+q)}\right)^i \qquad (6.4)$$

or a Negative Binomial distribution, normalised on the range $(0,\infty)$ and with mean $\varepsilon/\varepsilon_0$. The moments of this are readily obtained using (B.16) and are,

$$\bar{\mu}_n(\infty) = \sum_{i=n}^{\infty} \frac{(i)^{(n)}}{n!} P_\infty(i) = \frac{(p+q)_n}{n!} \left(\varepsilon/\varepsilon_0\right)^n \qquad (6.5)$$

The limiting cases of the kernel are identical to those of the last chapter and as in that case they will be seen to be obvious from the final form of the exact solution.

6.4 Moments of The Kernel

In Chapter 4 the analogy was drawn between the power of a continuous variable and the falling factorial function. For this reason the moments of the discrete kernel are defined as,

$$\bar{M}_n(i,k) = \sum_{j=0}^{i+k} (j)^{(n)} K(j,i;i+k) \tag{6.6}$$

and although there is no specific reason for assuming a homogeneous moment property it is assumed here and shown to hold later for this particular model. In this way the analogies with the continuous model can be more easily compared. Thus we put,

$$\bar{m}_n(i,k) = \sum_{l=0}^{n} \binom{n}{l} \bar{a}_{n,l}(k)^{(l)}(i)^{(n-l)} \tag{6.7}$$

6.4.1 Normalisation of the Kernel

The normalisation of the kernel is readily shown from (6.1) by changing the order of summation and noting the normalisation of the NHG (equation (B.13)).

$$\sum_{j=0}^{k} K(j,i;k) = \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k} W_{qp}(s-i;k-i) \cdot \sum_{j=r}^{s} W_{qq}(j-r;s-r)$$

$$= \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k} W_{qp}(s-i;k-i) \sum_{j=0}^{s-r} W_{qq}(j;s-r)$$

$$= \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=0}^{k-i} W_{qp}(s;k-i)$$

$$= \sum_{r=0}^{i} W_{pq}(r;i) = 1. \tag{6.8}$$

6.4.2 First Moment of the Kernel

The first moment of the kernel is defined as,

$$\bar{M}_1(i,k) = \sum_{j=1}^{k+i} j\, K(j,i;k+i) \tag{6.9}$$

We note the first moment of the NHG distribution,

$$\sum_{i=1}^{k} i\, W_{pq}(i;k) = \frac{pk}{p+q} \tag{6.10}$$

and hence on inserting (6.1) in (6.9) and rearranging the orders of summation we get,

$$\bar{M}_1(i,k) = \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k+i} W_{qp}(s-i;k) \sum_{j=r}^{s} j\, W_{qq}(j-r;s-r)$$

$$= \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k+i} W_{qp}(s-i;k) \sum_{j=0}^{s-r} (j+r) W_{qq}(j;s-r)$$

$$= \frac{1}{2} \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=0}^{k} W_{qp}(s;k)\ (s+i+r)$$

$$= \frac{qk + (2p+q)i}{2(p+q)} \tag{6.11}$$

$$\bar{m}_1(i,k) = \bar{a}_{10}\, i + \bar{a}_{11}\, k \qquad (6.12)$$

6.4.3 Second Moment of the Kernel

It initially turns out to be easier to calculate the second power moment of the kernel and then derive the second factorial moment from it. Following a procedure similar to that for the first moment we have,

$$\bar{m}_2'(i;k) = \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k+i} W_{qp}(s-i;k) \sum_{j=r}^{s} j^2\, W_{qq}(j-r;s-r)$$

We note that the second power moment of the NHG distribution is,

$$\begin{aligned}\sum_{i=0}^{k} i^2 W_{pq}(i;k) &= \sum_{i=0}^{k} \left(i(i-1)+i \right) W_{pq}(i;k)\\ &= \frac{p(p+1)}{(p+q)(p+q+1)}\, k(k-1) + \frac{p}{p+q}\, k\\ &= \frac{p(p+1)}{(p+q)(p+q+1)}\, k^2 + \frac{pq}{(p+q)(p+q+1)}\, k \qquad (6.13)\end{aligned}$$

and thus the second moment of the kernel is,

$$\begin{aligned}\bar{m}_2'(i,k) &= \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=i}^{k+i} W_{qp}(s-i;k) \sum_{j=0}^{s-r} (j^2+2jr+r^2)\, W_{qq}(j;s-r)\\ &= \sum_{r=0}^{i} W_{pq}(r;i) \sum_{s=0}^{k} W_{qp}(s;k) \left\{ \frac{q+1}{2(2q+1)}(s+i-r)^2 + r(s+i) \right.\\ &\qquad \left. + \frac{q}{2(2q+1)}(s+i-r) \right\}\end{aligned}$$

The two summations are now independent and thus on doing them we note that the following transformations occur,

$$s \rightarrow \frac{qk}{p+q}, \quad s^2 \rightarrow \frac{q(q+1)k^2 + pqk}{(p+q)(p+q+1)}$$

$$r \rightarrow \frac{pi}{p+q}, \quad r^2 \rightarrow \frac{(p+1)pi^2 + pqi}{(p+q)(p+q+1)} \tag{6.14}$$

This means that the second moment is,

$$\bar{m}_2'(i,k) = \nu_1 i^2 + \nu_2 i + \nu_3 ik + \nu_4 k + \nu_5 k^2 \tag{6.15}$$

where the ν_i are given by,

$$\nu_1 = \frac{q(q+1)^2 + 2p(2q+1)(p+q+1)}{2(2q+1)(p+q)(p+q+1)}$$

$$\nu_2 = \nu_4 = \frac{q(q^2+2pq+p+q)}{2(2q+1)(p+q)(p+q+1)}$$

$$\nu_3 = \frac{q((q+1)q + p(2q+1))}{(2q+1)(p+q)^2}$$

$$\nu_5 = \frac{q(q+1)^2}{2(2q+1)(p+q)(p+q+1)} \tag{6.16}$$

The second factorial moment is simply related to the second power moment by

$$\begin{aligned} \bar{m}_2(i,k) &= \bar{m}_2'(i,k) - \bar{m}_1(i,k) \\ &= \nu_1 i^2 + (\nu_2 - \bar{a}_{10})i + \nu_3 ik + (\nu_4 - \bar{a}_{11})k + \nu_5 k^2 \\ &= \bar{a}_{20}(i)^{(2)} + 2\bar{a}_{21}\, ik + \bar{a}_{22}(k)^{(2)} \end{aligned} \tag{6.17}$$

where,

$$\bar{a}_{20} = \frac{(p+q+1)(q^2+3pq+p+q) + p(p+1)(q+1)}{2(2q+1)(p+q)(p+q+1)}$$

$$\bar{a}_{21} = \frac{q(2pq+p+q+q^2)}{2(2q+1)(p+q)^2}$$

$$\bar{a}_{22} = \frac{q(q+1)^2}{2(2q+1)(p+q)(p+q+1)}$$

(6.18)

The similarity of this to the second moment of the continuous kernel is obvious and requires no further comment. Similarly on putting p=0 the second moment of the NHG is obtained in the same manner as for the continuous case.

6.5 Eigenvalues and Eigenfunctions

As mentioned before this kernel is a particular case of one studied by Hoare & Rahman (1979) who showed, in the present notation that the kernel has eigenfunctions and eigenvalues given by,

$$\sum_{i=0}^{\infty} \psi_n(i,k)\, K(i,j;k) = \lambda_n\, \psi_n(j,k)$$

(6.19)

where,

$$\psi_n(i,k) = {}_3F_2\left[\begin{matrix}-n, -i, 2p+2q-1 \\ p+q, -k\end{matrix}\,;1\right]$$

$$= Q_n(i; p+q-1, p+q; k)$$

(6.20)

and,

$$\lambda_n = {}_4F_3\left[\begin{matrix}-n,\ n+2p+2q-1,\ q,\ q\\ p+q,\ p+q,\ 2q\end{matrix}\ ;\ 1\right] \tag{6.21}$$

Note that the ${}_3F_2$ are Hahn polynomials (see Appendix C for more details of the properties and definitions). This implies that the kernel can be written as,

$$K(i,j;k) = \sum_{n=0}^{\infty}{}' \pi_n \lambda_n \psi_n(j,k)\, \psi_n(i,k)\, W_{p+q,p+q}(i,k) \tag{6.22}$$

and π_n is given by,

$$\pi_n = \frac{(-1)^n (-k)_n \quad (2p+2q)_n}{n!\ (2p+2q+1-k)_n} \tag{6.23}$$

Equations for the moment relaxation can be derived by a method identical to that in the previous chapter for the continuous case. However as we have seen they are of little use apart from formally giving the general solution and so we directly consider the construction of an exact similarity solution.

6.6 The Similarity Solution

As is now apparent an obvious form for the trial solution is,

$$P^s(i,t) = (A+Bi)\,(i+1)_{p+q-1}\,(1-\Psi)^i \tag{6.24}$$

with A(t), B(t) and Ψ(t) as time dependent functions. This is essentially the same as (4.20) for the diffuse scattering model and hence we can immediately write A and B in terms of Ψ using equations (4.25) and (4.26) as,

$$A = \Psi^{p+q}\,\Gamma(p+q)^{-1}\left[1+p+q-\left(\varepsilon/\varepsilon_0+p+q\right)\Psi\right] \tag{6.25}$$

$$B = \Psi^{p+q+1}\,\Gamma(p+q+1)^{-1}\left[\left(\varepsilon/\varepsilon_0+p+q\right)\Psi-p-q\right] \tag{6.26}$$

The method of finding Ψ closely parallels the methods used in the previous chapters. The left hand side (LHS) of the Boltzmann equation is directly translated from equation (4.27) to become,

$$(LHS) = (i+1)_{p+q-1}\,(1-\Psi)^{i}\left(\frac{-i}{1-\Psi}\frac{d\Psi}{dt}+\frac{\partial}{\partial t}+1\right)(A+Bi) \tag{6.27}$$

whilst the right hand side (RHS) can be written as,

$$(RHS) = \sum_{k=i}^{\infty}\sum_{j=0}^{k} K(i,j;k)\,(A+Bj)(A+B(k-j))\,(1-\Psi)^{k} \cdot (j+1)_{p+q-1}\,(k-j+1)_{p+q-1} \tag{6.28}$$

Using the detailed balance property (6.3) this becomes,

$$(RHS) = (i+1)_{p+q-1}\sum_{k=i}^{\infty}(k-i+1)_{p+q-1}\sum_{j=0}^{k} K(j,i;k)\,(A+Bj)(A+B(k-j))\,(1-\Psi)^{k} \tag{6.29}$$

Shifting the variable k to k+i and equating left and right hand sides gives,

$$\left(\frac{-i}{1-\Psi}\frac{d\Psi}{dt}+\frac{\partial}{\partial t}+1\right)(A+Bi) = \sum_{k=0}^{\infty}(k+1)_{p+q-1}\,(1-\Psi)^{k}\sum_{j=0}^{k+i} K(j,i;k+i)\,(A+Bj)(A+B(k-j)) \tag{6.30}$$

Expanding the brackets and doing the j summation by inserting the forms (6.12) and (6.17) for the first and second moments of the kernel gives,

$$(RHS) = \sum_{k=0}^{\infty} (k+1)_{p+q-1} (1-\Psi)^k \Big\{ B^2(\bar{a}_{11}-\bar{a}_{22})(k)^{(2)} + (AB + B^2(\bar{a}_{10}+\bar{a}_{11} - 2\bar{a}_{21})i)(k)^{(1)} + A^2 + ABi + B^2(a_{10}-a_{20})(i)^{(2)} \Big\}$$

(6.31)

Written in this way the k summation involves only factorial moments of the Negative Binomial distribution (equation (b.16)) . The result is,

$$\left(\frac{-i}{1-\Psi}\frac{d\Psi}{dt} + \frac{\partial}{\partial t} + 1\right)(A+Bi) = \frac{\Gamma(p+q)}{\Psi^{p+q+2}} \Big\{ B^2\Psi^2(\bar{a}_{10}-\bar{a}_{20})(i)^{(2)} + \left(AB\Psi^2 + B^2(p+q)(\bar{a}_{10}+\bar{a}_{11}-2\bar{a}_{21})\Psi(1-\Psi)\right)i + A^2\Psi^2 + AB(p+q)\Psi(1-\Psi) + B^2(\bar{a}_{11}-\bar{a}_{22})(p+q)(p+q+1)(1-\Psi)^2 \Big\}$$

(6.32)

For the trial solution to fit the Boltzmann equation we require that the coefficients of i^0, i and $(i)^{(2)}$ are all equal. These conditions are found to be satisfied and lead to the, by now familiar equation for Ψ.

$$\frac{d\Psi}{dt} = -\lambda\Psi\left[\left(\frac{\varepsilon+\varepsilon_0(p+q)}{\varepsilon_0(p+q)}\right)\Psi - 1\right]$$

(6.33)

where now,

$$\lambda = \frac{q(q^2+2pq+p+q)}{2(2q+1)(p+q)(p+q+1)}$$

(6.34)

This has the solution

$$\Psi = \frac{\varepsilon_0(p+q)}{\varepsilon+\varepsilon_0(p+q)}\left[1-\eta e^{-\lambda t}\right]^{-1}$$

(6.35)

with η parameterising the range of possible initial distributions. The final form of the solution is,

$$P^s(i,t) = \Psi^{p+q}\,\Gamma(p+q)^{-1}\,(i+1)_{p+q-1}\,(1-\Psi)^{i}$$
$$\cdot\{1+p+q-(\varepsilon/\varepsilon_0+p+q)\Psi+\frac{i\Psi}{1-\Psi}\left[\left(\frac{\varepsilon}{\varepsilon_0(p+q)}+1\right)\Psi-1\right]$$

(6.36)

Any remarks as to the validity or range of the solution are again dependent on (6.35) and the value of η , and have been adequately covered in previous chapters. This solution is of the same form as that for the discrete diffuse scattering model of chapter 4 and hence any initial distribution will relax in the same fashion with only the time scale depending on whether the model is of the diffuse or persistent scattering type (given the total number of degrees of freedom).

6.6.1 Limiting Cases of the Solution

In section 4.3 it was shown how continuous distributions could be derived from discrete ones by taking an appropriate limit (4.5) . We show here how this model encompasses all of those previously discussed and solved.

1. p→0. In this case it can be seen that the decay constant (6.34) reduces to that of the diffuse scattering case (4.32),

$$\lim_{p\to 0}\left\{\frac{q(q^2+2pq+p+q)}{2(2q+1)(p+q)(p+q+1)}\right\} = \frac{q}{2(2q+1)} \tag{6.37}$$

The rest of the solution is identical upon putting p=0 and hence in this limit the diffuse scattering model is the result. It was shown when discussing that model how the continuous diffuse scattering model could be obtained from it by taking the limit (4.5 section 4.4.3) and hence the discrete persistent scattering model contains both of the diffuse scattering models.

2. By taking the limit (4.5) in a manner similar to that in section 4.4.3 we can show that the solution (6.36) reduces to the solution (5.60) of the continuous persistent scattering model. The working is identical to that in section 4.4.3 except that p is replaced by p+q and hence is not given here. The continuous diffuse scattering model can also be obtained from the continuous persistent scattering model (see last chapter) thereby giving two routes to the solution of this model.

6.7 Computer Simulations

All of the remarks made in section 4.7 also apply here. However the emphasis on the various methods discussed there has changed due primarily to the complexity of the persistent scattering collision kernel. The method of Tjon & Wu (1979) is already expensive on computer time with a simple kernel like $K(x;u)=u^{-1}$, but if one has to perform a double summation (or integration) to get the value of the kernel then the method is clearly not of much use. Similarly the recently developed method of Barnsley & Turchetti (1979) which relies on knowledge of the polynomial moments is not aplicable here since they are not readily found in the persistent scattering case.

The method of direct substitution developed in Chapter 4 is of obvious application here since the model is almost as easily simulated as the diffuse one to give a qualitative description of the relaxation of an arbitrary initial distribution.

The number of molecules used in these simulations was 1000, and although trial runs with up to 10000 were tried it was found that there was little difference in the results obtained. Two energies i and k-i were chosen at random from the ensemble of 1000 energies and each of them split into two parts ((m,i-m) and (n-i,k-n) respectively) according to a random number on the range (0,i) or (0,k-i) (from the NHG distribution). The two interacting parts (i-m,n-i) were then added together and then split according to the above prescription with the results (j-m,n-j) being added to the non-interacting parts before the energies were replaced in i and k-i. Fig. 6.1 gives an explanation of this procedure.

The results of the relaxation of various initial distributions were monitored and plotted for up to 20 collision times and for various combinations of the parameters p and q. A selection of the resultant plots are shown in figs. 6.2 and 6.3 .

Firstly the obvious results that one would expect to find, such as the increasing rapidity of 'Maxwellisation' with the ratio q/p one does observe. Also the equilibrium distribution for p=1,q=1 is found to be quantitatively the same as the p=2 one from the diffuse scattering system. However a persistent scattering system takes slightly longer to reach the corresponding state of an equivalent diffuse scattering system. In particular the p=10, q=2 system takes about 10 collision times to relax whilst the almost equivalent p=10 diffuse scattering system takes about 5.

As in the diffuse scattering systems the entropy, variance and mean energy were monitored throughout the run. It was found that the total entropy increased monotonically until equilibrium when it fluctuated about a mean value and that the σ_2 part of the entropy (see section 2.10.1) decreased monotonically on the passage towards equilibrium. This can be shown to be a consequence of the similarity solution in a manner similar to that used in section 3.5 .

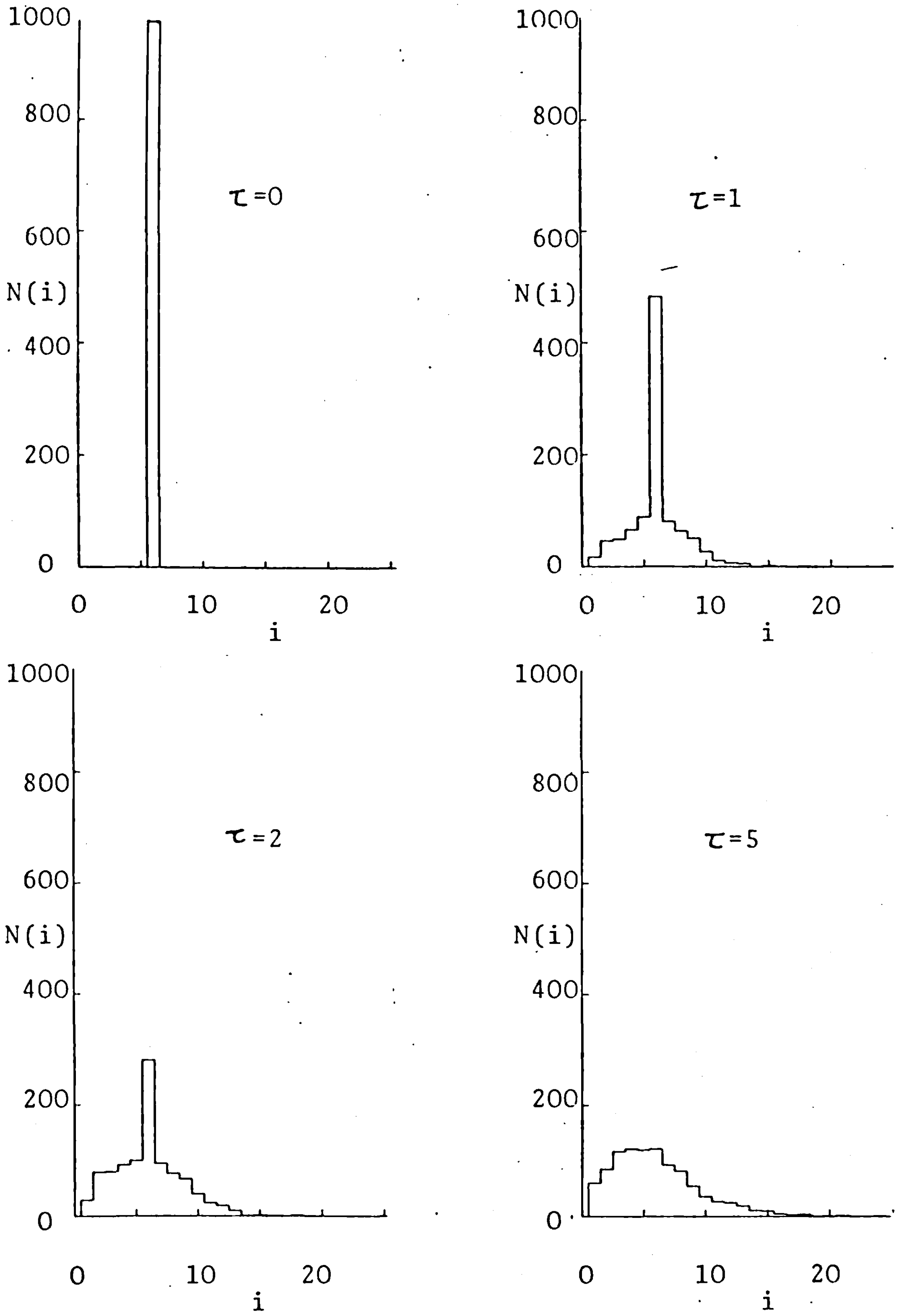

Fig. 6.2 : Computer Simulation of persistent scattering system ($p=1,q=1$) .

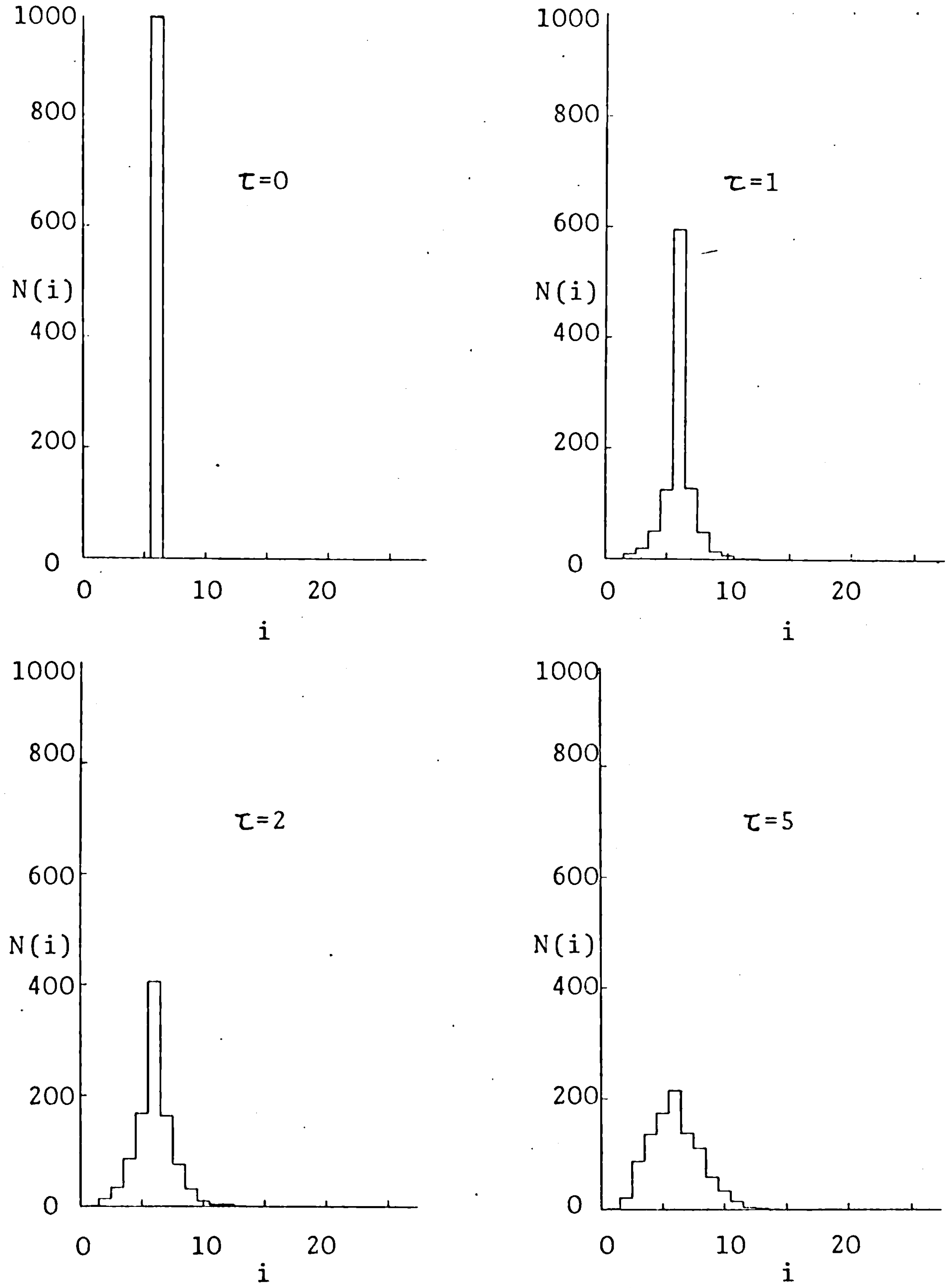

Fig. 6.3 : Computer simulation of persistent scattering system (p=10,q=2) .

APPENDIX A : FUNCTIONS

Many varied notations have been used for special functions in the literature and it is the purpose of Appendices A, B and C to show which ones have been used in this thesis, to define them and to give some relevant properties of them.

A.1 Pochhammer Functions

The falling Pochhammer function is defined as,

$$(a)^{(n)} = a(a-1)(a-2)\,\ldots\,(a-n+1) \tag{A.1}$$

and the rising Pochhammer function as,

$$(a)_n = a(a+1)(a+2)\,\ldots\,(a+n-1) \tag{A.2}$$

The relationship between them is,

$$(-a)_n = (-1)^n (a)^{(n)} \tag{A.3}$$

For a large number of properties of the rising Pochhammer function see Slater (1966).

A.2 Hypergeometric Functions

All of the polynomials can be defined in terms of Hypergeometric distributions and we use this basic unambiguous starting point to define them. The general Hypergeometric function is defined as,

$$ {}_nF_m\left[\begin{matrix} a_1, a_2, \cdots a_n \\ b_1, b_2, \cdots b_m \end{matrix} ; x\right] = \sum_{\nu=0}^{\infty} \left\{ \frac{\prod_{i=0}^{n} (a_i)_\nu}{\prod_{i=0}^{m} (b_i)_\nu \, \nu!} x^\nu \right\} \tag{A.4} $$

For some of the lower order ones there are summation properties and for further details one is again refered to Slater (1966).

APPENDIX B : DISTRIBUTIONS

B.1 Beta Distribution

We begin by considering a small physical system which is described by a macrostate E which is comprised of microstates ε_i distributed amongst that system's degrees of freedom. The ε_i are additively conserved although not individually so and thus,

$$0 \leq \varepsilon_i \leq E \quad , \quad \sum_{i=0}^{s} \varepsilon_i = E \tag{B.1}$$

where there are a total of s microstates ε_i. The total volume of state space accessible to systems in dE about E can be specified by a structure function $G_s(E)$ defined by,

$$G_s(E)\,dE = \underset{\{E \leq \varepsilon_1 + \varepsilon_2 + \dots + \varepsilon_s \leq E + dE\}}{\int \cdots \int d\varepsilon_1 \cdots d\varepsilon_s} \tag{B.2}$$

If these microstates are unbiased and uncorrelated then the result of the integral is,

$$G_s(E) = E^{s-1}\,\Gamma(s)^{-1} \tag{B.3}$$

We can now find the probability transition kernel that we need for Chapter 3.i.e.

$$W_{pq}(x;E)\,dx = \mathrm{Pr.}\left\{\begin{array}{l}\text{p subsystems of a total p+q have a}\\ \text{share in dx about x when p+q contain E.}\end{array}\right\}$$

$$= \frac{G_p(x)\;G_q(E-x)}{G_{p+q}(E)}\,dx \tag{B.4}$$

$$W_{p,q}(x;E) = \frac{\Gamma(p+q)}{\Gamma(p)\Gamma(q)} \frac{x^{p-1}(E-x)^{q-1}}{E^{p+q-1}}$$ (B.5)

which is the Beta distribution normalised on the range $0 \leqslant x \leqslant E$.

$$\int_0^E W_{p,q}(x;E)\,dx = 1$$ (B.6)

The moments of the distribution are,

$$\int_0^E x^n W_{p,q}(x;E)\,dx = \frac{(p)_n}{(p+q)_n} E^n$$ (B.7)

Also of interest are the moments of the symmetric Beta distribution (p=q),

$$\int_0^E x^n W_{p,p}(x;E)\,dx = \frac{(p)_n}{(2p)_n} E^n$$ (B.8)

B.2 Gamma Distribution

This is defined as,

$$W_{p,\infty}(x,\beta) = \Gamma(p)^{-1} \beta^p x^{p-1} e^{-\beta x}$$ (B.9)

where x lies on the range $(0,\infty)$. The moments of the distribution are,

$$\int_0^\infty x^n W_{p,\infty}(x,\beta)\,dx = \frac{(p)_n}{\beta^n}$$ (B.10)

B.3 Negative Hypergeometric Distribution

The problem of discrete occupancy is rather more common than that of continuous occupancy which was discussed in part 1 of this Appendix since it is a 'balls in boxes' type problem. The structure function giving the number of ways i quanta are distributed in s degrees of freedom is

$$\Omega_s(i) = \frac{\Gamma(i+s)}{\Gamma(i+1)\Gamma(s)} = \frac{(i+1)_{s-1}}{\Gamma(s)} \tag{B.11}$$

where as usual $(a)_n$ is the rising Pochhammer function. Thus the occupancy distribution for i quanta in p degrees of freedom given a total N in p+q degrees of freedom is,

$$W_{pq}(i;N) = \frac{\Omega_p(i)\ \ \Omega_q(N-i)}{\Omega_{p+q}(N)}$$

$$= \frac{\Gamma(p+q)}{\Gamma(p)\Gamma(q)} \frac{(i+1)_{p-1}\ \ (N-i+1)_{q-1}}{(N+1)_{p+q-1}} \tag{B.12}$$

or the Negative Hypergeometric distribution (NHG) normalised and valid on the set of integers $(i \in 0,1,2...N)$.

$$\sum_{i=0}^{N} W_{p,q}(i;N) = 1 \tag{B.13}$$

The moments of the distribution are,

$$\sum_{i=0}^{N} (i)^{(n)} W_{pq}(i,N) = \frac{(p)_n}{(2p)_n} (N)^{(n)}. \tag{B.14}$$

where we note that the sum can equally well start from n since the falling Pochhammer function ensures that the first n terms of the present series are zero.

B.4 Negative Binomial Distribution

This distribution is the discrete analogue of the Gamma distribution and is defined as,

$$W_{p,\infty}(i,\alpha) = \Gamma(p)^{-1}(i+1)_{p-1}(1-\alpha)^{p}\alpha^{i} \tag{B.15}$$

It is the weight function for Meixner polynomials and it's moments are,

$$\sum_{i=0}^{\infty} (i)^{(n)} W_{p,\infty}(i,\alpha) = \frac{(p)_n \alpha^n}{(1-\alpha)^n} \tag{B.16}$$

APPENDIX C : POLYNOMIALS

C.1 Jacobi Polynomials

Definition,

$$J_n(a,b;x) = {}_2F_1(-n, n+a; b; x) \tag{C.1}$$

$$= \sum_{\nu=0}^{n} \frac{(-n)_\nu \; (n+a)_\nu}{(b)_\nu \; \nu!} x^\nu \tag{c.2}$$

Rodrigues Formula,

$$J_n(a,b;x) = x^{1-b}(1-x)^{b-a} \frac{\Gamma(b)}{\Gamma(b+n)} \frac{d^n}{dx^n}\left\{x^{b+n-1}(1-x)^{a+n-b}\right\} \tag{C.3}$$

Orthogonality and Normalisation,

$$\int_0^1 x^{b-1}(1-x)^{a-b} J_n(a,b;x) J_m(a,b;x)\, dx$$

$$= \frac{n! \; \Gamma(b)^2 \, \Gamma(n+a-b+1)}{(a+2n)\, \Gamma(a+n)\, \Gamma(b+n)} \delta_{n,m} \tag{C.4}$$

C.2 Laguerre Polynomials

Definition,

$$L_n^{(\alpha)}(x) = \binom{n+\alpha}{n} {}_1F_1\left[-n, \alpha+1; x\right] \tag{C.5}$$

$$= \binom{n+\alpha}{n} \sum_{\nu=0}^{n} \frac{(-n)_\nu}{(\alpha+1)_\nu \, \nu!} x^\nu \tag{C.6}$$

Generating Function,

$$\sum_{n=0}^{\infty} L_n^{(\alpha)}(x)\, z^n = (1-z)^{-\alpha-1} \exp^{\frac{xz}{z-1}}$$

(C.7)

Orthogonality and Normalisation,

$$\int_0^{\infty} e^{-x} x^{\alpha} L_n^{(\alpha)}(x)\, L_m^{(\alpha)}(x) = \frac{\Gamma(\alpha+n+1)}{n!}\, \delta_{n,m}$$

(C.8)

Addition Formula,

$$\sum_{m=0}^{n} L_m^{(\alpha)}(x) \cdot L_{n-m}^{(\beta)}(y) = L_n^{(\alpha+\beta+1)}(x+y)$$

(C.9)

Rodrigues Formula,

$$n!\, e^{-x} x^{\alpha} L_n^{(\alpha)}(x) = \frac{d^n}{dx^n}\left\{ e^{-x} x^{n+\alpha} \right\}$$

(C.10)

C.3 Meixner Polynomials

Definition,

$$M_k(i, p, c) = {}_2F_1\left(-i, -k; p; 1-\tfrac{1}{c}\right)$$

(C.11)

Orthogonality and Normalisation,

$$\frac{(1-c)^p}{\Gamma(p)} \sum_{i=0}^{\infty} (i+1)_{p-1}\, c^i\, M_k(i,p,c)\, M_l(i,p,c) = \frac{k!}{c^k (p)_k}\, \delta_{k,l}$$

(C.12)

Generating Function,

$$\Gamma(p)^{-1} \sum_{i=0}^{\infty} (i+1)_{p-1}\, t^i\, M_k(i,p,c) = \frac{(1-t/c)^k}{(1-t)^{p+k}}$$

(C.13)

Addition Property,

$$\sum_{r=0}^{n} W_{pp}(r;n)\, M_{n-r}(\alpha,p,c)\, M_r(\beta,p,c) = M_n(\alpha+\beta,2p,c) \tag{C.14}$$

Continuous Limit,

$$\lim_{\left[\begin{smallmatrix} i\to\infty,\ c\to 1 \\ c^{i} = e^{x} \end{smallmatrix}\right]} M_k(i,p,c) = {}_1F_1(-k,p,x) = \frac{k!}{(p)_k} L_k^{(p-1)}(x) \tag{C.15}$$

Rodrigues Formula,

$$M_k(i,p,c) = \frac{c^{-i-k}}{(p)_k (i+1)_{p-1}} \Delta_i^k \left[c^i (i-k+1)_{p+k-1}\right] \tag{C.16}$$

Self Duality Property,

$$M_k(i,p,c) = M_i(k,p,c) \tag{C.17}$$

C.4 Hahn Polynomials

Definition,

$$Q_n(x;\alpha,\beta,N) = {}_3F_2\left[\begin{matrix} -n,\ n+\alpha+\beta+1,\ -x \\ \alpha+1,\ -N \end{matrix};1\right] \tag{C.18}$$

$$= \sum_{\nu=0}^{n} \frac{(-n)_\nu (n+\alpha+\beta+1)_\nu (-x)_\nu}{(\alpha+1)_\nu (-N)_\nu\ \nu!} \tag{C.19}$$

Orthogonality and Normalisation,

$$\sum_{x=0}^{N} W_{\alpha+1,\beta+1}(x,N)\, Q_m(x;\alpha,\beta,N)\, Q_n(x;\alpha,\beta,N) = \frac{\delta_{mn}}{\pi_n(\alpha,\beta,N)} \tag{C.20}$$

for m,n = 0,1,2....N and where,

$$\pi_n(\alpha,\beta,N) = \frac{(-1)^n(-N)_n(\alpha+1)_n(\alpha+\beta+1)_n}{n!\,(N+\alpha+\beta+2)_n\,(\beta+1)_n} \cdot \frac{2n+\alpha+\beta+1}{\alpha+\beta+1} \tag{C.21}$$

These polynomials are the discrete analogue of the Jacobi polynomials and the Meixner polynomials can be obtained from them by taking the limit N ⟶ ∞.

APPENDIX D : DIFFUSE SCATTERING MOMENTS

The moments can be calculated sequentially from the infinite set of equations (2.38). The boundary conditions of these equations are given by (3.12) and hence the equation for the second moment is,

$$\frac{d\mu_2(t)}{dt} + (1-2c_2)\mu_2(t) = c_2\varepsilon^2 \tag{D.1}$$

which has the solution,

$$\mu_2(t) - \mu_2(\infty) = (\mu_2(0) - \mu_2(\infty))\, e^{-(1-2c_2)t} \tag{D.2}$$

where,

$$\mu_2(\infty) = \frac{c_2\varepsilon^2}{1-2c_2} \tag{D.3}$$

The equation for the third moment is,

$$\frac{d\mu_3(t)}{dt} + (1-2c_3)\mu_3(t) = 2\varepsilon\mu_2(t)c_3 \tag{D.4}$$

which has the solution,

$$\mu_3(t) - \mu_3(\infty) = (\mu_3(0) - \mu_3(\infty))\, e^{-(1-2c_3)t} + \frac{c_3\varepsilon}{c_2 - c_3}(\mu_2(0) - \mu_2(\infty))\left(e^{-(1-2c_2)t} - e^{-(1-2c_3)t}\right) \tag{D.5}$$

where,

$$\mu_3(\infty) = \frac{2\varepsilon\,\mu_2(\infty)\,c_3}{1-2c_3} = \frac{2\varepsilon^3 c_2 c_3}{(1-2c_2)(1-2c_3)} \tag{D.6}$$

For the special case of either of the two diffuse scattering models,

$$c_2 = \frac{p+1}{2(2p+1)} \quad , \quad c_3 = \frac{p+2}{4(2p+1)} \tag{D.7}$$

and,

$$\left(\mu_2(t) - \frac{p+1}{2p}\varepsilon^2\right) = \left(\mu_2(0) - \frac{p+1}{2p}\varepsilon^2\right) e^{-\frac{pt}{2p+1}} \tag{D.8}$$

$$\begin{aligned}\left(\mu_3(t) - \frac{(p+1)(p+2)\varepsilon^3}{6p^2}\right) &= \left(\mu_3(0) - \frac{(p+1)(p+2)\varepsilon^2}{6p^2}\right) e^{-\frac{3pt}{2(2p+1)}} \\ &\quad + \frac{(p+1)\varepsilon}{p}\left(\mu_2(0) - \frac{p+1}{2p}\varepsilon^2\right)\left(e^{\frac{-pt}{2p+1}} - e^{\frac{-3pt}{2(2p+1)}}\right)\end{aligned} \tag{D.9}$$

APPENDIX E : AN ECONOMIC MODEL

The purpose of this problem is to show how, by the use of a particular kernel a general solution to the non-linear Boltzmann equation (2.11) can be obtained. The process is of the diffuse scattering type but there is no possibility of a reverse collision and hence the model must be studied under the guise of an economic model.

E.1 The Model

The model is simply defined by people playing two person , zero sum games where the 'rule' of each game is that each player must bet all of their money and the winnings (winner chosen at random) are the total stake. (Note that the obvious result of this is that everyone ends up with no money apart from one person who owns all of the money in the collective.) A variation of this model where the winnings are half of the total stake (i.e. each player wins the same amount) is equivalent to the Ehrenfest 'wind tree' model for which the Krook-Wu solution is also a solution (Ernst (1979a)). The transition kernel is

$$K(x;u) = \frac{1}{2}\left\{\delta(x-u) + \delta(x)\right\} \tag{E.1}$$

where δ is the usual Dirac delta function. This kernel still obeys the necessary interactional symmetry (2.2).

Noting that,

$$f(x)\,\delta(x-\alpha) = f(\alpha)\,\delta(x-\alpha)$$

(E.2)

and substituting (E.1) into (2.11) gives,

$$\left(\frac{\partial}{\partial t}+1\right) P(x,t) = \frac{1}{2}\delta(x)\int_0^\infty du \int_0^u dy\, P(y,t)\,P(u-y,t)$$
$$+\frac{1}{2}\int_x^\infty du\, \delta(u-x)\int_0^x dy\, P(y,t)\,P(u-y,t)$$
$$= \frac{1}{2}\,\delta(x) + \frac{1}{2}\int_0^x dy\, P(y,t)\,P(x-y,t)$$

(E.3)

The Laplace transform of P(x,t) is defined as,

$$G(s,t) = \int_0^\infty dx\, e^{-sx}\, P(x,t)$$

(E.4)

Thus,

$$\left(\frac{\partial}{\partial t}+1\right) G(s,t) = \frac{1}{2}\left(1+G^2(s,t)\right)$$

(E.5)

This equation can be partially integrated with respect to time to give,

$$\left[G(s,t)-1\right]^{-1} = -t/2 + \left[G(s,0)-1\right]^{-1}$$

(E.6)

which can be rearranged to give,

$$G(s,t) = \frac{G(s,0) - t/2\,(G(s,0)-1)}{1 - t/2\,(G(s,0)-1)}$$

(E.7)

It is obvious that putting $\frac{\partial G}{\partial t}$ =0 in (E.5) implies that,

$$G(s,\infty) = 1 \tag{E.8}$$

and hence,

$$P_\infty(x) = \delta(x) \tag{E.9}$$

the equilibrium distribution that would be expected.

There are a few important points about the model,

1. Detailed balance does not exist due to the fact that there cannot always be a reverse collision.
2. Th equilibrium distribution does not conserve energy, or the energy must be zero thus reducing the interest of the problem.
3. The solution (E.7) can be written as,

$$P(x,t) = \delta(x) + \mathcal{L}^{-1}\left\{\frac{1}{[G(s,0)-1]^{-1} - t/2}\right\} \tag{E.10}$$

which implies that the delta function is always present and that the effect of the initial distribution decreases monotonically as t increases.

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